



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:41 AM UTC

PDB ID : 3A5D / pdb_00003a5d
Title : Inter-subunit interaction and quaternary rearrangement defined by the central stalk of prokaryotic V1-ATPase
Authors : Numoto, N.; Hasegawa, Y.; Takeda, K.; Miki, K.
Deposited on : 2009-08-06
Resolution : 4.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

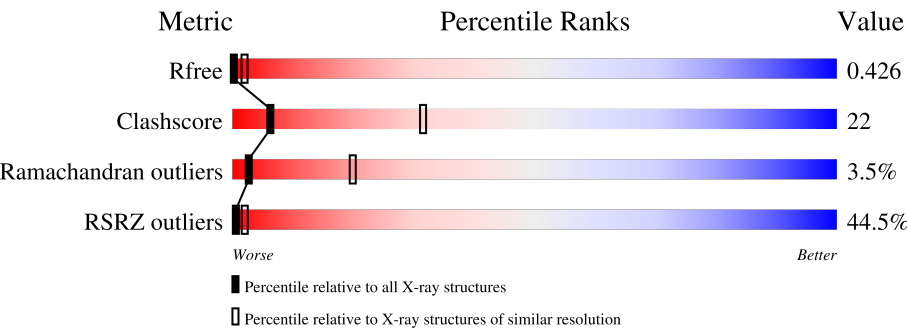
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1018 (5.66-3.94)
Clashscore	190562	1001 (5.60-3.98)
Ramachandran outliers	187476	1104 (5.70-3.90)
RSRZ outliers	180081	1013 (5.66-3.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	578	47% 82% 13% ...
1	B	578	24% 83% 12% ...
1	C	578	55% 79% 15% ...
1	I	578	54% 80% 14% ...
1	J	578	31% 81% 13% ...
1	K	578	59% 80% 14% ...
2	D	478	36% 82% 10% 6%

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Mol	Chain	Length	Quality of chain
2	E	478	
2	F	478	
2	L	478	
2	M	478	
2	N	478	
3	G	223	
3	O	223	
4	H	104	
4	P	104	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32080 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called V-type ATP synthase alpha chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	B	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	C	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	I	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	J	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	K	561	Total	C	N	O	0	0	0
			2752	1630	561	561			

- Molecule 2 is a protein called V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	E	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	F	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	L	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	M	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	N	450	Total	C	N	O	0	0	0
			2212	1312	450	450			

- Molecule 3 is a protein called V-type ATP synthase subunit D.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	129	Total 639	C 381	N 129	O 129	0	0	0
3	O	129	Total 639	C 381	N 129	O 129	0	0	0

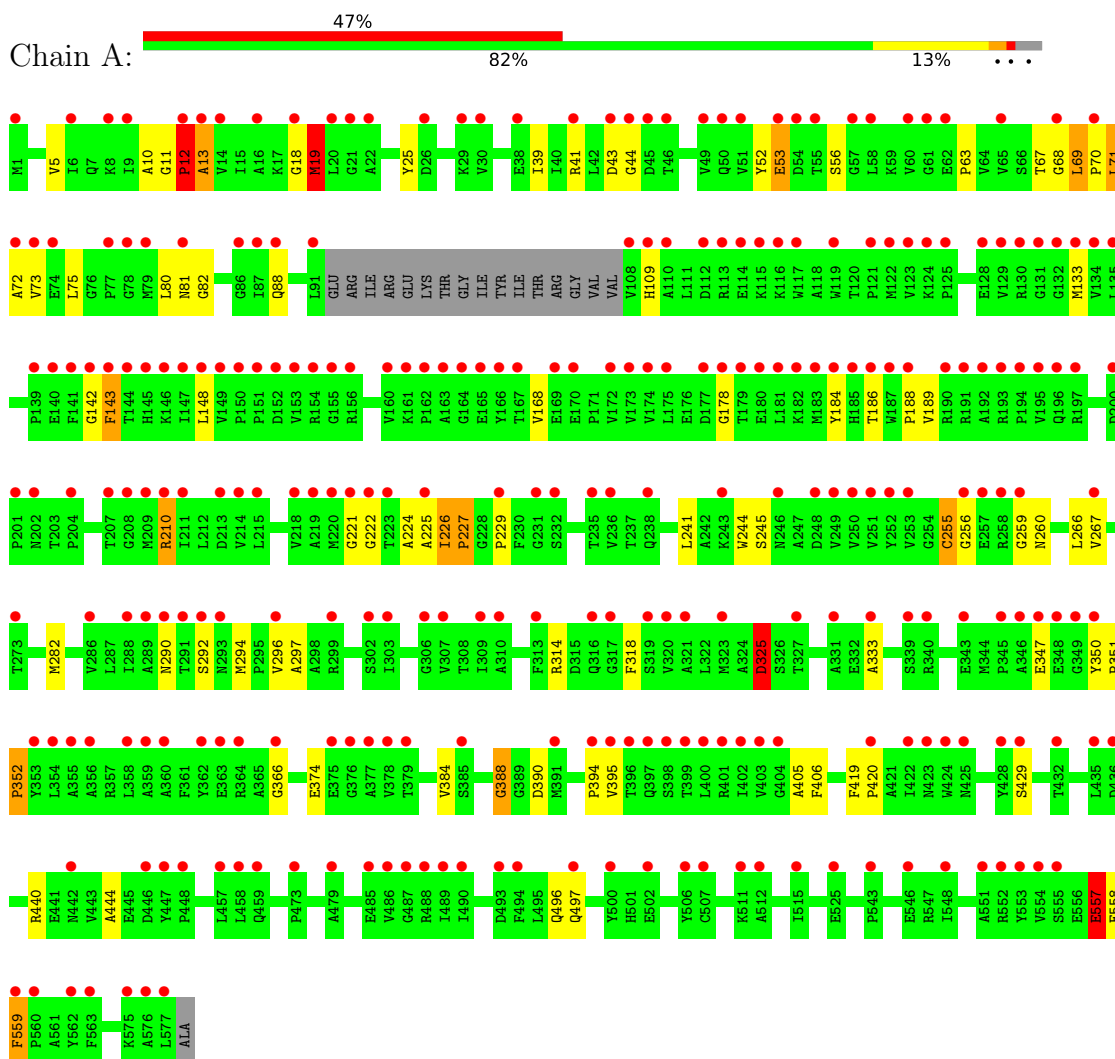
- Molecule 4 is a protein called V-type ATP synthase subunit F.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	104	Total 509	C 301	N 104	O 104	0	0	0
4	P	104	Total 509	C 301	N 104	O 104	0	0	0

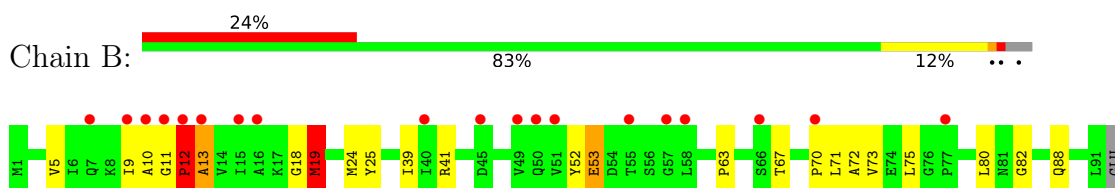
3 Residue-property plots [i](#)

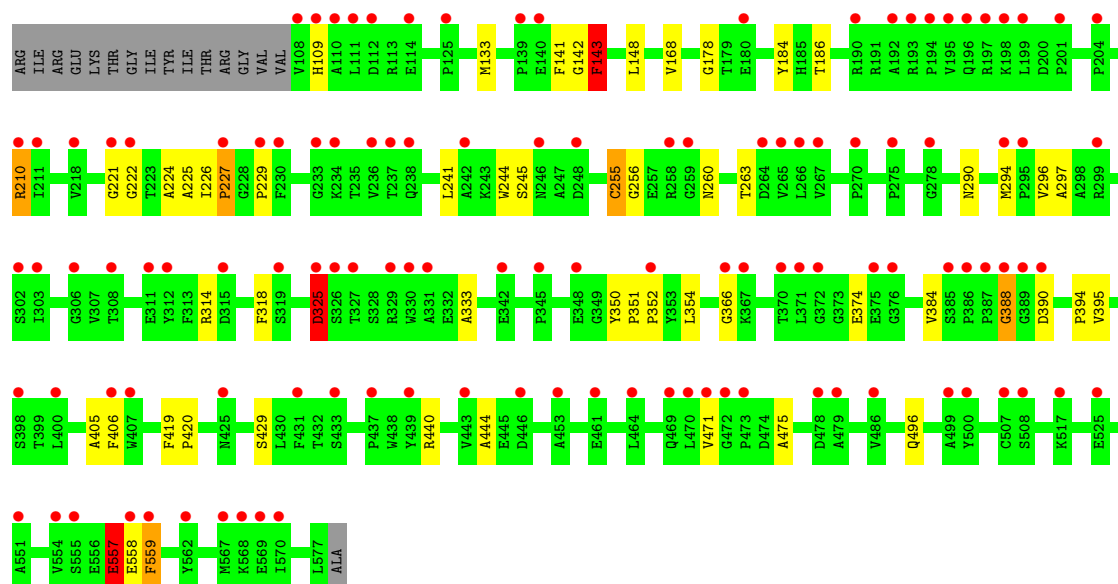
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: V-type ATP synthase alpha chain

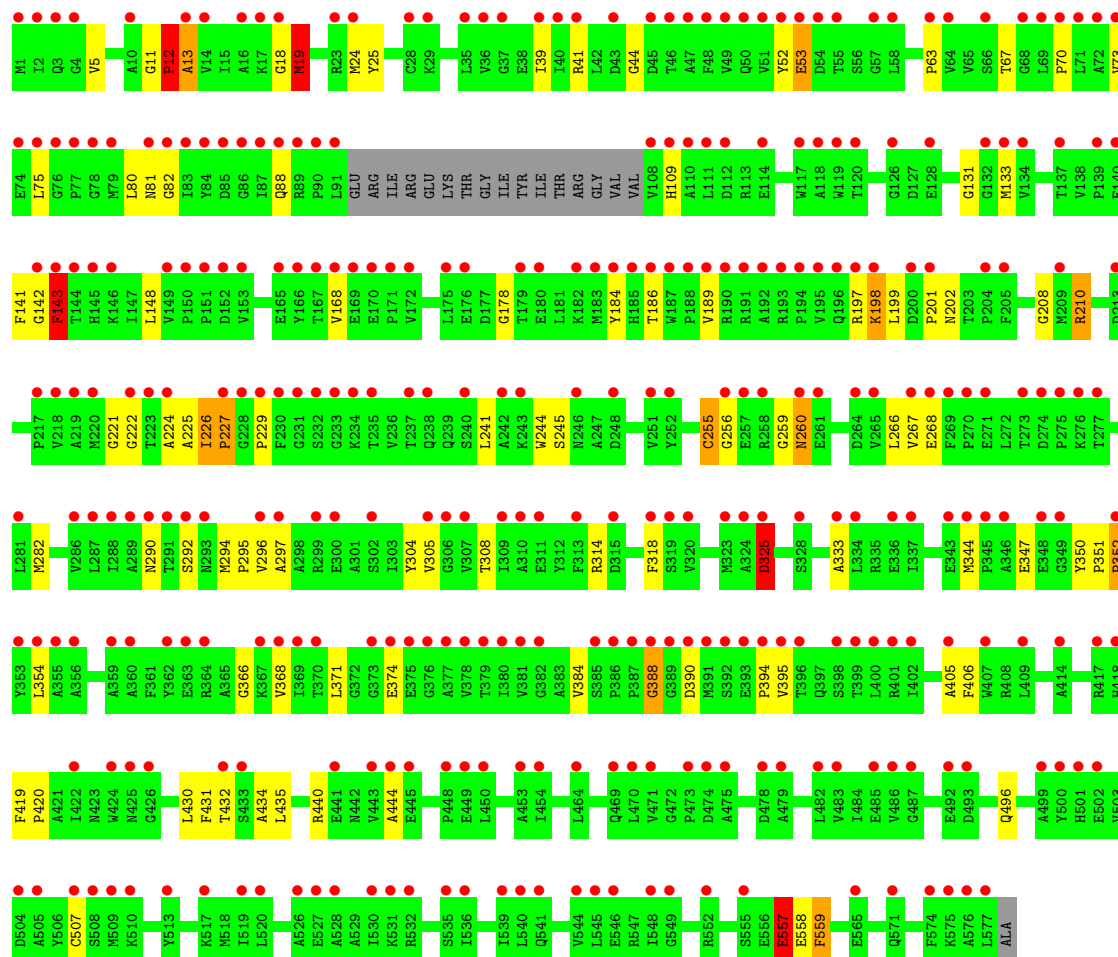
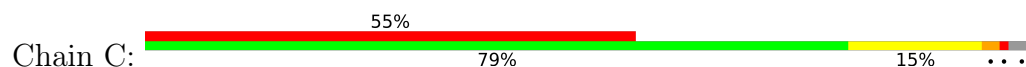


• Molecule 1: V-type ATP synthase alpha chain

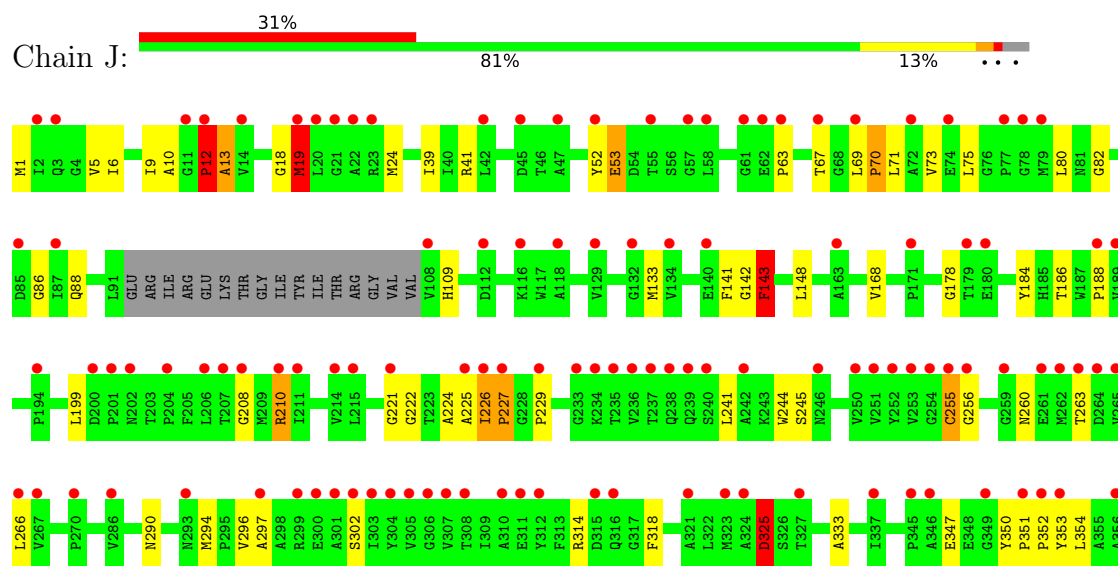


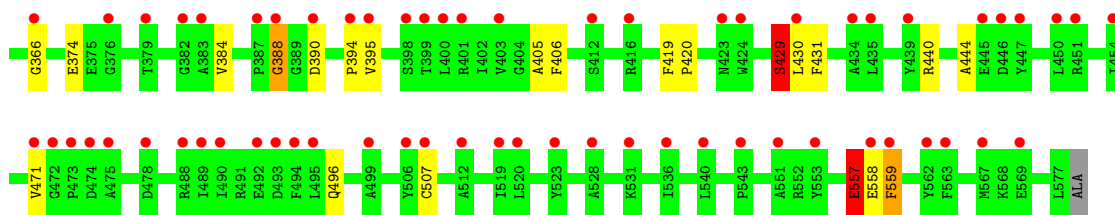


• Molecule 1: V-type ATP synthase alpha chain

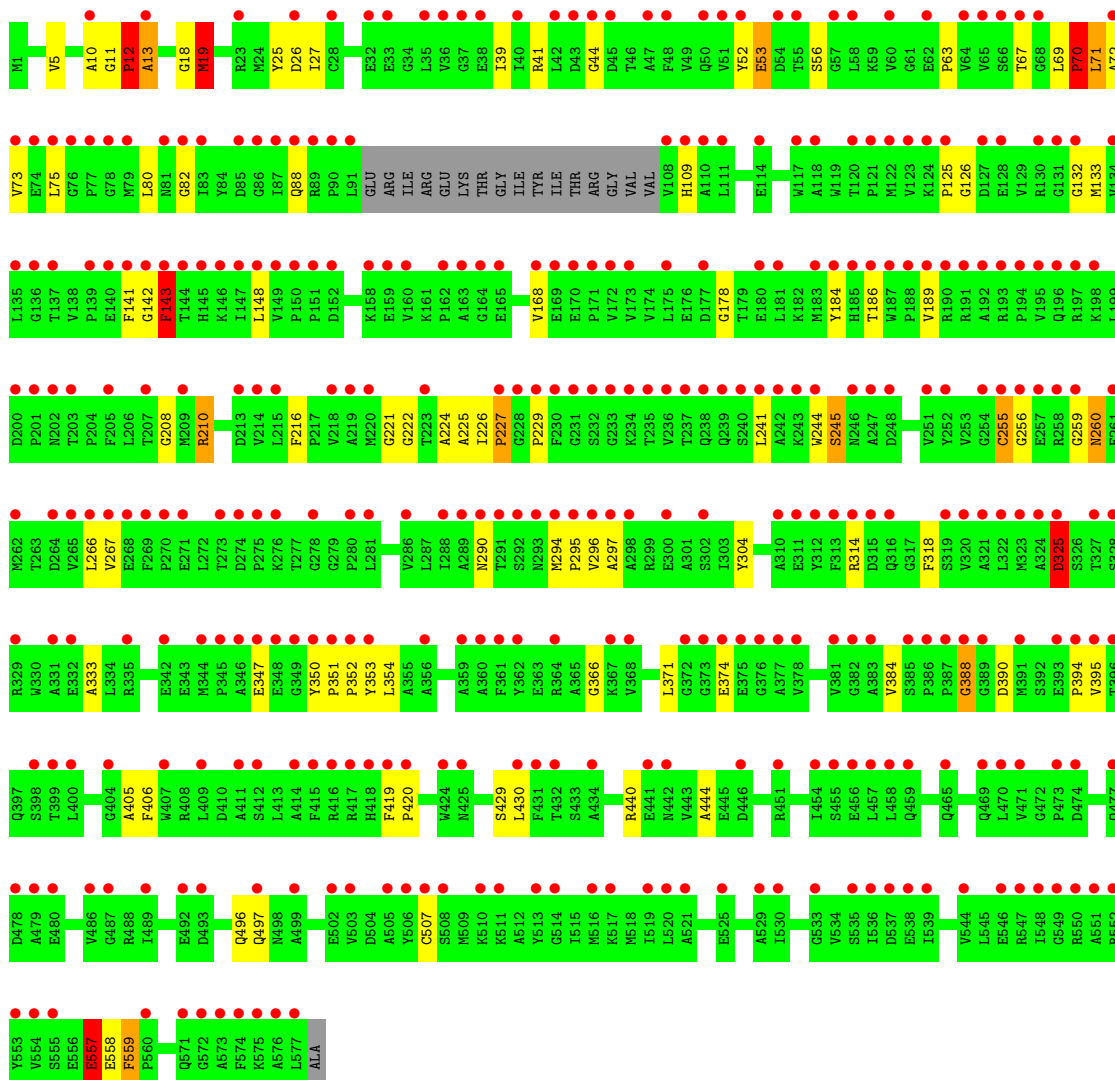
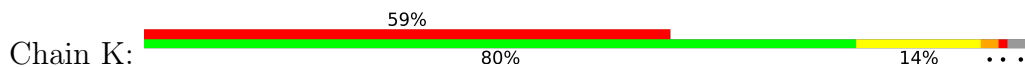


• Molecule 1: V-type ATP synthase alpha chain

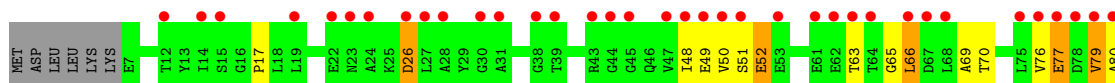
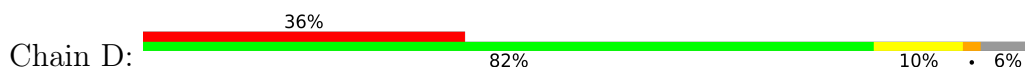


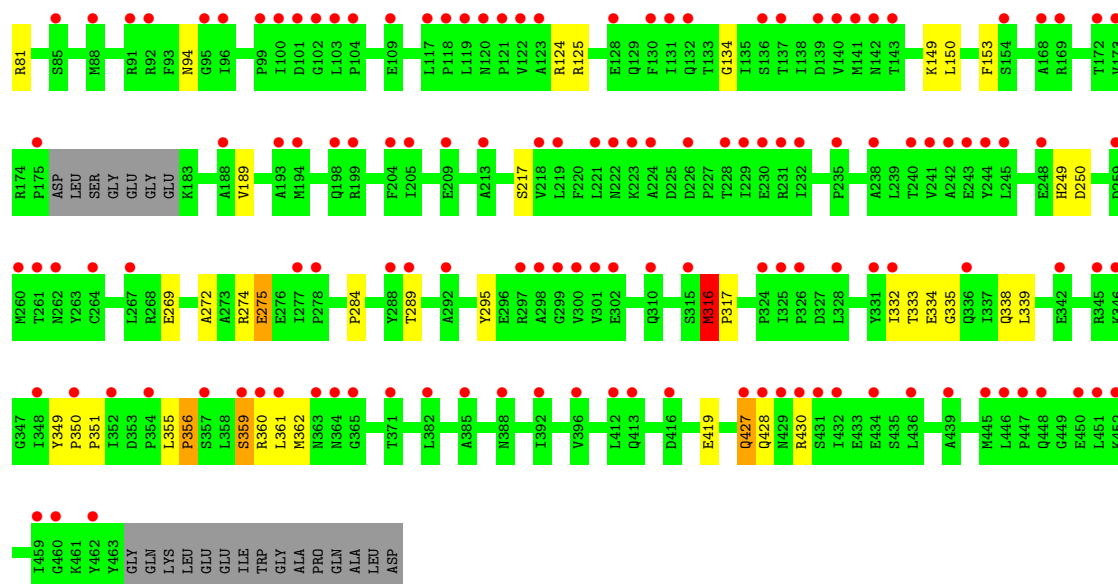


• Molecule 1: V-type ATP synthase alpha chain

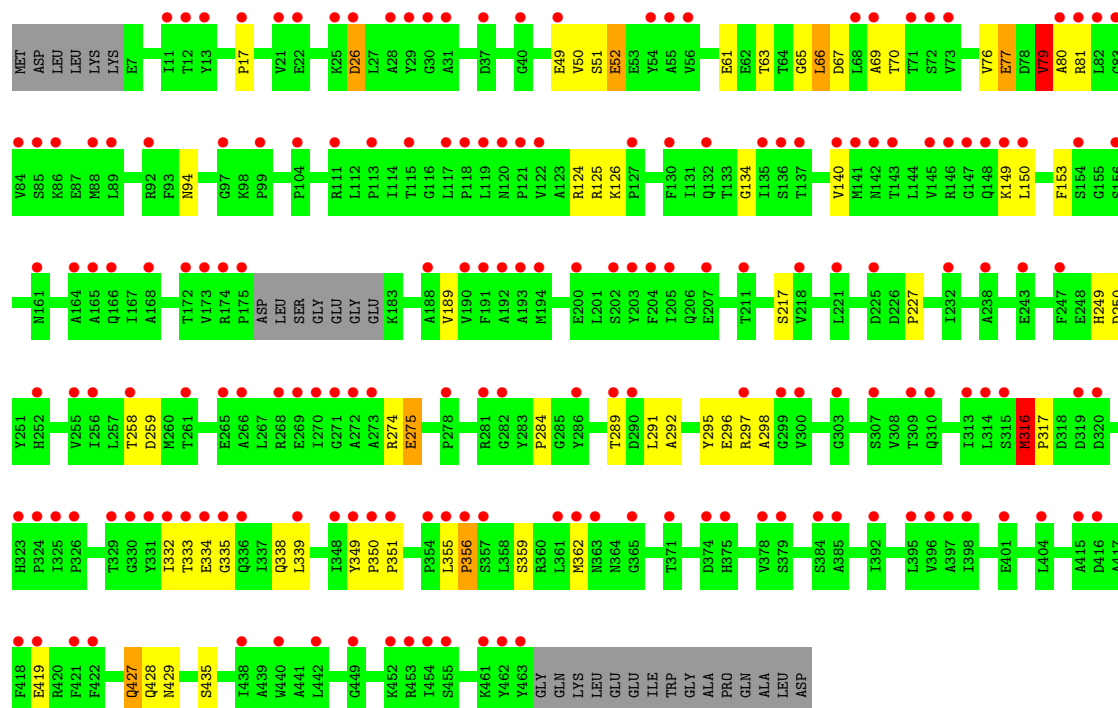
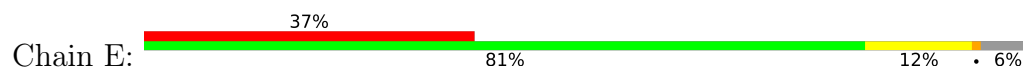


• Molecule 2: V-type ATP synthase beta chain

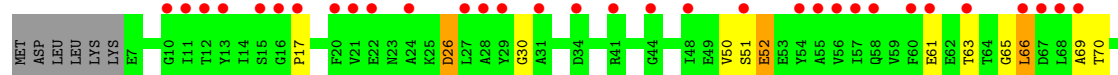
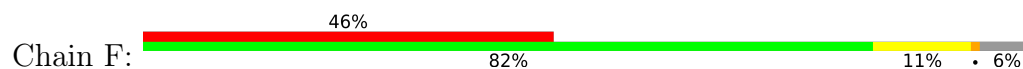


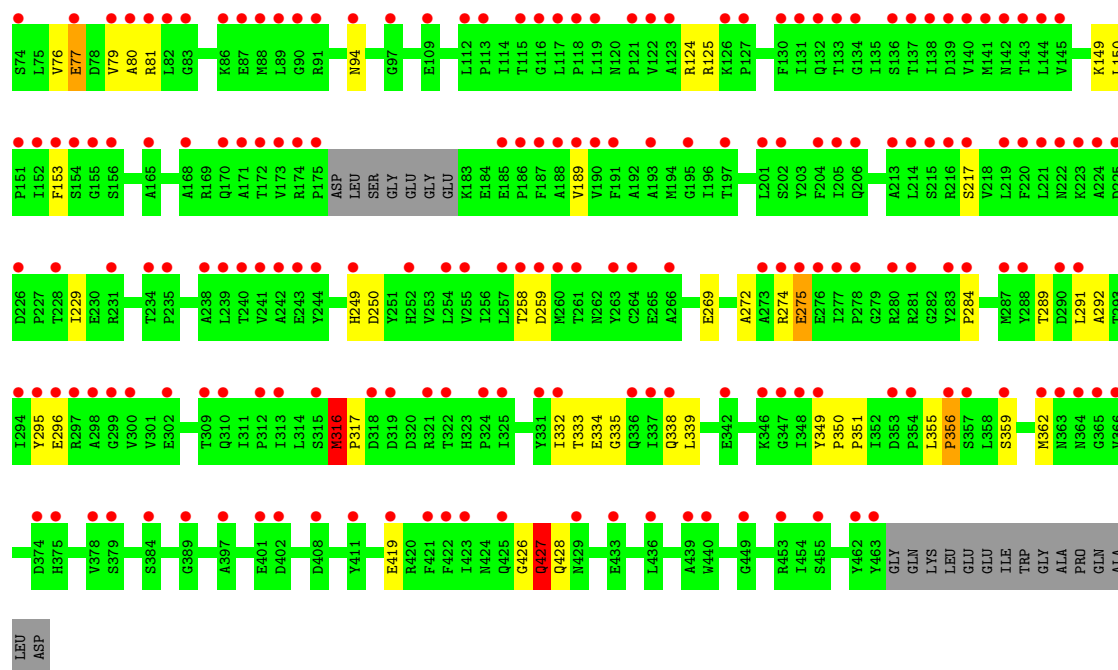


• Molecule 2: V-type ATP synthase beta chain

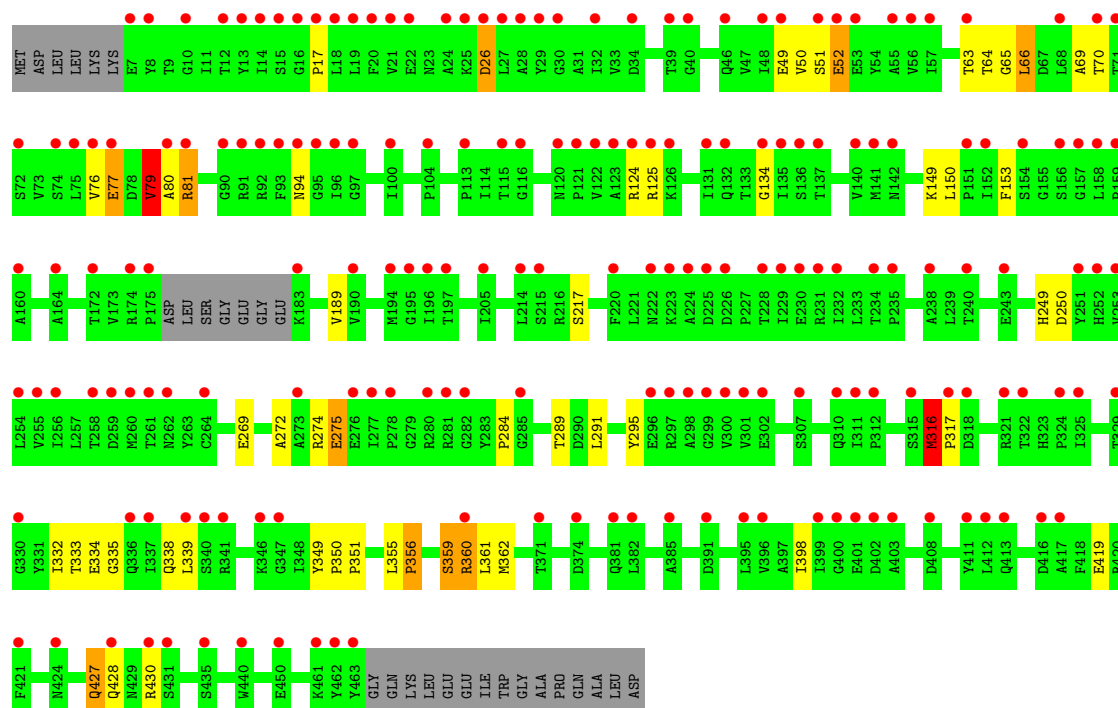
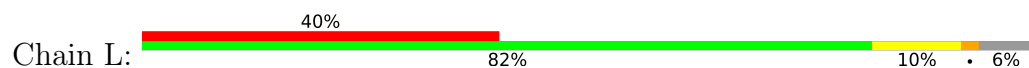


• Molecule 2: V-type ATP synthase beta chain

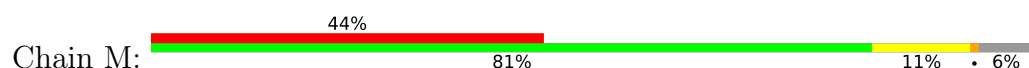


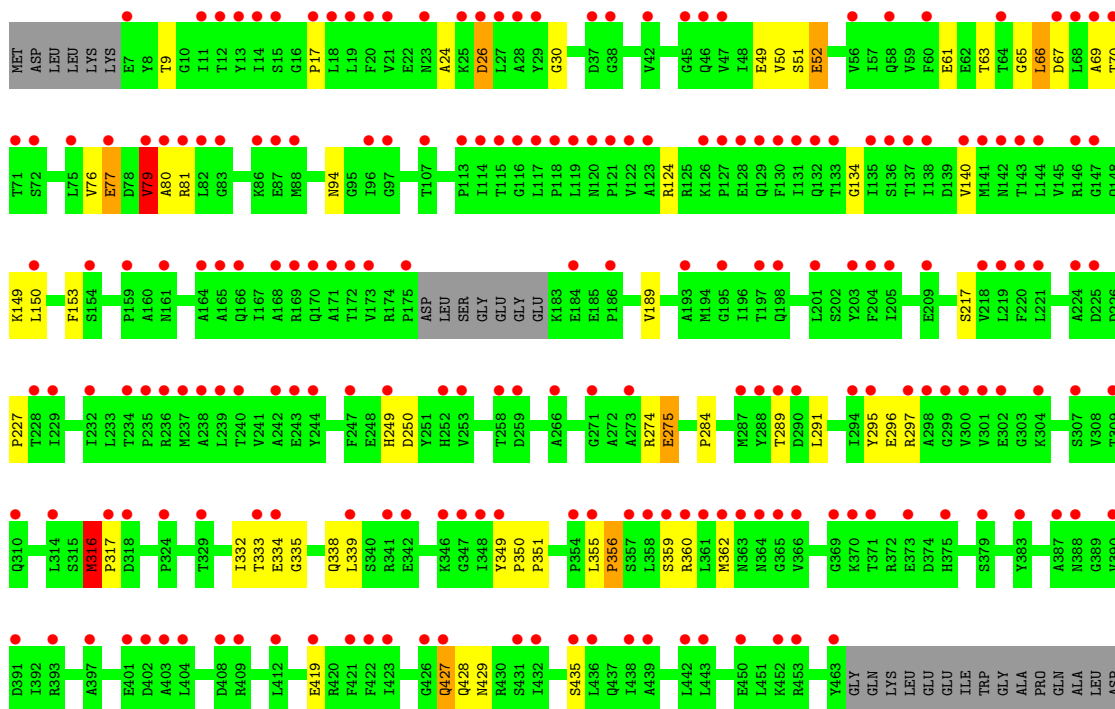


• Molecule 2: V-type ATP synthase beta chain

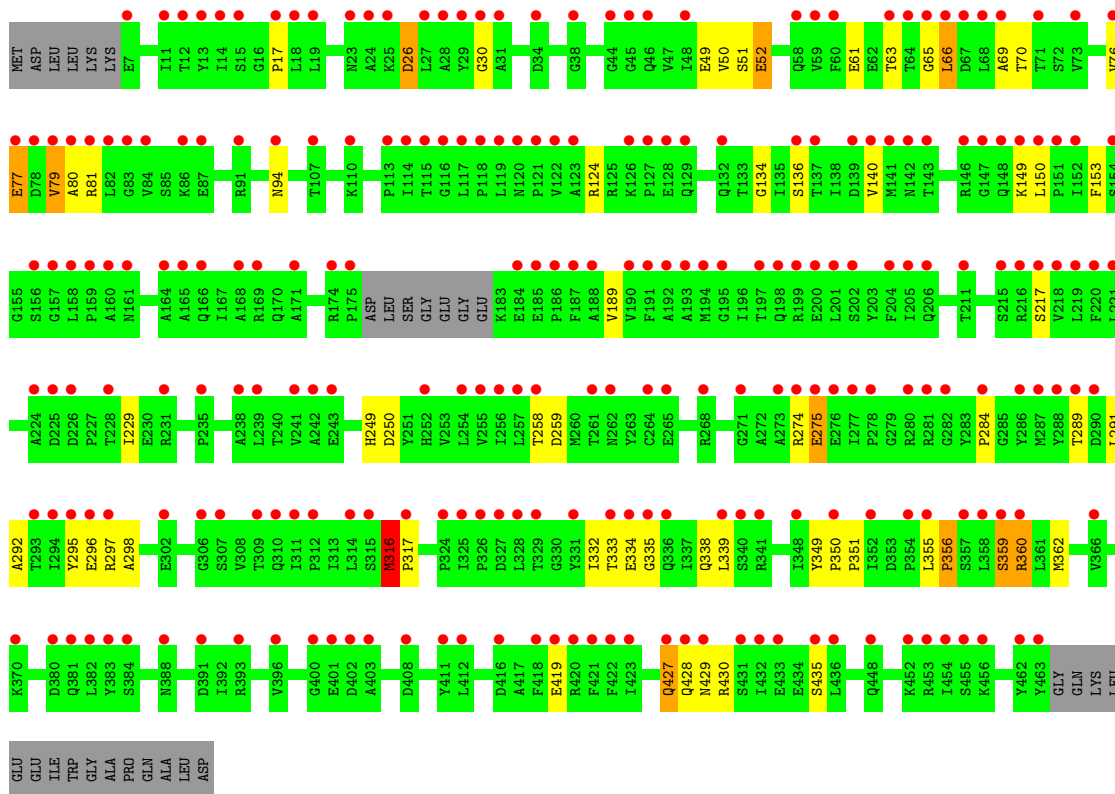
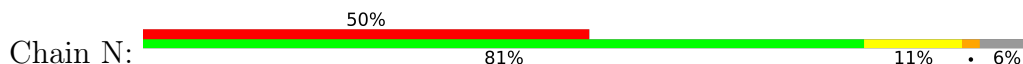


• Molecule 2: V-type ATP synthase beta chain

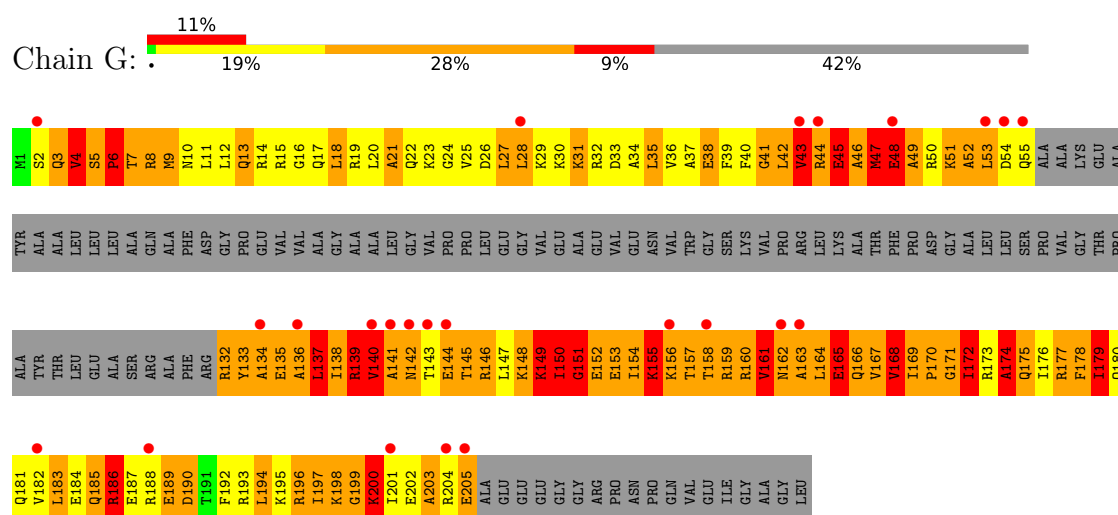




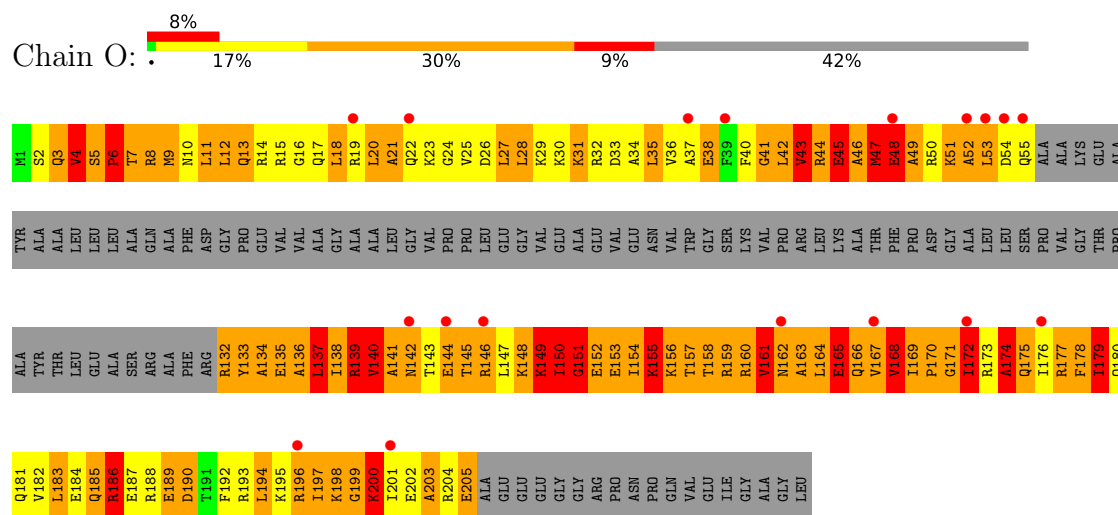
• Molecule 2: V-type ATP synthase beta chain



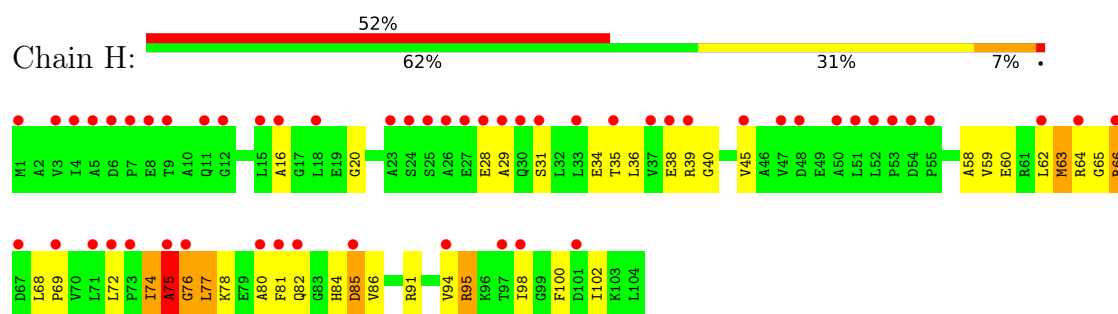
• Molecule 3: V-type ATP synthase subunit D



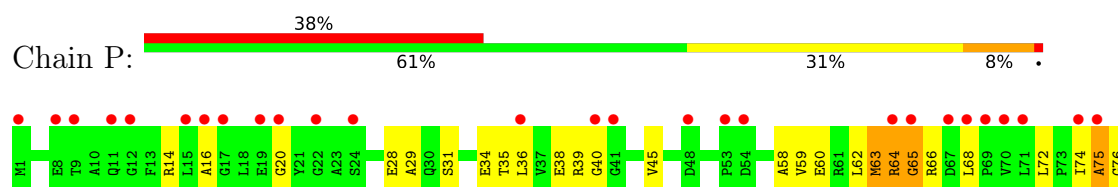
• Molecule 3: V-type ATP synthase subunit D

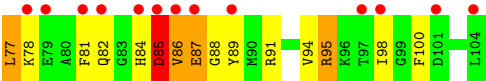


• Molecule 4: V-type ATP synthase subunit F



• Molecule 4: V-type ATP synthase subunit F





4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	380.70Å 380.70Å 147.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.97 – 4.80 29.97 – 4.80	Depositor EDS
% Data completeness (in resolution range)	95.3 (29.97-4.80) 94.9 (29.97-4.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 4.86Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.441 , 0.454 0.413 , 0.426	Depositor DCC
R_{free} test set	2935 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	173.9	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.14 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.28$, $\langle L^2 \rangle = 0.12$	Xtriage
Estimated twinning fraction	0.217 for -h,-k,l	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	32080	wwPDB-VP
Average B, all atoms (Å ²)	191.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.93	4/2750 (0.1%)	1.83	34/3815 (0.9%)
1	B	0.98	5/2750 (0.2%)	1.76	31/3815 (0.8%)
1	C	0.95	5/2750 (0.2%)	1.77	33/3815 (0.9%)
1	I	0.97	7/2750 (0.3%)	1.91	45/3815 (1.2%)
1	J	0.97	6/2750 (0.2%)	1.81	35/3815 (0.9%)
1	K	0.97	6/2750 (0.2%)	2.10	36/3815 (0.9%)
2	D	1.22	14/2210 (0.6%)	1.60	16/3068 (0.5%)
2	E	1.21	14/2210 (0.6%)	1.56	14/3068 (0.5%)
2	F	1.12	9/2210 (0.4%)	1.54	14/3068 (0.5%)
2	L	1.23	15/2210 (0.7%)	1.67	22/3068 (0.7%)
2	M	1.18	13/2210 (0.6%)	1.56	14/3068 (0.5%)
2	N	1.16	14/2210 (0.6%)	1.56	14/3068 (0.5%)
3	G	6.39	252/637 (39.6%)	4.10	159/885 (18.0%)
3	O	6.38	248/637 (38.9%)	4.09	159/885 (18.0%)
4	H	2.31	20/508 (3.9%)	2.31	23/703 (3.3%)
4	P	2.48	23/508 (4.5%)	3.04	29/703 (4.1%)
All	All	1.69	655/32050 (2.0%)	1.93	678/44474 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	5
1	C	0	6
1	I	0	6
1	J	0	6
1	K	0	6
2	D	0	3
2	E	0	3
2	F	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	3
2	M	0	3
2	N	0	3
4	H	0	2
4	P	0	2
All	All	0	55

All (655) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	47	MET	CA-CB	-32.19	0.99	1.53
3	G	47	MET	CA-CB	-32.18	0.99	1.53
3	G	196	ARG	CA-C	23.91	1.84	1.52
3	O	196	ARG	CA-C	23.83	1.84	1.52
3	G	167	VAL	CA-C	23.30	1.81	1.52
3	O	167	VAL	CA-C	23.24	1.81	1.52
3	G	138	ILE	CA-CB	-21.65	1.26	1.54
3	O	138	ILE	CA-CB	-21.56	1.27	1.54
3	O	7	THR	CA-CB	20.40	1.86	1.53
3	O	4	VAL	CA-C	20.17	1.78	1.52
3	G	7	THR	CA-CB	20.16	1.86	1.53
3	G	4	VAL	CA-C	20.11	1.78	1.52
3	O	27	LEU	CA-CB	19.85	1.87	1.53
3	G	27	LEU	CA-CB	19.74	1.87	1.53
3	O	31	LYS	N-CA	19.32	1.71	1.46
3	G	31	LYS	N-CA	18.93	1.70	1.46
2	L	80	ALA	CA-C	17.50	1.71	1.53
3	G	194	LEU	CA-C	17.30	1.75	1.52
3	O	194	LEU	CA-C	17.11	1.75	1.52
3	G	168	VAL	CA-CB	-16.91	1.31	1.54
4	P	34	GLU	C-O	16.86	1.43	1.24
4	H	34	GLU	C-O	16.82	1.43	1.24
3	O	168	VAL	CA-CB	-16.74	1.31	1.54
3	G	163	ALA	CA-C	16.39	1.74	1.52
3	O	163	ALA	CA-C	16.23	1.74	1.52
4	P	75	ALA	CA-C	15.57	1.72	1.52
3	O	19	ARG	N-CA	15.21	1.65	1.46
3	G	19	ARG	N-CA	15.20	1.65	1.46
1	B	429	SER	C-N	14.95	1.54	1.33
3	G	184	GLU	N-CA	14.90	1.64	1.46
3	O	20	LEU	CA-C	14.88	1.71	1.52
3	O	184	GLU	N-CA	14.86	1.64	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	20	LEU	CA-C	14.85	1.71	1.52
3	G	16	GLY	CA-C	14.60	1.69	1.51
3	O	16	GLY	CA-C	14.58	1.69	1.51
3	O	52	ALA	CA-CB	14.47	1.75	1.53
3	G	52	ALA	CA-CB	14.37	1.75	1.53
3	O	32	ARG	C-O	14.19	1.40	1.24
3	G	189	GLU	CA-CB	14.16	1.76	1.53
3	G	32	ARG	C-O	14.16	1.40	1.24
3	O	38	GLU	N-CA	14.10	1.63	1.46
3	O	142	ASN	CA-CB	14.09	1.75	1.53
3	O	189	GLU	CA-CB	14.07	1.76	1.53
3	G	32	ARG	CA-C	13.98	1.71	1.52
3	G	142	ASN	CA-CB	13.98	1.75	1.53
3	G	38	GLU	N-CA	13.96	1.62	1.46
3	G	156	LYS	CA-C	13.96	1.71	1.52
3	O	32	ARG	CA-C	13.91	1.70	1.52
3	O	156	LYS	CA-C	13.88	1.70	1.52
2	D	80	ALA	CA-C	13.51	1.69	1.52
3	G	167	VAL	CA-CB	13.42	1.70	1.54
3	G	164	LEU	C-O	13.23	1.40	1.24
3	O	164	LEU	C-O	13.21	1.40	1.24
3	G	6	PRO	C-O	13.21	1.41	1.24
3	O	167	VAL	CA-CB	13.18	1.69	1.54
3	G	189	GLU	CA-C	13.15	1.69	1.52
4	P	75	ALA	N-CA	13.15	1.62	1.46
3	G	184	GLU	CA-CB	13.11	1.73	1.53
3	O	184	GLU	CA-CB	13.09	1.73	1.53
3	O	189	GLU	CA-C	13.04	1.69	1.52
3	O	163	ALA	C-O	12.93	1.40	1.24
3	O	6	PRO	C-O	12.81	1.40	1.24
3	G	195	LYS	N-CA	12.77	1.62	1.46
3	G	163	ALA	C-O	12.76	1.40	1.24
3	G	182	VAL	N-CA	12.62	1.62	1.46
3	O	195	LYS	N-CA	12.61	1.62	1.46
3	O	182	VAL	N-CA	12.60	1.62	1.46
3	O	50	ARG	C-O	12.57	1.41	1.24
3	O	205	GLU	CA-CB	12.56	1.78	1.53
3	O	155	LYS	N-CA	12.55	1.62	1.46
1	J	429	SER	C-N	12.53	1.51	1.33
3	G	155	LYS	N-CA	12.52	1.62	1.46
3	G	183	LEU	C-O	12.47	1.39	1.24
3	O	170	PRO	CA-C	12.46	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	70	PRO	C-N	12.44	1.51	1.33
3	O	169	ILE	C-O	12.36	1.40	1.24
3	O	183	LEU	C-O	12.35	1.39	1.24
3	G	205	GLU	CA-CB	12.34	1.78	1.53
3	G	50	ARG	C-O	12.32	1.40	1.24
3	O	33	ASP	N-CA	12.32	1.61	1.46
3	G	33	ASP	N-CA	12.32	1.61	1.46
3	G	169	ILE	C-O	12.28	1.39	1.24
3	G	170	PRO	CA-C	12.24	1.68	1.52
2	E	81	ARG	CA-C	12.23	1.67	1.52
3	G	28	LEU	CA-C	12.22	1.69	1.52
3	O	9	MET	CA-C	-12.22	1.36	1.52
2	D	81	ARG	CA-C	12.19	1.67	1.52
3	G	9	MET	CA-C	-12.07	1.36	1.52
3	O	171	GLY	CA-C	11.95	1.68	1.51
3	G	169	ILE	CA-C	11.91	1.65	1.52
3	O	28	LEU	CA-C	11.90	1.69	1.52
3	O	192	PHE	CA-C	11.90	1.69	1.52
3	G	171	GLY	CA-C	11.88	1.68	1.51
4	P	76	GLY	N-CA	11.88	1.57	1.45
2	E	80	ALA	CA-C	11.83	1.68	1.52
3	G	192	PHE	CA-C	11.79	1.68	1.52
2	D	81	ARG	N-CA	11.75	1.60	1.46
3	O	169	ILE	CA-C	11.74	1.65	1.52
2	E	81	ARG	N-CA	11.71	1.59	1.46
3	O	4	VAL	CA-CB	11.70	1.70	1.54
3	G	4	VAL	CA-CB	11.66	1.70	1.54
3	G	188	ARG	N-CA	11.65	1.60	1.46
3	O	52	ALA	N-CA	11.64	1.60	1.46
3	O	188	ARG	N-CA	11.63	1.60	1.46
3	G	52	ALA	N-CA	11.56	1.60	1.46
3	O	134	ALA	N-CA	11.50	1.61	1.46
3	O	187	GLU	CA-C	11.48	1.67	1.52
3	G	134	ALA	N-CA	11.47	1.60	1.46
3	G	7	THR	CA-C	11.47	1.68	1.52
3	O	16	GLY	C-O	11.46	1.40	1.23
3	O	7	THR	CA-C	11.44	1.68	1.52
3	G	193	ARG	N-CA	11.42	1.60	1.46
3	O	53	LEU	N-CA	11.40	1.60	1.46
3	O	32	ARG	C-N	11.40	1.49	1.33
3	O	172	ILE	N-CA	11.38	1.60	1.46
3	O	185	GLN	C-O	11.38	1.38	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	193	ARG	N-CA	11.36	1.60	1.46
3	G	172	ILE	N-CA	11.35	1.60	1.46
3	G	32	ARG	C-N	11.33	1.49	1.33
3	G	185	GLN	C-O	11.32	1.38	1.24
3	G	16	GLY	C-O	11.19	1.39	1.23
3	O	198	LYS	C-O	11.15	1.38	1.24
3	G	198	LYS	C-O	11.12	1.38	1.24
3	G	53	LEU	N-CA	11.08	1.60	1.46
3	G	187	GLU	CA-C	11.03	1.67	1.52
3	G	36	VAL	CA-C	11.00	1.67	1.52
3	G	46	ALA	C-O	10.98	1.37	1.24
3	O	46	ALA	C-O	10.90	1.37	1.24
3	O	36	VAL	CA-C	10.88	1.67	1.52
4	P	40	GLY	C-O	10.83	1.36	1.24
4	H	75	ALA	CA-C	10.82	1.67	1.52
3	G	14	ARG	N-CA	10.75	1.59	1.46
3	O	27	LEU	N-CA	10.75	1.60	1.46
3	O	51	LYS	C-O	10.75	1.37	1.24
3	G	27	LEU	N-CA	10.71	1.60	1.46
4	H	40	GLY	C-O	10.70	1.36	1.24
2	M	81	ARG	CA-C	10.68	1.65	1.52
3	G	154	ILE	C-O	10.65	1.36	1.24
3	O	49	ALA	CA-C	-10.64	1.39	1.52
3	G	24	GLY	CA-C	10.62	1.64	1.51
3	O	169	ILE	N-CA	10.61	1.59	1.46
3	G	51	LYS	C-O	10.61	1.37	1.24
3	O	34	ALA	CA-CB	-10.60	1.35	1.53
3	G	192	PHE	C-O	10.59	1.37	1.24
3	G	34	ALA	CA-CB	-10.57	1.35	1.53
3	G	49	ALA	CA-C	-10.56	1.39	1.52
3	O	192	PHE	C-O	10.55	1.37	1.24
3	G	179	ILE	C-O	10.50	1.36	1.24
3	G	22	GLN	C-O	10.49	1.37	1.24
3	G	4	VAL	C-O	10.48	1.36	1.24
3	O	201	ILE	CA-CB	-10.44	1.41	1.54
3	O	24	GLY	CA-C	10.44	1.64	1.51
3	O	22	GLN	C-O	10.41	1.37	1.24
3	O	179	ILE	C-O	10.41	1.36	1.24
3	G	169	ILE	N-CA	10.40	1.59	1.46
3	O	14	ARG	N-CA	10.40	1.58	1.46
3	O	138	ILE	CA-C	-10.37	1.39	1.52
3	G	204	ARG	N-CA	10.35	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	4	VAL	C-O	10.35	1.36	1.24
3	G	201	ILE	CA-CB	-10.32	1.41	1.54
3	O	204	ARG	N-CA	10.29	1.59	1.46
3	O	154	ILE	C-O	10.29	1.36	1.24
3	G	200	LYS	CA-C	10.16	1.66	1.52
2	L	289	THR	C-N	10.14	1.46	1.33
3	G	6	PRO	CA-CB	10.12	1.68	1.53
2	M	81	ARG	N-CA	10.10	1.57	1.46
4	P	76	GLY	CA-C	10.09	1.63	1.51
3	O	200	LYS	CA-C	10.03	1.66	1.52
3	G	138	ILE	CA-C	-9.99	1.39	1.52
3	O	6	PRO	CA-CB	9.93	1.67	1.53
3	G	14	ARG	C-O	9.85	1.35	1.24
2	M	66	LEU	CA-CB	-9.83	1.42	1.54
2	M	289	THR	C-N	9.81	1.46	1.33
3	O	146	ARG	CA-CB	9.79	1.70	1.53
2	D	289	THR	C-N	9.79	1.46	1.33
2	N	289	THR	C-N	9.79	1.46	1.33
2	N	66	LEU	CA-CB	-9.78	1.42	1.54
3	O	205	GLU	CA-C	9.75	1.73	1.52
3	G	164	LEU	N-CA	9.74	1.58	1.46
3	G	146	ARG	CA-CB	9.74	1.70	1.53
3	O	14	ARG	C-O	9.74	1.35	1.24
2	E	66	LEU	CA-CB	-9.73	1.42	1.54
3	O	164	LEU	N-CA	9.72	1.58	1.46
2	L	66	LEU	CA-CB	-9.71	1.42	1.54
2	E	289	THR	C-N	9.70	1.46	1.33
2	F	289	THR	C-N	9.70	1.46	1.33
2	F	66	LEU	CA-CB	-9.69	1.42	1.54
3	G	205	GLU	CA-C	9.68	1.73	1.52
3	O	11	LEU	CA-CB	9.67	1.69	1.53
2	D	66	LEU	CA-CB	-9.65	1.42	1.54
3	G	11	LEU	CA-CB	9.64	1.69	1.53
4	H	75	ALA	N-CA	9.62	1.58	1.46
3	O	184	GLU	CA-C	9.58	1.65	1.52
3	G	35	LEU	CA-C	9.56	1.65	1.52
3	O	35	LEU	CA-C	9.54	1.65	1.52
3	G	184	GLU	CA-C	9.53	1.65	1.52
3	G	49	ALA	N-CA	9.44	1.57	1.46
3	G	50	ARG	CA-C	9.40	1.66	1.52
3	G	163	ALA	C-N	9.39	1.46	1.34
3	O	163	ALA	C-N	9.38	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	50	ARG	CA-C	9.35	1.65	1.52
3	O	203	ALA	N-CA	-9.34	1.34	1.46
3	G	17	GLN	CA-CB	-9.25	1.39	1.53
3	O	49	ALA	N-CA	9.18	1.57	1.46
2	L	81	ARG	CA-C	9.16	1.72	1.52
3	O	17	GLN	CA-CB	-9.15	1.39	1.53
3	O	5	SER	CA-C	-9.12	1.41	1.52
2	M	80	ALA	CA-C	9.08	1.66	1.53
3	O	194	LEU	C-O	9.08	1.34	1.24
3	G	203	ALA	N-CA	-9.06	1.34	1.46
3	O	31	LYS	C-O	9.04	1.35	1.24
3	G	194	LEU	C-O	9.01	1.34	1.24
3	O	196	ARG	CA-CB	9.01	1.68	1.53
3	G	23	LYS	N-CA	8.98	1.57	1.46
3	G	5	SER	CA-C	-8.96	1.41	1.52
3	G	196	ARG	CA-CB	8.96	1.67	1.53
3	O	23	LYS	N-CA	8.94	1.57	1.46
3	O	51	LYS	CA-C	8.93	1.64	1.52
3	G	158	THR	CA-CB	-8.91	1.38	1.53
3	O	22	GLN	CA-C	8.90	1.64	1.52
3	O	18	LEU	CA-C	8.84	1.64	1.52
3	O	175	GLN	CA-CB	-8.82	1.39	1.53
3	G	31	LYS	C-O	8.82	1.35	1.24
3	G	51	LYS	CA-C	8.78	1.64	1.52
3	O	52	ALA	C-O	8.77	1.34	1.24
3	G	52	ALA	C-O	8.76	1.34	1.24
3	O	45	GLU	C-O	8.74	1.34	1.24
3	G	22	GLN	CA-C	8.70	1.64	1.52
3	G	18	LEU	CA-C	8.68	1.64	1.52
3	G	198	LYS	CA-C	8.68	1.64	1.52
3	G	175	GLN	CA-CB	-8.67	1.39	1.53
3	G	134	ALA	CA-CB	8.66	1.68	1.53
1	C	198	LYS	C-N	8.61	1.45	1.33
3	O	158	THR	CA-CB	-8.61	1.39	1.53
3	O	14	ARG	CA-CB	8.61	1.66	1.53
3	O	193	ARG	CA-C	-8.60	1.41	1.52
3	G	22	GLN	C-N	8.56	1.45	1.34
3	O	36	VAL	CA-CB	8.56	1.65	1.54
4	H	76	GLY	CA-C	8.55	1.60	1.51
3	O	134	ALA	CA-CB	8.55	1.68	1.53
3	O	148	LYS	CA-CB	8.53	1.68	1.53
3	O	166	GLN	CA-C	8.53	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	45	GLU	C-O	8.53	1.34	1.24
4	H	76	GLY	N-CA	8.52	1.54	1.45
3	G	148	LYS	CA-CB	8.51	1.68	1.53
3	O	164	LEU	CA-C	8.50	1.64	1.52
3	O	22	GLN	C-N	8.49	1.45	1.34
3	G	166	GLN	CA-C	8.48	1.64	1.52
3	O	12	LEU	CA-C	-8.47	1.42	1.52
3	G	148	LYS	N-CA	8.47	1.57	1.46
3	G	143	THR	N-CA	8.46	1.56	1.46
3	G	193	ARG	CA-C	-8.46	1.41	1.52
3	G	36	VAL	CA-CB	8.44	1.65	1.54
3	G	183	LEU	C-N	8.39	1.44	1.33
3	O	148	LYS	N-CA	8.39	1.57	1.46
3	G	164	LEU	CA-C	8.38	1.64	1.52
3	O	183	LEU	C-N	8.38	1.44	1.33
3	O	198	LYS	CA-C	8.36	1.64	1.52
3	G	170	PRO	N-CA	8.33	1.56	1.47
3	O	143	THR	N-CA	8.32	1.56	1.46
3	G	25	VAL	N-CA	8.32	1.57	1.46
3	O	25	VAL	N-CA	8.31	1.57	1.46
3	G	14	ARG	CA-CB	8.30	1.66	1.53
3	G	12	LEU	CA-C	-8.28	1.42	1.52
3	O	24	GLY	C-O	8.27	1.33	1.23
3	G	21	ALA	C-O	8.26	1.34	1.24
3	O	48	GLU	CA-C	8.26	1.63	1.52
1	K	13	ALA	CA-CB	-8.18	1.39	1.53
1	J	13	ALA	CA-CB	-8.17	1.39	1.53
3	O	170	PRO	N-CA	8.17	1.56	1.47
1	B	13	ALA	CA-CB	-8.16	1.39	1.53
3	O	7	THR	N-CA	8.16	1.56	1.46
3	G	149	LYS	CA-C	8.12	1.63	1.52
1	C	13	ALA	CA-CB	-8.12	1.39	1.53
3	G	7	THR	N-CA	8.11	1.56	1.46
3	G	142	ASN	CA-C	8.10	1.63	1.52
3	O	175	GLN	N-CA	-8.09	1.36	1.46
1	A	13	ALA	CA-CB	-8.08	1.39	1.53
3	G	15	ARG	CA-CB	8.08	1.66	1.53
3	O	21	ALA	C-O	8.08	1.34	1.24
3	G	48	GLU	CA-C	8.08	1.63	1.52
3	O	15	ARG	CA-CB	8.07	1.66	1.53
3	O	142	ASN	CA-C	8.06	1.63	1.52
3	G	49	ALA	CA-CB	-8.03	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	13	ALA	CA-CB	-8.03	1.39	1.53
3	G	15	ARG	C-O	8.01	1.33	1.24
3	O	165	GLU	N-CA	7.99	1.56	1.46
3	O	153	GLU	N-CA	7.96	1.56	1.46
3	G	153	GLU	N-CA	7.95	1.56	1.46
3	O	149	LYS	CA-C	7.94	1.63	1.52
3	O	47	MET	C-O	7.94	1.33	1.24
3	G	166	GLN	CA-CB	-7.93	1.40	1.53
3	G	175	GLN	N-CA	-7.93	1.36	1.46
3	G	24	GLY	C-O	7.90	1.33	1.23
3	G	47	MET	C-O	7.90	1.33	1.24
3	O	166	GLN	CA-CB	-7.88	1.41	1.53
3	O	136	ALA	N-CA	7.85	1.56	1.46
3	G	195	LYS	CA-C	-7.85	1.42	1.52
3	O	195	LYS	CA-C	-7.82	1.42	1.52
3	O	49	ALA	CA-CB	-7.81	1.41	1.53
2	M	77	GLU	CA-CB	-7.79	1.43	1.54
3	G	160	ARG	CA-C	7.79	1.63	1.52
2	N	77	GLU	CA-CB	-7.79	1.43	1.54
3	G	17	GLN	N-CA	7.78	1.56	1.46
3	O	15	ARG	C-O	7.77	1.33	1.24
1	I	352	PRO	CA-CB	-7.76	1.43	1.53
3	O	160	ARG	CA-C	7.75	1.63	1.52
3	O	168	VAL	N-CA	7.75	1.56	1.46
3	G	165	GLU	N-CA	7.72	1.56	1.46
2	F	77	GLU	CA-CB	-7.71	1.43	1.54
3	G	187	GLU	C-N	7.71	1.44	1.33
3	G	168	VAL	N-CA	7.70	1.55	1.46
2	L	81	ARG	N-CA	7.70	1.60	1.46
3	O	187	GLU	C-N	7.69	1.44	1.33
1	A	352	PRO	CA-CB	-7.69	1.43	1.53
3	G	199	GLY	N-CA	7.67	1.56	1.45
2	D	77	GLU	CA-CB	-7.66	1.44	1.54
3	O	183	LEU	CA-C	7.65	1.63	1.52
2	E	77	GLU	CA-CB	-7.65	1.44	1.54
3	G	12	LEU	N-CA	7.63	1.55	1.46
3	G	52	ALA	CA-C	7.62	1.62	1.52
3	G	136	ALA	N-CA	7.61	1.56	1.46
3	G	26	ASP	C-O	7.60	1.32	1.24
1	C	325	ASP	C-N	-7.60	1.23	1.33
1	I	325	ASP	C-N	-7.60	1.23	1.33
3	G	201	ILE	C-O	7.58	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	29	ALA	CA-CB	-7.58	1.41	1.53
1	A	325	ASP	C-N	-7.57	1.23	1.33
3	O	194	LEU	C-N	7.56	1.44	1.34
3	O	17	GLN	N-CA	7.56	1.55	1.46
3	O	196	ARG	C-O	7.55	1.33	1.24
2	N	81	ARG	CA-C	7.55	1.61	1.52
1	K	325	ASP	C-N	-7.54	1.23	1.33
3	G	36	VAL	C-O	7.54	1.33	1.24
1	B	325	ASP	C-N	-7.53	1.24	1.33
4	H	29	ALA	CA-CB	-7.52	1.41	1.53
3	O	19	ARG	CA-C	7.52	1.62	1.52
3	G	194	LEU	C-N	7.51	1.44	1.34
2	L	77	GLU	CA-CB	-7.51	1.44	1.54
3	O	201	ILE	C-O	7.50	1.33	1.24
3	G	183	LEU	CA-C	7.50	1.62	1.52
3	O	12	LEU	N-CA	7.49	1.55	1.46
1	I	70	PRO	CA-C	7.47	1.63	1.52
4	H	29	ALA	N-CA	-7.47	1.37	1.46
1	I	429	SER	C-N	-7.46	1.24	1.33
1	J	325	ASP	C-N	-7.46	1.24	1.33
3	G	30	LYS	C-N	7.46	1.44	1.33
3	G	196	ARG	C-O	7.44	1.33	1.24
4	P	29	ALA	N-CA	-7.44	1.37	1.46
3	O	36	VAL	C-O	7.44	1.32	1.24
3	G	167	VAL	C-O	7.44	1.32	1.24
3	O	7	THR	C-O	7.43	1.33	1.24
3	G	19	ARG	CA-C	7.42	1.62	1.52
3	O	26	ASP	C-O	7.41	1.32	1.24
3	O	199	GLY	N-CA	7.41	1.56	1.45
3	G	7	THR	C-O	7.40	1.33	1.24
3	O	16	GLY	C-N	7.40	1.43	1.33
3	O	52	ALA	CA-C	7.39	1.62	1.52
3	G	37	ALA	CA-CB	-7.38	1.40	1.53
4	P	77	LEU	N-CA	7.37	1.60	1.46
2	N	81	ARG	N-CA	7.37	1.55	1.45
3	G	162	ASN	CA-CB	-7.36	1.41	1.53
3	G	170	PRO	C-O	7.35	1.33	1.24
3	G	49	ALA	C-O	7.35	1.32	1.24
3	O	28	LEU	C-O	7.31	1.33	1.24
2	D	80	ALA	N-CA	7.31	1.54	1.45
3	G	162	ASN	C-O	7.31	1.33	1.24
3	G	192	PHE	C-N	7.28	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	162	ASN	CA-CB	-7.28	1.41	1.53
1	J	352	PRO	CA-CB	-7.28	1.43	1.53
3	O	29	LYS	CA-C	7.28	1.61	1.52
3	O	38	GLU	C-O	7.27	1.32	1.24
3	G	16	GLY	C-N	7.27	1.43	1.33
2	L	81	ARG	C-N	7.27	1.43	1.33
3	O	165	GLU	C-O	7.27	1.33	1.24
3	G	48	GLU	C-N	7.25	1.43	1.33
3	O	49	ALA	C-O	7.24	1.32	1.24
3	O	133	TYR	CA-C	7.24	1.62	1.52
3	O	167	VAL	C-O	7.24	1.32	1.24
3	G	38	GLU	C-O	7.23	1.32	1.24
4	H	36	LEU	C-N	7.22	1.43	1.33
3	O	162	ASN	C-O	7.21	1.33	1.24
3	G	189	GLU	C-O	7.21	1.32	1.24
3	O	37	ALA	CA-CB	-7.21	1.40	1.53
1	K	352	PRO	CA-CB	-7.20	1.43	1.53
3	O	22	GLN	N-CA	7.19	1.55	1.46
1	B	352	PRO	CA-CB	-7.19	1.43	1.53
3	O	170	PRO	C-O	7.19	1.32	1.24
3	G	165	GLU	C-O	7.18	1.33	1.24
3	G	133	TYR	CA-C	7.18	1.62	1.52
3	O	192	PHE	C-N	7.18	1.43	1.34
3	G	28	LEU	C-O	7.17	1.33	1.24
2	L	80	ALA	C-N	7.17	1.43	1.33
3	O	30	LYS	C-N	7.16	1.43	1.33
2	E	80	ALA	N-CA	7.16	1.54	1.45
3	G	22	GLN	N-CA	7.15	1.55	1.46
2	N	275	GLU	CA-CB	-7.11	1.41	1.53
4	P	36	LEU	C-N	7.11	1.42	1.33
3	O	48	GLU	C-N	7.11	1.43	1.33
3	G	144	GLU	N-CA	-7.10	1.37	1.46
3	G	25	VAL	CA-CB	7.09	1.64	1.54
3	O	189	GLU	C-O	7.08	1.32	1.24
2	L	275	GLU	CA-CB	-7.06	1.41	1.53
3	G	37	ALA	C-O	7.06	1.33	1.24
3	G	29	LYS	CA-C	7.05	1.61	1.52
2	M	275	GLU	CA-CB	-7.05	1.41	1.53
3	O	144	GLU	N-CA	-7.02	1.37	1.46
2	E	275	GLU	CA-CB	-7.00	1.41	1.53
1	C	352	PRO	CA-CB	-6.98	1.43	1.53
3	O	160	ARG	C-O	6.97	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	80	ALA	CA-C	6.97	1.62	1.53
3	O	20	LEU	C-O	6.97	1.32	1.24
2	F	275	GLU	CA-CB	-6.96	1.41	1.53
3	G	139	ARG	CA-CB	6.95	1.65	1.53
3	O	172	ILE	CA-C	-6.92	1.44	1.52
2	D	275	GLU	CA-CB	-6.92	1.41	1.53
3	O	37	ALA	C-O	6.91	1.32	1.24
3	G	20	LEU	C-O	6.87	1.31	1.24
3	G	160	ARG	C-O	6.87	1.32	1.24
3	O	154	ILE	C-N	6.84	1.43	1.33
3	O	184	GLU	C-O	6.84	1.31	1.24
3	G	203	ALA	CA-CB	-6.83	1.42	1.53
3	O	25	VAL	CA-CB	6.82	1.63	1.54
3	G	154	ILE	C-N	6.81	1.43	1.33
3	O	203	ALA	CA-CB	-6.81	1.42	1.53
3	O	139	ARG	CA-CB	6.79	1.65	1.53
3	G	155	LYS	CA-CB	6.76	1.64	1.53
1	K	19	MET	CA-CB	-6.73	1.42	1.53
1	I	19	MET	CA-CB	-6.71	1.42	1.53
3	O	188	ARG	C-O	6.71	1.31	1.24
3	G	184	GLU	C-O	6.70	1.31	1.24
1	A	19	MET	CA-CB	-6.70	1.42	1.53
1	J	19	MET	CA-CB	-6.70	1.42	1.53
1	B	19	MET	CA-CB	-6.69	1.42	1.53
1	C	19	MET	CA-CB	-6.68	1.42	1.53
3	G	150	ILE	N-CA	6.62	1.54	1.46
3	G	172	ILE	CA-C	-6.62	1.44	1.52
3	G	188	ARG	C-O	6.61	1.31	1.24
4	H	58	ALA	CA-CB	-6.61	1.42	1.53
3	G	190	ASP	C-O	6.59	1.31	1.24
3	O	155	LYS	CA-CB	6.59	1.64	1.53
3	O	181	GLN	C-O	6.57	1.32	1.24
4	P	76	GLY	C-N	6.55	1.42	1.33
3	O	133	TYR	C-N	6.54	1.42	1.33
3	G	178	PHE	C-O	6.50	1.31	1.24
4	P	58	ALA	CA-CB	-6.50	1.43	1.53
3	O	35	LEU	C-O	6.50	1.32	1.24
3	O	150	ILE	N-CA	6.47	1.54	1.46
3	G	133	TYR	C-N	6.45	1.42	1.33
3	G	141	ALA	N-CA	6.44	1.54	1.46
3	O	190	ASP	C-O	6.42	1.31	1.24
3	O	141	ALA	N-CA	6.41	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	171	GLY	C-O	6.41	1.32	1.23
3	O	178	PHE	C-O	6.40	1.31	1.24
3	G	181	GLN	CA-C	6.39	1.61	1.52
3	O	161	VAL	C-O	6.37	1.31	1.24
3	G	142	ASN	C-O	6.36	1.31	1.24
3	G	171	GLY	C-O	6.32	1.32	1.23
3	O	181	GLN	CA-C	6.32	1.61	1.52
3	G	35	LEU	C-O	6.32	1.31	1.24
3	G	181	GLN	C-O	6.31	1.32	1.24
3	G	202	GLU	N-CA	6.31	1.53	1.46
3	O	183	LEU	N-CA	6.30	1.54	1.46
3	G	149	LYS	N-CA	-6.29	1.38	1.46
2	N	359	SER	CA-C	6.29	1.60	1.52
3	G	135	GLU	CA-CB	6.28	1.63	1.53
3	G	186	ARG	C-O	6.25	1.31	1.24
3	O	202	GLU	N-CA	6.25	1.53	1.46
3	G	133	TYR	C-O	6.24	1.32	1.24
3	O	149	LYS	N-CA	-6.24	1.38	1.46
3	O	141	ALA	CA-CB	6.23	1.64	1.53
4	P	75	ALA	C-N	6.23	1.41	1.33
3	G	188	ARG	C-N	6.22	1.42	1.33
3	O	13	GLN	C-N	6.20	1.41	1.33
4	H	28	GLU	CA-C	6.18	1.60	1.52
4	P	28	GLU	CA-C	6.18	1.60	1.52
3	O	188	ARG	C-N	6.18	1.42	1.33
3	O	133	TYR	C-O	6.17	1.31	1.24
3	G	31	LYS	CA-CB	6.17	1.63	1.53
4	H	40	GLY	C-N	6.15	1.44	1.33
3	G	190	ASP	CA-C	6.13	1.60	1.52
3	G	183	LEU	N-CA	6.12	1.54	1.46
3	O	142	ASN	C-O	6.10	1.31	1.24
4	P	77	LEU	C-N	6.09	1.42	1.34
4	H	75	ALA	C-N	6.09	1.39	1.32
4	P	40	GLY	C-N	6.08	1.44	1.33
3	G	141	ALA	CA-CB	6.07	1.64	1.53
3	O	190	ASP	CA-C	6.06	1.60	1.52
3	G	42	LEU	C-O	6.05	1.31	1.24
3	O	38	GLU	CA-C	6.05	1.60	1.52
3	O	159	ARG	C-O	6.05	1.31	1.24
2	N	250	ASP	C-O	-6.04	1.15	1.23
3	O	31	LYS	CA-CB	6.03	1.63	1.53
2	M	250	ASP	C-O	-6.00	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	250	ASP	C-O	-5.99	1.15	1.23
2	E	250	ASP	C-O	-5.98	1.15	1.23
2	D	250	ASP	C-O	-5.98	1.15	1.23
3	O	42	LEU	C-O	5.97	1.31	1.24
4	P	45	VAL	CA-C	-5.96	1.45	1.52
3	G	161	VAL	C-O	5.95	1.31	1.24
3	G	5	SER	CA-CB	5.95	1.62	1.53
3	O	29	LYS	C-O	5.94	1.30	1.24
4	H	31	SER	N-CA	-5.93	1.39	1.46
3	G	38	GLU	CA-C	5.92	1.60	1.52
3	G	200	LYS	CA-CB	5.92	1.63	1.53
3	O	135	GLU	CA-CB	5.92	1.62	1.53
3	G	13	GLN	C-N	5.91	1.41	1.33
2	F	250	ASP	C-O	-5.90	1.15	1.23
3	O	200	LYS	CA-CB	5.88	1.63	1.53
4	H	45	VAL	CA-C	-5.88	1.45	1.52
3	O	139	ARG	CA-C	5.87	1.60	1.52
4	P	31	SER	N-CA	-5.85	1.39	1.46
3	G	159	ARG	C-O	5.85	1.30	1.24
4	P	77	LEU	CA-C	5.85	1.65	1.52
2	E	26	ASP	CA-CB	-5.81	1.43	1.53
3	G	139	ARG	CA-C	5.81	1.60	1.52
2	M	80	ALA	N-CA	5.81	1.52	1.45
4	P	35	THR	CA-C	5.80	1.60	1.52
3	O	186	ARG	C-O	5.79	1.31	1.24
2	L	26	ASP	CA-CB	-5.77	1.43	1.53
3	O	5	SER	CA-CB	5.77	1.62	1.53
4	H	35	THR	CA-C	5.76	1.60	1.52
3	G	30	LYS	N-CA	5.75	1.53	1.46
2	D	249	HIS	C-O	-5.73	1.16	1.24
3	O	41	GLY	C-O	5.72	1.31	1.23
3	G	159	ARG	N-CA	5.71	1.53	1.46
3	O	142	ASN	C-N	5.70	1.41	1.33
3	G	135	GLU	CA-C	5.70	1.60	1.52
3	G	43	VAL	N-CA	5.68	1.53	1.46
3	O	166	GLN	C-O	5.68	1.30	1.24
3	G	166	GLN	N-CA	-5.67	1.39	1.46
2	D	26	ASP	CA-CB	-5.67	1.43	1.53
2	N	26	ASP	CA-CB	-5.67	1.43	1.53
3	G	182	VAL	C-O	5.66	1.30	1.24
3	O	182	VAL	C-O	5.65	1.30	1.24
2	M	26	ASP	CA-CB	-5.65	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	30	LYS	N-CA	5.64	1.53	1.46
3	O	177	ARG	N-CA	5.64	1.53	1.46
3	O	11	LEU	C-N	5.63	1.40	1.33
2	E	249	HIS	C-O	-5.62	1.16	1.24
3	G	166	GLN	C-O	5.62	1.30	1.24
3	O	43	VAL	N-CA	5.61	1.53	1.46
2	F	249	HIS	C-O	-5.60	1.16	1.24
3	O	43	VAL	C-O	5.60	1.30	1.24
3	G	177	ARG	N-CA	5.60	1.53	1.46
3	O	159	ARG	N-CA	5.60	1.53	1.46
3	G	43	VAL	CA-CB	5.59	1.62	1.54
3	G	205	GLU	C-O	5.58	1.34	1.23
3	O	205	GLU	C-O	5.58	1.34	1.23
3	G	15	ARG	N-CA	5.57	1.52	1.46
2	F	26	ASP	CA-CB	-5.56	1.44	1.53
2	M	249	HIS	C-O	-5.56	1.16	1.24
3	O	43	VAL	CA-CB	5.55	1.62	1.54
3	G	24	GLY	N-CA	5.55	1.52	1.45
3	G	8	ARG	CA-C	5.53	1.60	1.52
3	O	190	ASP	CA-CB	-5.53	1.44	1.53
3	G	133	TYR	N-CA	-5.52	1.39	1.46
3	G	41	GLY	C-O	5.51	1.31	1.23
3	O	15	ARG	N-CA	5.51	1.52	1.46
3	O	181	GLN	C-N	5.50	1.40	1.33
2	N	249	HIS	C-O	-5.50	1.16	1.24
2	L	249	HIS	C-O	-5.50	1.16	1.24
3	G	158	THR	N-CA	5.49	1.53	1.46
3	O	158	THR	N-CA	5.48	1.53	1.46
3	G	11	LEU	C-N	5.48	1.40	1.33
3	G	29	LYS	C-O	5.48	1.30	1.24
2	L	80	ALA	N-CA	5.47	1.53	1.46
3	G	190	ASP	CA-CB	-5.46	1.44	1.53
4	P	91	ARG	C-O	5.45	1.30	1.24
3	O	156	LYS	CA-CB	5.44	1.62	1.54
3	O	204	ARG	C-O	5.43	1.30	1.24
2	M	63	THR	CA-CB	-5.42	1.44	1.53
3	G	177	ARG	C-O	5.40	1.30	1.24
4	H	91	ARG	C-O	5.39	1.30	1.24
3	O	198	LYS	C-N	5.38	1.41	1.33
3	O	133	TYR	N-CA	-5.37	1.39	1.46
3	O	135	GLU	CA-C	5.37	1.59	1.52
3	G	182	VAL	C-N	5.37	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	166	GLN	N-CA	-5.36	1.39	1.46
2	F	291	LEU	C-O	-5.36	1.17	1.24
3	G	204	ARG	C-O	5.36	1.30	1.24
3	O	38	GLU	CA-CB	5.36	1.61	1.53
3	O	8	ARG	CA-C	5.35	1.60	1.52
3	O	186	ARG	CA-CB	5.35	1.62	1.53
3	G	186	ARG	CA-CB	5.35	1.62	1.53
3	G	198	LYS	C-N	5.34	1.41	1.33
3	G	149	LYS	CA-CB	-5.33	1.44	1.53
3	O	24	GLY	N-CA	5.33	1.52	1.45
2	N	63	THR	CA-CB	-5.33	1.44	1.53
3	O	44	ARG	CA-CB	-5.32	1.43	1.53
3	G	38	GLU	CA-CB	5.32	1.61	1.53
2	L	63	THR	CA-CB	-5.32	1.44	1.53
3	G	179	ILE	CA-C	5.31	1.59	1.52
3	O	21	ALA	C-N	5.30	1.41	1.33
2	E	63	THR	CA-CB	-5.30	1.44	1.53
3	O	179	ILE	CA-C	5.29	1.59	1.52
2	F	63	THR	CA-CB	-5.29	1.44	1.53
3	G	181	GLN	C-N	5.29	1.40	1.33
3	G	27	LEU	C-O	5.28	1.30	1.24
3	G	43	VAL	C-O	5.27	1.30	1.24
3	G	44	ARG	CA-CB	-5.27	1.43	1.53
3	G	22	GLN	CA-CB	5.26	1.62	1.53
4	P	20	GLY	C-O	-5.26	1.16	1.23
3	G	157	THR	CA-CB	-5.26	1.44	1.53
3	O	135	GLU	N-CA	5.26	1.52	1.46
3	G	21	ALA	N-CA	5.25	1.52	1.46
3	O	149	LYS	CA-CB	-5.25	1.44	1.53
3	O	177	ARG	C-O	5.25	1.30	1.24
3	O	194	LEU	N-CA	5.25	1.52	1.46
2	D	81	ARG	C-N	5.24	1.40	1.33
3	G	140	VAL	N-CA	5.23	1.52	1.46
2	N	360	ARG	N-CA	5.23	1.52	1.46
2	E	81	ARG	C-N	5.22	1.40	1.33
3	O	37	ALA	C-N	5.22	1.40	1.33
3	G	134	ALA	CA-C	5.22	1.59	1.52
3	O	11	LEU	CA-C	5.22	1.59	1.52
3	O	134	ALA	CA-C	5.22	1.59	1.52
3	G	21	ALA	C-N	5.21	1.41	1.33
3	G	142	ASN	C-N	5.21	1.40	1.33
1	J	244	TRP	CA-C	5.21	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	63	THR	CA-CB	-5.20	1.44	1.53
3	O	145	THR	C-O	5.20	1.30	1.24
2	M	291	LEU	C-O	-5.19	1.17	1.24
3	G	11	LEU	CA-C	5.19	1.59	1.52
1	I	244	TRP	CA-C	5.19	1.59	1.52
3	O	42	LEU	CA-C	5.18	1.59	1.52
2	N	291	LEU	C-O	-5.17	1.17	1.24
3	O	22	GLN	CA-CB	5.17	1.62	1.53
3	G	156	LYS	CA-CB	5.16	1.62	1.54
3	O	182	VAL	C-N	5.14	1.40	1.33
3	G	37	ALA	C-N	5.13	1.40	1.33
1	K	244	TRP	CA-C	5.12	1.59	1.52
4	H	20	GLY	C-O	-5.11	1.16	1.23
3	G	194	LEU	N-CA	5.11	1.52	1.46
3	O	199	GLY	CA-C	-5.10	1.44	1.51
3	O	47	MET	CA-C	5.09	1.59	1.52
3	O	157	THR	CA-CB	-5.08	1.44	1.53
3	O	139	ARG	C-O	5.08	1.30	1.24
3	G	53	LEU	CA-CB	5.08	1.62	1.53
3	G	144	GLU	CA-C	5.07	1.59	1.52
3	O	21	ALA	N-CA	5.07	1.52	1.46
4	P	72	LEU	N-CA	-5.07	1.41	1.46
3	G	42	LEU	CA-C	5.06	1.59	1.52
2	D	80	ALA	C-N	5.06	1.39	1.33
3	G	139	ARG	C-O	5.05	1.30	1.24
3	G	174	ALA	CA-C	5.05	1.59	1.52
2	E	291	LEU	C-O	-5.04	1.17	1.24
2	L	291	LEU	C-O	-5.03	1.17	1.24
3	G	51	LYS	C-N	5.03	1.40	1.33
3	G	192	PHE	N-CA	5.02	1.52	1.46
3	G	47	MET	CA-C	5.02	1.59	1.52
4	H	72	LEU	N-CA	-5.02	1.41	1.46
3	G	30	LYS	CA-C	5.01	1.59	1.52
3	O	14	ARG	CA-C	5.01	1.59	1.52
4	H	77	LEU	N-CA	5.01	1.55	1.46

All (678) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	325	ASP	O-C-N	-47.91	58.87	122.59
1	J	325	ASP	O-C-N	-47.91	58.87	122.59
1	A	325	ASP	O-C-N	-47.89	58.90	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	325	ASP	O-C-N	-47.89	58.90	122.59
1	B	325	ASP	O-C-N	-47.85	58.94	122.59
1	K	325	ASP	O-C-N	-47.85	58.94	122.59
1	K	70	PRO	CA-C-N	-43.74	37.99	121.54
1	K	70	PRO	C-N-CA	-43.74	37.99	121.54
1	K	70	PRO	O-C-N	31.64	159.40	123.01
1	C	325	ASP	CA-C-N	-28.02	75.92	121.87
1	C	325	ASP	C-N-CA	-28.02	75.92	121.87
1	A	325	ASP	CA-C-N	-27.96	76.01	121.87
1	A	325	ASP	C-N-CA	-27.96	76.01	121.87
1	K	325	ASP	CA-C-N	-27.92	76.08	121.87
1	K	325	ASP	C-N-CA	-27.92	76.08	121.87
1	B	325	ASP	CA-C-N	-27.88	76.14	121.87
1	B	325	ASP	C-N-CA	-27.88	76.14	121.87
1	J	325	ASP	CA-C-N	-27.87	76.16	121.87
1	J	325	ASP	C-N-CA	-27.87	76.16	121.87
1	I	325	ASP	CA-C-N	-27.82	76.25	121.87
1	I	325	ASP	C-N-CA	-27.82	76.25	121.87
2	D	316	MET	O-C-N	-26.08	91.32	121.32
2	L	316	MET	O-C-N	-26.02	91.40	121.32
2	E	316	MET	O-C-N	-25.97	91.45	121.32
2	F	316	MET	O-C-N	-25.92	91.52	121.32
2	N	316	MET	O-C-N	-25.89	91.55	121.32
2	M	316	MET	O-C-N	-25.88	91.56	121.32
4	P	77	LEU	CA-C-N	-25.09	82.18	120.31
4	P	77	LEU	C-N-CA	-25.09	82.18	120.31
4	P	85	ASP	O-C-N	23.36	153.66	122.59
1	A	429	SER	O-C-N	-23.32	94.90	123.36
4	P	85	ASP	CA-C-O	-23.15	87.40	120.51
4	P	74	ILE	O-C-N	-20.15	101.54	123.10
4	H	77	LEU	CA-C-N	-19.74	87.13	120.68
4	H	77	LEU	C-N-CA	-19.74	87.13	120.68
4	P	75	ALA	N-CA-C	18.29	134.01	110.24
1	I	429	SER	CA-C-N	-17.62	94.66	122.67
1	I	429	SER	C-N-CA	-17.62	94.66	122.67
1	I	429	SER	O-C-N	17.24	143.27	123.27
1	J	429	SER	O-C-N	-17.02	91.47	122.44
3	O	133	TYR	N-CA-C	-16.80	91.89	112.38
3	O	157	THR	N-CA-C	-16.76	92.09	112.54
3	G	133	TYR	N-CA-C	-16.75	91.94	112.38
3	G	157	THR	N-CA-C	-16.74	92.12	112.54
2	L	360	ARG	N-CA-C	-16.70	92.83	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	12	LEU	N-CA-C	-16.57	92.91	110.97
3	O	12	LEU	N-CA-C	-16.42	93.07	110.97
1	I	198	LYS	O-C-N	16.00	143.00	122.68
3	O	203	ALA	N-CA-C	-15.36	89.92	112.04
3	G	203	ALA	N-CA-C	-15.34	89.96	112.04
2	L	80	ALA	CA-C-N	14.62	148.01	121.70
2	L	80	ALA	C-N-CA	14.62	148.01	121.70
3	G	142	ASN	N-CA-C	-14.38	95.69	111.36
3	O	142	ASN	N-CA-C	-14.19	95.89	111.36
4	P	76	GLY	CA-C-N	13.95	146.80	121.70
4	P	76	GLY	C-N-CA	13.95	146.80	121.70
3	G	153	GLU	N-CA-C	13.90	130.13	112.89
3	O	6	PRO	CA-C-N	-13.84	97.16	120.68
3	O	6	PRO	C-N-CA	-13.84	97.16	120.68
3	O	153	GLU	N-CA-C	13.77	129.96	112.89
3	O	187	GLU	N-CA-C	13.77	133.53	113.02
3	G	6	PRO	CA-C-N	-13.72	97.36	120.68
3	G	6	PRO	C-N-CA	-13.72	97.36	120.68
2	D	81	ARG	N-CA-C	13.71	126.88	108.38
1	I	198	LYS	CA-C-N	-13.59	101.42	120.71
1	I	198	LYS	C-N-CA	-13.59	101.42	120.71
3	O	47	MET	N-CA-C	13.58	139.72	110.80
3	G	47	MET	N-CA-C	13.56	139.69	110.80
2	D	360	ARG	N-CA-C	-13.21	96.27	112.38
3	O	139	ARG	N-CA-C	-13.16	82.76	110.80
3	G	139	ARG	N-CA-C	-13.15	82.79	110.80
3	G	194	LEU	N-CA-C	12.86	127.09	111.40
3	O	194	LEU	N-CA-C	12.81	127.03	111.40
4	H	74	ILE	O-C-N	-12.80	109.38	123.20
3	O	186	ARG	CA-C-N	-12.61	102.03	122.08
3	O	186	ARG	C-N-CA	-12.61	102.03	122.08
2	E	81	ARG	N-CA-C	12.60	127.00	108.60
3	G	187	GLU	N-CA-C	12.57	133.75	113.89
3	G	186	ARG	CA-C-N	-12.44	102.58	121.99
3	G	186	ARG	C-N-CA	-12.44	102.58	121.99
2	M	81	ARG	N-CA-C	12.41	126.72	108.60
1	A	429	SER	CA-C-N	11.99	146.89	122.55
1	A	429	SER	C-N-CA	11.99	146.89	122.55
3	G	188	ARG	N-CA-C	-11.97	98.23	111.28
4	P	76	GLY	CA-C-O	-11.93	107.74	121.46
3	O	9	MET	CA-C-N	-11.83	98.29	121.94
3	O	9	MET	C-N-CA	-11.83	98.29	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	9	MET	CA-C-N	-11.82	98.29	121.94
3	G	9	MET	C-N-CA	-11.82	98.29	121.94
3	O	188	ARG	N-CA-C	-11.80	98.42	111.28
4	H	76	GLY	CA-C-O	-11.59	110.46	122.05
3	O	49	ALA	CA-C-N	-11.55	98.83	121.94
3	O	49	ALA	C-N-CA	-11.55	98.83	121.94
3	G	49	ALA	CA-C-N	-11.52	98.91	121.94
3	G	49	ALA	C-N-CA	-11.52	98.91	121.94
3	G	167	VAL	O-C-N	-11.42	110.71	121.91
3	G	7	THR	CA-C-N	-11.41	103.72	120.38
3	G	7	THR	C-N-CA	-11.41	103.72	120.38
3	O	167	VAL	O-C-N	-11.39	110.75	121.91
1	I	70	PRO	N-CA-C	-11.36	89.06	112.47
2	N	351	PRO	N-CA-CB	11.31	110.39	102.81
3	O	7	THR	CA-C-N	-11.31	103.86	120.38
3	O	7	THR	C-N-CA	-11.31	103.86	120.38
1	A	70	PRO	N-CA-C	-11.26	98.31	113.40
2	M	351	PRO	N-CA-CB	11.24	110.34	102.81
4	H	76	GLY	CA-C-N	11.20	141.86	121.70
4	H	76	GLY	C-N-CA	11.20	141.86	121.70
2	D	351	PRO	N-CA-CB	11.17	110.30	102.81
3	G	6	PRO	N-CA-CB	11.14	114.95	103.25
1	I	63	PRO	N-CA-CB	11.14	113.77	103.19
3	O	47	MET	CA-C-N	-11.13	100.28	121.54
3	O	47	MET	C-N-CA	-11.13	100.28	121.54
3	G	47	MET	CA-C-N	-11.12	100.30	121.54
3	G	47	MET	C-N-CA	-11.12	100.30	121.54
2	L	351	PRO	N-CA-CB	11.11	110.25	102.81
1	K	63	PRO	N-CA-CB	11.07	113.71	103.19
1	C	63	PRO	N-CA-CB	11.06	113.70	103.19
2	E	351	PRO	N-CA-CB	11.01	110.18	102.81
2	F	351	PRO	N-CA-CB	10.95	110.15	102.81
1	B	63	PRO	N-CA-CB	10.94	113.58	103.19
1	J	63	PRO	N-CA-CB	10.91	113.56	103.19
1	A	63	PRO	N-CA-CB	10.89	113.54	103.19
1	J	429	SER	CA-C-N	10.87	142.31	121.54
1	J	429	SER	C-N-CA	10.87	142.31	121.54
3	O	6	PRO	N-CA-CB	10.81	114.60	103.25
2	L	359	SER	N-CA-C	-10.66	93.63	109.62
3	O	38	GLU	N-CA-C	10.55	122.36	111.07
3	G	38	GLU	N-CA-C	10.47	122.27	111.07
3	O	163	ALA	N-CA-C	10.30	123.77	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	163	ALA	N-CA-C	10.29	123.75	111.82
3	O	167	VAL	CA-C-N	-10.25	103.51	121.97
3	O	167	VAL	C-N-CA	-10.25	103.51	121.97
3	G	167	VAL	CA-C-N	-10.23	103.55	121.97
3	G	167	VAL	C-N-CA	-10.23	103.55	121.97
4	P	65	GLY	N-CA-C	-10.13	96.20	112.31
1	I	69	LEU	CA-C-N	10.13	132.50	119.84
1	I	69	LEU	C-N-CA	10.13	132.50	119.84
3	G	183	LEU	CA-C-N	10.11	134.19	120.54
3	G	183	LEU	C-N-CA	10.11	134.19	120.54
3	O	183	LEU	CA-C-N	10.10	134.18	120.54
3	O	183	LEU	C-N-CA	10.10	134.18	120.54
1	I	69	LEU	O-C-N	9.98	133.16	121.39
3	O	156	LYS	N-CA-C	9.96	129.63	113.89
3	G	156	LYS	N-CA-C	9.96	129.63	113.89
3	G	19	ARG	N-CA-C	9.94	123.14	111.71
2	N	81	ARG	N-CA-C	9.90	123.71	108.96
3	O	19	ARG	N-CA-C	9.88	123.07	111.71
4	P	68	LEU	CA-C-N	9.64	130.24	119.93
4	P	68	LEU	C-N-CA	9.64	130.24	119.93
4	H	68	LEU	CA-C-N	9.58	130.18	119.93
4	H	68	LEU	C-N-CA	9.58	130.18	119.93
3	G	204	ARG	N-CA-C	9.45	122.78	111.82
3	G	178	PHE	N-CA-C	-9.42	99.94	111.33
2	L	80	ALA	O-C-N	-9.41	112.76	123.40
3	O	30	LYS	CA-C-N	9.36	139.41	121.54
3	O	30	LYS	C-N-CA	9.36	139.41	121.54
3	G	30	LYS	CA-C-N	9.35	139.39	121.54
3	G	30	LYS	C-N-CA	9.35	139.39	121.54
3	O	204	ARG	N-CA-C	9.27	122.58	111.82
3	O	178	PHE	N-CA-C	-9.26	100.12	111.33
1	K	244	TRP	N-CA-C	9.22	125.94	112.94
1	J	244	TRP	N-CA-C	9.21	125.93	112.94
3	G	49	ALA	CA-C-O	9.21	130.18	120.70
3	G	37	ALA	CA-C-N	9.19	132.39	120.44
3	G	37	ALA	C-N-CA	9.19	132.39	120.44
1	I	244	TRP	N-CA-C	9.18	125.88	112.94
3	O	11	LEU	N-CA-C	-9.11	101.59	112.89
3	G	11	LEU	N-CA-C	-9.11	101.60	112.89
1	C	70	PRO	N-CA-C	-9.10	100.45	113.47
3	O	14	ARG	N-CA-C	9.10	120.81	111.07
3	G	156	LYS	CA-C-N	-9.09	105.53	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	156	LYS	C-N-CA	-9.09	105.53	120.72
3	O	156	LYS	CA-C-N	-9.07	105.58	120.72
3	O	156	LYS	C-N-CA	-9.07	105.58	120.72
3	O	37	ALA	CA-C-N	9.05	132.21	120.44
3	O	37	ALA	C-N-CA	9.05	132.21	120.44
3	O	49	ALA	CA-C-O	9.03	130.00	120.70
3	O	181	GLN	N-CA-C	9.02	123.83	113.01
3	G	14	ARG	N-CA-C	9.01	120.71	111.07
3	G	181	GLN	N-CA-C	8.97	123.78	113.01
3	G	174	ALA	CA-C-N	-8.94	108.14	120.38
3	G	174	ALA	C-N-CA	-8.94	108.14	120.38
3	G	192	PHE	N-CA-C	8.93	123.49	112.23
3	O	31	LYS	O-C-N	8.91	134.45	122.59
3	G	31	LYS	O-C-N	8.86	134.37	122.59
2	L	80	ALA	CA-C-O	-8.85	109.30	120.27
3	O	192	PHE	N-CA-C	8.83	123.36	112.23
3	O	174	ALA	CA-C-N	-8.81	108.31	120.38
3	O	174	ALA	C-N-CA	-8.81	108.31	120.38
3	O	155	LYS	CA-C-N	-8.79	108.28	121.99
3	O	155	LYS	C-N-CA	-8.79	108.28	121.99
4	H	75	ALA	N-CA-C	8.79	129.51	110.80
3	G	155	LYS	CA-C-N	-8.72	108.39	121.99
3	G	155	LYS	C-N-CA	-8.72	108.39	121.99
4	P	64	ARG	N-CA-C	-8.70	94.14	108.49
4	P	35	THR	CB-CA-C	-8.63	96.99	110.81
4	H	35	THR	CB-CA-C	-8.63	97.01	110.81
1	C	244	TRP	N-CA-C	8.42	126.24	113.61
1	B	244	TRP	N-CA-C	8.38	126.18	113.61
2	L	289	THR	O-C-N	-8.38	111.11	122.33
1	C	198	LYS	O-C-N	-8.35	112.53	122.46
2	D	289	THR	O-C-N	-8.32	111.17	122.33
2	E	289	THR	O-C-N	-8.29	111.23	122.33
2	N	289	THR	O-C-N	-8.27	111.25	122.33
2	M	289	THR	O-C-N	-8.26	111.26	122.33
2	D	359	SER	N-CA-C	-8.26	94.19	108.56
1	K	430	LEU	N-CA-C	-8.24	102.78	112.92
2	F	289	THR	O-C-N	-8.18	111.37	122.33
3	O	170	PRO	N-CA-CB	8.17	111.79	102.88
3	G	170	PRO	N-CA-CB	8.13	111.75	102.88
2	D	284	PRO	N-CA-CB	8.13	110.41	103.25
2	L	284	PRO	N-CA-CB	8.12	110.39	103.25
2	N	284	PRO	N-CA-CB	8.11	110.39	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	158	THR	N-CA-C	8.06	122.39	112.23
3	G	12	LEU	O-C-N	8.05	130.40	122.03
2	E	284	PRO	N-CA-CB	8.04	110.32	103.25
3	O	13	GLN	CA-C-N	7.99	130.83	120.44
3	O	13	GLN	C-N-CA	7.99	130.83	120.44
2	M	284	PRO	N-CA-CB	7.97	110.26	103.25
2	F	284	PRO	N-CA-CB	7.97	110.26	103.25
2	L	81	ARG	CA-C-N	-7.94	112.04	123.00
2	L	81	ARG	C-N-CA	-7.94	112.04	123.00
1	J	70	PRO	N-CA-C	-7.92	96.16	112.47
3	G	13	GLN	CA-C-N	7.91	130.72	120.44
3	G	13	GLN	C-N-CA	7.91	130.72	120.44
3	O	12	LEU	O-C-N	7.89	130.24	122.03
3	O	158	THR	N-CA-C	7.88	122.66	112.89
3	O	182	VAL	O-C-N	7.88	133.85	122.04
1	I	351	PRO	N-CA-CB	7.82	107.57	103.19
1	K	351	PRO	N-CA-CB	7.82	107.57	103.19
3	G	163	ALA	CA-C-N	7.78	131.49	120.28
3	G	163	ALA	C-N-CA	7.78	131.49	120.28
3	O	160	ARG	N-CA-C	-7.77	102.89	112.38
1	C	12	PRO	N-CA-CB	7.76	111.39	103.25
1	A	351	PRO	N-CA-CB	7.75	107.53	103.19
3	O	140	VAL	N-CA-C	7.75	125.45	109.34
3	O	163	ALA	CA-C-N	7.74	131.42	120.28
3	O	163	ALA	C-N-CA	7.74	131.42	120.28
3	G	47	MET	CA-C-O	7.74	131.57	120.51
3	G	160	ARG	N-CA-C	-7.74	102.94	112.38
3	G	140	VAL	N-CA-C	7.71	125.37	109.34
3	G	182	VAL	O-C-N	7.71	133.60	122.04
3	G	165	GLU	CA-C-N	-7.70	109.84	120.38
3	G	165	GLU	C-N-CA	-7.70	109.84	120.38
2	F	17	PRO	N-CA-CB	7.69	110.51	103.20
1	K	12	PRO	N-CA-CB	7.67	111.31	103.25
2	E	17	PRO	N-CA-CB	7.66	110.48	103.20
2	D	17	PRO	N-CA-CB	7.65	110.47	103.20
3	O	165	GLU	CA-C-N	-7.64	109.92	120.38
3	O	165	GLU	C-N-CA	-7.64	109.92	120.38
1	C	351	PRO	N-CA-CB	7.62	107.45	103.19
3	O	47	MET	CA-C-O	7.61	131.40	120.51
1	B	12	PRO	N-CA-CB	7.61	111.24	103.25
3	G	154	ILE	N-CA-C	-7.61	93.52	109.34
1	A	12	PRO	N-CA-CB	7.60	111.23	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	12	PRO	N-CA-CB	7.59	111.22	103.25
1	I	12	PRO	N-CA-CB	7.57	111.20	103.25
2	L	17	PRO	N-CA-CB	7.56	110.38	103.20
1	B	351	PRO	N-CA-CB	7.56	107.42	103.19
3	O	154	ILE	N-CA-C	-7.55	93.63	109.34
2	N	17	PRO	N-CA-CB	7.53	110.36	103.20
2	M	17	PRO	N-CA-CB	7.52	110.34	103.20
3	G	188	ARG	N-CA-CB	7.50	121.14	110.12
1	J	351	PRO	N-CA-CB	7.50	107.39	103.19
3	G	166	GLN	CA-C-N	-7.48	111.13	120.56
3	G	166	GLN	C-N-CA	-7.48	111.13	120.56
3	O	196	ARG	N-CA-CB	-7.47	99.06	110.20
3	G	196	ARG	N-CA-CB	-7.46	99.09	110.20
3	G	202	GLU	CA-C-O	7.45	128.42	119.78
3	O	21	ALA	O-C-N	7.43	132.48	122.59
4	P	76	GLY	O-C-N	-7.42	115.42	123.29
3	O	32	ARG	CA-C-O	-7.41	112.70	120.55
3	O	149	LYS	N-CA-C	-7.41	95.03	110.80
3	O	166	GLN	CA-C-N	-7.41	111.23	120.56
3	O	166	GLN	C-N-CA	-7.41	111.23	120.56
1	K	353	TYR	N-CA-C	7.36	121.84	113.01
3	G	149	LYS	N-CA-C	-7.36	95.13	110.80
3	G	21	ALA	O-C-N	7.36	132.37	122.59
3	O	188	ARG	N-CA-CB	7.35	120.92	110.12
3	G	193	ARG	N-CA-C	-7.30	103.31	111.71
3	G	151	GLY	N-CA-C	-7.29	95.90	113.18
1	I	353	TYR	N-CA-C	7.29	121.75	113.01
3	G	32	ARG	CA-C-O	-7.27	112.85	120.55
1	J	353	TYR	N-CA-C	7.25	121.71	113.01
3	O	151	GLY	N-CA-C	-7.25	96.00	113.18
3	O	202	GLU	CA-C-O	7.25	128.19	119.78
3	G	5	SER	O-C-N	7.22	129.62	121.32
3	O	136	ALA	N-CA-C	-7.21	95.45	110.80
3	O	51	LYS	CA-C-N	7.18	130.23	120.54
3	O	51	LYS	C-N-CA	7.18	130.23	120.54
3	O	5	SER	O-C-N	7.17	129.56	121.32
3	O	51	LYS	N-CA-C	-7.11	103.53	111.71
3	G	51	LYS	CA-C-N	7.10	130.12	120.54
3	G	51	LYS	C-N-CA	7.10	130.12	120.54
3	G	51	LYS	N-CA-C	-7.09	103.56	111.71
3	G	136	ALA	N-CA-C	-7.07	95.74	110.80
3	G	137	LEU	CA-C-N	-7.07	109.95	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	137	LEU	C-N-CA	-7.07	109.95	121.19
3	O	137	LEU	CA-C-N	-7.05	109.98	121.19
3	O	137	LEU	C-N-CA	-7.05	109.98	121.19
1	A	69	LEU	N-CA-C	7.03	122.33	107.91
3	G	31	LYS	CA-C-N	6.99	129.65	120.28
3	G	31	LYS	C-N-CA	6.99	129.65	120.28
1	K	354	LEU	N-CA-C	6.98	120.89	112.38
4	P	77	LEU	CA-C-O	-6.97	108.95	120.80
3	O	193	ARG	N-CA-C	-6.97	103.70	111.71
3	G	15	ARG	N-CA-C	-6.95	103.32	111.03
1	J	354	LEU	N-CA-C	6.95	120.86	112.38
3	G	195	LYS	CA-C-O	6.94	127.94	120.10
3	O	195	LYS	CA-C-O	6.93	127.93	120.10
1	I	354	LEU	N-CA-C	6.93	120.83	112.38
1	J	557	GLU	O-C-N	-6.90	113.42	122.39
3	O	31	LYS	CA-C-N	6.89	129.52	120.28
3	O	31	LYS	C-N-CA	6.89	129.52	120.28
3	G	196	ARG	CB-CA-C	6.86	123.26	110.70
1	C	557	GLU	O-C-N	-6.85	113.49	122.39
1	B	557	GLU	O-C-N	-6.83	113.51	122.39
4	P	40	GLY	N-CA-C	6.83	120.88	113.58
3	O	15	ARG	N-CA-C	-6.82	103.46	111.03
4	H	40	GLY	O-C-N	6.81	128.16	122.71
3	O	196	ARG	CB-CA-C	6.80	123.14	110.70
2	L	80	ALA	N-CA-C	6.80	118.58	107.23
4	H	81	PHE	N-CA-C	-6.79	104.63	113.12
1	K	557	GLU	O-C-N	-6.79	113.57	122.39
2	F	81	ARG	N-CA-C	6.78	119.47	109.24
4	H	40	GLY	N-CA-C	6.78	120.83	113.58
1	I	557	GLU	O-C-N	-6.77	113.58	122.39
1	A	557	GLU	O-C-N	-6.77	113.59	122.39
3	O	187	GLU	CA-C-O	-6.75	111.98	119.34
4	P	40	GLY	O-C-N	6.72	128.09	122.71
3	G	32	ARG	CA-C-N	6.67	129.52	120.44
3	G	32	ARG	C-N-CA	6.67	129.52	120.44
3	O	179	ILE	CA-C-N	-6.67	111.24	120.38
3	O	179	ILE	C-N-CA	-6.67	111.24	120.38
4	P	81	PHE	N-CA-C	-6.66	104.80	113.12
3	G	199	GLY	N-CA-C	-6.64	97.45	113.18
3	O	199	GLY	N-CA-C	-6.62	97.48	113.18
4	P	65	GLY	CA-C-N	6.59	133.56	121.70
4	P	65	GLY	C-N-CA	6.59	133.56	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	70	PRO	CA-C-N	6.57	134.10	121.54
1	I	70	PRO	C-N-CA	6.57	134.10	121.54
2	M	66	LEU	N-CA-CB	-6.57	107.53	114.10
3	G	179	ILE	CA-C-N	-6.55	111.41	120.38
3	G	179	ILE	C-N-CA	-6.55	111.41	120.38
2	N	66	LEU	N-CA-CB	-6.55	107.55	114.10
2	D	66	LEU	N-CA-CB	-6.54	107.56	114.10
3	O	32	ARG	CA-C-N	6.54	129.33	120.44
3	O	32	ARG	C-N-CA	6.54	129.33	120.44
2	L	66	LEU	N-CA-CB	-6.53	107.57	114.10
4	P	77	LEU	O-C-N	-6.53	112.55	123.00
2	E	66	LEU	N-CA-CB	-6.51	107.59	114.10
2	F	66	LEU	N-CA-CB	-6.51	107.59	114.10
1	A	142	GLY	CA-C-N	6.46	133.34	121.70
1	A	142	GLY	C-N-CA	6.46	133.34	121.70
3	O	161	VAL	O-C-N	6.45	130.64	122.57
3	G	161	VAL	O-C-N	6.42	130.59	122.57
2	E	79	VAL	O-C-N	-6.39	114.58	122.57
4	P	95	ARG	N-CA-C	-6.37	104.25	111.07
4	H	95	ARG	N-CA-C	-6.36	104.26	111.07
1	B	39	ILE	CB-CA-C	-6.35	104.43	111.35
3	G	182	VAL	CB-CA-C	-6.34	102.71	111.65
3	G	145	THR	N-CA-C	6.34	118.19	111.28
4	P	34	GLU	CA-C-O	-6.33	114.17	120.82
1	K	142	GLY	CA-C-N	6.32	133.08	121.70
1	K	142	GLY	C-N-CA	6.32	133.08	121.70
3	G	10	ASN	CA-C-N	-6.32	110.08	121.14
3	G	10	ASN	C-N-CA	-6.32	110.08	121.14
1	K	39	ILE	CB-CA-C	-6.32	104.46	111.35
2	N	360	ARG	N-CA-C	6.32	117.96	111.14
1	C	142	GLY	CA-C-N	6.31	133.06	121.70
1	C	142	GLY	C-N-CA	6.31	133.06	121.70
1	C	226	ILE	N-CA-CB	6.31	119.80	111.40
1	I	142	GLY	CA-C-N	6.31	133.06	121.70
1	I	142	GLY	C-N-CA	6.31	133.06	121.70
1	J	226	ILE	N-CA-CB	6.30	119.78	111.40
1	A	39	ILE	CB-CA-C	-6.29	104.50	111.35
1	J	142	GLY	CA-C-N	6.29	133.02	121.70
1	J	142	GLY	C-N-CA	6.29	133.02	121.70
1	B	142	GLY	CA-C-N	6.28	133.01	121.70
1	B	142	GLY	C-N-CA	6.28	133.01	121.70
3	O	10	ASN	CA-C-N	-6.28	110.15	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	10	ASN	C-N-CA	-6.28	110.15	121.14
3	O	145	THR	N-CA-C	6.28	118.13	111.28
4	H	34	GLU	CA-C-O	-6.27	114.24	120.82
3	O	167	VAL	CB-CA-C	6.26	119.99	111.97
1	I	39	ILE	CB-CA-C	-6.25	104.53	111.35
3	G	169	ILE	N-CA-C	6.24	122.36	108.88
3	O	182	VAL	CB-CA-C	-6.24	102.85	111.65
1	I	226	ILE	N-CA-CB	6.24	119.69	111.40
1	J	39	ILE	CB-CA-C	-6.23	104.56	111.35
1	C	229	PRO	N-CA-CB	6.22	110.97	103.45
4	P	75	ALA	CA-C-N	6.21	133.54	121.93
4	P	75	ALA	C-N-CA	6.21	133.54	121.93
1	I	143	PHE	N-CA-C	6.21	128.38	111.00
3	G	167	VAL	CB-CA-C	6.20	119.90	111.97
1	C	39	ILE	CB-CA-C	-6.19	104.61	111.35
4	H	77	LEU	CA-C-O	-6.18	110.30	120.80
1	A	226	ILE	N-CA-CB	6.17	119.61	111.40
1	K	226	ILE	N-CA-CB	6.17	119.60	111.40
3	O	169	ILE	N-CA-C	6.17	122.20	108.88
1	I	229	PRO	N-CA-CB	6.16	110.91	103.45
3	G	138	ILE	N-CA-C	6.16	121.01	113.00
3	G	172	ILE	O-C-N	6.16	130.26	122.57
1	C	143	PHE	N-CA-C	6.15	128.22	111.00
1	K	143	PHE	N-CA-C	6.15	128.22	111.00
1	J	143	PHE	N-CA-C	6.15	128.22	111.00
3	O	138	ILE	N-CA-C	6.15	121.00	113.00
1	B	143	PHE	N-CA-C	6.14	128.20	111.00
3	O	172	ILE	O-C-N	6.14	130.24	122.57
3	O	203	ALA	CA-C-N	6.12	129.62	120.31
3	O	203	ALA	C-N-CA	6.12	129.62	120.31
1	B	226	ILE	N-CA-CB	6.12	119.54	111.40
1	C	354	LEU	N-CA-C	6.11	117.94	111.28
1	B	354	LEU	N-CA-C	6.11	117.94	111.28
1	B	229	PRO	N-CA-CB	6.10	110.83	103.45
1	C	559	PHE	CA-C-N	6.10	125.78	119.56
1	C	559	PHE	C-N-CA	6.10	125.78	119.56
1	J	229	PRO	N-CA-CB	6.09	110.82	103.45
1	K	210	ARG	CA-C-O	-6.07	114.45	120.82
3	O	137	LEU	O-C-N	-6.07	114.52	122.59
1	I	559	PHE	CA-C-N	6.06	125.75	119.56
1	I	559	PHE	C-N-CA	6.06	125.75	119.56
3	G	164	LEU	CA-C-O	6.06	126.95	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	229	PRO	N-CA-CB	6.06	110.78	103.45
1	B	559	PHE	CA-C-N	6.06	125.74	119.56
1	B	559	PHE	C-N-CA	6.06	125.74	119.56
1	A	143	PHE	N-CA-C	6.05	127.94	111.00
1	A	210	ARG	CA-C-O	-6.04	114.47	120.82
1	K	559	PHE	CA-C-N	6.04	125.72	119.56
1	K	559	PHE	C-N-CA	6.04	125.72	119.56
3	O	29	LYS	N-CA-C	-6.03	104.39	110.97
3	O	164	LEU	CA-C-O	6.01	126.90	120.10
1	I	350	TYR	CA-C-N	6.00	124.04	119.66
1	I	350	TYR	C-N-CA	6.00	124.04	119.66
3	G	187	GLU	CA-C-O	-5.99	112.27	119.03
2	F	94	ASN	CA-C-N	5.98	127.67	120.13
2	F	94	ASN	C-N-CA	5.98	127.67	120.13
1	A	559	PHE	CA-C-N	5.96	125.64	119.56
1	A	559	PHE	C-N-CA	5.96	125.64	119.56
3	O	47	MET	N-CA-CB	-5.96	100.41	110.49
3	G	47	MET	N-CA-CB	-5.96	100.42	110.49
3	G	203	ALA	CA-C-N	5.94	129.34	120.31
3	G	203	ALA	C-N-CA	5.94	129.34	120.31
1	B	210	ARG	CA-C-O	-5.93	114.60	120.82
3	O	47	MET	O-C-N	-5.92	114.71	122.59
1	J	559	PHE	CA-C-N	5.92	125.60	119.56
1	J	559	PHE	C-N-CA	5.92	125.60	119.56
1	A	229	PRO	N-CA-CB	5.92	110.61	103.45
1	J	210	ARG	CA-C-O	-5.92	114.61	120.82
3	G	27	LEU	N-CA-C	5.91	119.75	112.54
2	E	94	ASN	CA-C-N	5.91	127.58	120.13
2	E	94	ASN	C-N-CA	5.91	127.58	120.13
3	G	29	LYS	N-CA-C	-5.91	104.53	110.97
3	O	193	ARG	O-C-N	5.90	129.13	122.22
3	O	201	ILE	CA-C-O	5.90	127.10	120.85
3	G	201	ILE	CA-C-O	5.89	127.09	120.85
2	N	94	ASN	CA-C-N	5.88	127.54	120.13
2	N	94	ASN	C-N-CA	5.88	127.54	120.13
3	O	27	LEU	N-CA-C	5.88	119.71	112.54
3	G	47	MET	O-C-N	-5.88	114.77	122.59
3	G	137	LEU	O-C-N	-5.87	114.78	122.59
1	I	210	ARG	CA-C-O	-5.87	114.66	120.82
1	C	210	ARG	CA-C-O	-5.86	114.66	120.82
3	G	193	ARG	O-C-N	5.86	129.08	122.22
2	M	94	ASN	CA-C-N	5.83	127.47	120.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	94	ASN	C-N-CA	5.83	127.47	120.13
3	G	7	THR	N-CA-C	5.83	119.57	112.23
2	D	94	ASN	CA-C-N	5.81	127.45	120.13
2	D	94	ASN	C-N-CA	5.81	127.45	120.13
4	H	77	LEU	O-C-N	-5.80	113.71	123.00
1	B	41	ARG	CA-C-O	-5.80	114.15	120.36
1	B	168	VAL	N-CA-CB	-5.80	104.07	110.51
2	L	94	ASN	CA-C-N	5.79	127.43	120.13
2	L	94	ASN	C-N-CA	5.79	127.43	120.13
3	O	143	THR	CA-C-O	5.79	127.57	120.56
1	K	168	VAL	N-CA-CB	-5.79	104.08	110.51
3	O	7	THR	N-CA-C	5.78	119.51	112.23
3	G	143	THR	CA-C-O	5.77	127.54	120.56
1	I	168	VAL	N-CA-CB	-5.77	104.11	110.51
1	A	143	PHE	CA-C-O	5.76	130.59	120.80
2	F	80	ALA	N-CA-C	-5.75	102.94	110.53
4	H	76	GLY	O-C-N	-5.74	116.91	123.23
1	I	41	ARG	CA-C-O	-5.74	114.22	120.36
3	O	196	ARG	N-CA-C	5.74	118.75	111.69
1	C	143	PHE	CA-C-O	5.73	130.54	120.80
3	O	201	ILE	N-CA-C	5.71	116.49	110.72
4	H	76	GLY	N-CA-C	5.69	117.73	110.96
1	K	143	PHE	CA-C-O	5.69	130.47	120.80
1	C	41	ARG	CA-C-O	-5.69	114.27	120.36
2	N	289	THR	CA-C-N	5.69	127.83	120.44
2	N	289	THR	C-N-CA	5.69	127.83	120.44
2	D	289	THR	CA-C-N	5.68	127.83	120.44
2	D	289	THR	C-N-CA	5.68	127.83	120.44
2	L	289	THR	CA-C-N	5.68	127.83	120.44
2	L	289	THR	C-N-CA	5.68	127.83	120.44
3	G	7	THR	O-C-N	-5.67	114.73	122.33
3	G	165	GLU	N-CA-C	5.67	122.88	110.80
3	O	7	THR	O-C-N	-5.67	114.73	122.33
1	J	143	PHE	CA-C-O	5.67	130.43	120.80
1	B	143	PHE	CA-C-O	5.67	130.43	120.80
3	G	140	VAL	CA-C-N	5.66	131.89	122.54
3	G	140	VAL	C-N-CA	5.66	131.89	122.54
1	I	71	LEU	CA-C-N	5.66	131.89	121.70
1	I	71	LEU	C-N-CA	5.66	131.89	121.70
3	O	165	GLU	N-CA-C	5.66	122.85	110.80
3	G	159	ARG	O-C-N	5.65	128.66	122.11
1	A	41	ARG	CA-C-O	-5.64	114.32	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	201	ILE	N-CA-C	5.64	116.42	110.72
1	C	168	VAL	N-CA-CB	-5.64	104.25	110.51
2	F	289	THR	CA-C-N	5.64	127.77	120.44
2	F	289	THR	C-N-CA	5.64	127.77	120.44
3	O	140	VAL	CA-C-N	5.63	131.83	122.54
3	O	140	VAL	C-N-CA	5.63	131.83	122.54
1	A	350	TYR	CA-C-N	5.63	123.77	119.66
1	A	350	TYR	C-N-CA	5.63	123.77	119.66
1	A	168	VAL	N-CA-CB	-5.62	104.27	110.51
1	C	350	TYR	CA-C-N	5.62	123.77	119.66
1	C	350	TYR	C-N-CA	5.62	123.77	119.66
1	I	143	PHE	CA-C-O	5.62	130.36	120.80
1	J	168	VAL	N-CA-CB	-5.62	104.27	110.51
1	K	350	TYR	CA-C-N	5.62	123.76	119.66
1	K	350	TYR	C-N-CA	5.62	123.76	119.66
1	A	68	GLY	CA-C-N	-5.62	115.03	122.56
1	A	68	GLY	C-N-CA	-5.62	115.03	122.56
2	M	289	THR	CA-C-N	5.61	127.73	120.44
2	M	289	THR	C-N-CA	5.61	127.73	120.44
1	K	41	ARG	CA-C-O	-5.61	114.36	120.36
1	J	41	ARG	CA-C-O	-5.60	114.36	120.36
3	G	46	ALA	N-CA-C	-5.60	98.86	110.80
3	G	163	ALA	CA-C-O	-5.58	113.55	119.97
3	O	163	ALA	CA-C-O	-5.58	113.56	119.97
2	E	289	THR	CA-C-N	5.57	127.69	120.44
2	E	289	THR	C-N-CA	5.57	127.69	120.44
3	O	159	ARG	O-C-N	5.57	128.57	122.11
3	G	182	VAL	CA-C-N	5.57	132.18	121.54
3	G	182	VAL	C-N-CA	5.57	132.18	121.54
4	P	38	GLU	N-CA-C	-5.56	105.37	111.82
3	G	157	THR	N-CA-CB	5.56	119.62	110.39
3	G	196	ARG	N-CA-C	5.56	118.52	111.69
3	O	182	VAL	CA-C-N	5.54	132.12	121.54
3	O	182	VAL	C-N-CA	5.54	132.12	121.54
3	G	132	ARG	CA-C-N	-5.54	111.74	120.60
3	G	132	ARG	C-N-CA	-5.54	111.74	120.60
1	I	222	GLY	CA-C-N	-5.54	115.30	123.05
1	I	222	GLY	C-N-CA	-5.54	115.30	123.05
3	O	171	GLY	N-CA-C	-5.53	100.06	113.18
3	O	202	GLU	O-C-N	5.53	129.83	122.26
3	G	15	ARG	CA-C-O	-5.53	115.21	120.90
1	A	222	GLY	CA-C-N	-5.52	115.32	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	GLY	C-N-CA	-5.52	115.32	123.05
1	J	350	TYR	CA-C-N	5.52	123.69	119.66
1	J	350	TYR	C-N-CA	5.52	123.69	119.66
3	G	31	LYS	N-CA-C	5.52	122.55	110.80
3	O	31	LYS	N-CA-C	5.51	122.54	110.80
4	H	38	GLU	N-CA-C	-5.50	105.44	111.82
3	O	46	ALA	N-CA-C	-5.50	99.08	110.80
3	O	157	THR	N-CA-CB	5.50	119.51	110.39
3	G	23	LYS	N-CA-C	-5.49	105.45	111.82
3	O	15	ARG	CA-C-O	-5.49	115.25	120.90
1	B	222	GLY	CA-C-N	-5.47	115.39	123.05
1	B	222	GLY	C-N-CA	-5.47	115.39	123.05
1	C	222	GLY	CA-C-N	-5.47	115.39	123.05
1	C	222	GLY	C-N-CA	-5.47	115.39	123.05
4	H	75	ALA	CA-C-N	5.46	130.08	121.62
4	H	75	ALA	C-N-CA	5.46	130.08	121.62
1	K	222	GLY	CA-C-N	-5.45	115.42	123.05
1	K	222	GLY	C-N-CA	-5.45	115.42	123.05
3	G	171	GLY	N-CA-C	-5.45	100.27	113.18
2	L	79	VAL	O-C-N	-5.45	115.76	122.57
1	B	350	TYR	CA-C-N	5.45	123.64	119.66
1	B	350	TYR	C-N-CA	5.45	123.64	119.66
3	G	202	GLU	O-C-N	5.42	129.69	122.26
3	O	23	LYS	N-CA-C	-5.42	105.53	111.82
1	J	222	GLY	CA-C-N	-5.41	115.47	123.05
1	J	222	GLY	C-N-CA	-5.41	115.47	123.05
2	D	356	PRO	N-CA-CB	5.40	108.92	103.25
3	G	178	PHE	O-C-N	5.40	127.84	122.12
3	G	172	ILE	CB-CA-C	-5.39	102.45	111.29
3	O	30	LYS	O-C-N	5.39	127.83	122.12
3	O	132	ARG	CA-C-N	-5.39	111.97	120.60
3	O	132	ARG	C-N-CA	-5.39	111.97	120.60
3	G	165	GLU	CA-C-O	5.38	128.20	120.51
1	B	67	THR	N-CA-CB	5.36	118.11	110.67
1	J	199	LEU	N-CA-C	5.35	117.77	110.55
1	J	294	MET	CA-C-N	5.34	125.28	119.78
1	J	294	MET	C-N-CA	5.34	125.28	119.78
1	C	294	MET	CA-C-N	5.33	125.28	119.78
1	C	294	MET	C-N-CA	5.33	125.28	119.78
4	P	76	GLY	N-CA-C	5.33	120.86	110.73
3	O	172	ILE	CB-CA-C	-5.33	102.55	111.29
1	B	294	MET	CA-C-N	5.32	125.26	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	294	MET	C-N-CA	5.32	125.26	119.78
1	K	294	MET	CA-C-N	5.32	125.26	119.78
1	K	294	MET	C-N-CA	5.32	125.26	119.78
2	L	419	GLU	CA-C-O	5.30	126.04	120.42
1	C	67	THR	N-CA-CB	5.30	118.04	110.67
3	O	178	PHE	O-C-N	5.29	127.73	122.12
3	G	30	LYS	O-C-N	5.28	127.71	122.12
3	O	165	GLU	CA-C-O	5.27	128.05	120.51
2	L	356	PRO	N-CA-CB	5.27	108.78	103.25
1	A	294	MET	CA-C-N	5.27	125.21	119.78
1	A	294	MET	C-N-CA	5.27	125.21	119.78
1	I	67	THR	N-CA-CB	5.26	117.99	110.67
2	D	81	ARG	CA-C-O	-5.26	115.68	121.31
3	G	43	VAL	CA-C-N	-5.26	112.17	120.63
3	G	43	VAL	C-N-CA	-5.26	112.17	120.63
2	M	356	PRO	N-CA-CB	5.26	108.77	103.25
3	G	194	LEU	CA-C-O	-5.25	114.93	120.55
3	G	31	LYS	CB-CA-C	-5.25	99.98	110.42
2	M	419	GLU	CA-C-O	5.25	125.98	120.42
2	E	356	PRO	N-CA-CB	5.24	108.75	103.25
1	B	429	SER	O-C-N	-5.23	116.58	123.28
1	K	67	THR	N-CA-CB	5.23	117.94	110.67
3	O	203	ALA	CA-C-O	-5.22	113.78	120.31
2	F	419	GLU	CA-C-O	5.22	125.95	120.42
1	I	294	MET	CA-C-N	5.22	125.16	119.78
1	I	294	MET	C-N-CA	5.22	125.16	119.78
3	G	144	GLU	CA-C-N	5.21	127.27	120.28
3	G	144	GLU	C-N-CA	5.21	127.27	120.28
3	O	194	LEU	CA-C-O	-5.21	114.97	120.55
3	O	31	LYS	CB-CA-C	-5.21	100.05	110.42
3	O	136	ALA	O-C-N	5.21	129.52	122.59
1	K	347	GLU	CA-C-O	-5.20	115.29	120.96
1	J	67	THR	N-CA-CB	5.20	117.90	110.67
2	N	356	PRO	N-CA-CB	5.19	108.70	103.25
3	O	156	LYS	O-C-N	-5.19	116.57	122.23
3	G	203	ALA	CA-C-O	-5.18	113.83	120.31
3	O	170	PRO	CA-C-O	5.18	125.29	118.98
1	A	347	GLU	CA-C-O	-5.17	115.32	120.96
3	O	25	VAL	CA-C-O	5.17	125.83	120.25
1	A	67	THR	N-CA-CB	5.17	117.85	110.67
3	O	189	GLU	CB-CA-C	5.17	119.47	110.79
3	O	174	ALA	N-CA-C	5.16	121.80	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	13	ALA	CA-C-N	-5.16	116.43	122.93
1	C	13	ALA	C-N-CA	-5.16	116.43	122.93
2	E	419	GLU	CA-C-O	5.16	125.89	120.42
4	H	69	PRO	CA-C-O	-5.16	115.70	121.32
3	G	54	ASP	CA-C-N	-5.15	112.43	121.70
3	G	54	ASP	C-N-CA	-5.15	112.43	121.70
3	G	136	ALA	O-C-N	5.15	129.44	122.59
3	G	189	GLU	CB-CA-C	5.15	119.45	110.79
3	G	174	ALA	N-CA-C	5.15	121.77	110.80
2	D	419	GLU	CA-C-O	5.12	125.85	120.42
2	M	79	VAL	O-C-N	-5.12	116.16	122.57
3	O	54	ASP	CA-C-N	-5.12	112.48	121.70
3	O	54	ASP	C-N-CA	-5.12	112.48	121.70
3	O	49	ALA	CB-CA-C	-5.12	102.81	110.90
3	G	26	ASP	O-C-N	5.11	127.55	122.08
2	F	356	PRO	N-CA-CB	5.11	108.61	103.25
3	G	156	LYS	O-C-N	-5.11	116.66	122.23
1	C	347	GLU	CA-C-O	-5.10	115.40	120.96
3	O	144	GLU	CA-C-N	5.09	127.10	120.28
3	O	144	GLU	C-N-CA	5.09	127.10	120.28
3	G	49	ALA	CB-CA-C	-5.09	102.86	110.90
1	J	347	GLU	CA-C-O	-5.08	115.42	120.96
3	O	23	LYS	CA-C-N	5.08	125.73	119.99
3	O	23	LYS	C-N-CA	5.08	125.73	119.99
3	O	43	VAL	CA-C-N	-5.07	112.46	120.63
3	O	43	VAL	C-N-CA	-5.07	112.46	120.63
3	G	170	PRO	CA-C-O	5.07	125.16	118.98
3	G	4	VAL	N-CA-C	5.06	119.87	109.34
3	O	26	ASP	O-C-N	5.06	127.50	122.08
3	O	185	GLN	N-CA-C	-5.05	100.03	110.80
4	P	14	ARG	N-CA-C	5.05	116.78	111.28
3	O	47	MET	CB-CA-C	-5.04	100.38	110.42
3	G	47	MET	CB-CA-C	-5.04	100.39	110.42
1	I	13	ALA	CA-C-N	-5.04	116.58	122.93
1	I	13	ALA	C-N-CA	-5.04	116.58	122.93
3	O	4	VAL	N-CA-C	5.04	119.82	109.34
2	N	419	GLU	CA-C-O	5.04	125.76	120.42
3	G	204	ARG	O-C-N	5.03	128.46	122.27
1	B	13	ALA	CA-C-N	-5.01	116.62	122.93
1	B	13	ALA	C-N-CA	-5.01	116.62	122.93
3	G	25	VAL	CA-C-O	5.01	125.66	120.25
1	K	245	SER	CA-C-N	-5.01	113.00	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	245	SER	C-N-CA	-5.01	113.00	122.27
3	G	23	LYS	CA-C-N	5.01	125.65	119.99
3	G	23	LYS	C-N-CA	5.01	125.65	119.99

There are no chirality outliers.

All (55) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	GLY	Peptide
1	A	210	ARG	Mainchain
1	A	297	ALA	Mainchain
1	A	325	ASP	Mainchain
1	A	557	GLU	Mainchain
1	B	178	GLY	Peptide
1	B	210	ARG	Mainchain
1	B	297	ALA	Mainchain
1	B	325	ASP	Mainchain
1	B	557	GLU	Mainchain
1	C	178	GLY	Peptide
1	C	198	LYS	Mainchain
1	C	210	ARG	Mainchain
1	C	297	ALA	Mainchain
1	C	325	ASP	Mainchain
1	C	557	GLU	Mainchain
2	D	316	MET	Mainchain
2	D	427	GLN	Peptide
2	D	79	VAL	Mainchain
2	E	316	MET	Mainchain
2	E	427	GLN	Peptide
2	E	79	VAL	Mainchain
2	F	316	MET	Mainchain
2	F	427	GLN	Peptide
4	H	39	ARG	Peptide
4	H	82	GLN	Peptide
1	I	178	GLY	Peptide
1	I	210	ARG	Mainchain
1	I	297	ALA	Mainchain
1	I	325	ASP	Mainchain
1	I	429	SER	Mainchain
1	I	557	GLU	Mainchain
1	J	178	GLY	Peptide
1	J	210	ARG	Mainchain

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Mol	Chain	Res	Type	Group
1	J	297	ALA	Mainchain
1	J	325	ASP	Mainchain
1	J	429	SER	Mainchain
1	J	557	GLU	Mainchain
1	K	178	GLY	Peptide
1	K	210	ARG	Mainchain
1	K	297	ALA	Mainchain
1	K	325	ASP	Mainchain
1	K	557	GLU	Mainchain
1	K	70	PRO	Mainchain
2	L	316	MET	Mainchain
2	L	427	GLN	Peptide
2	L	79	VAL	Mainchain
2	M	316	MET	Mainchain
2	M	427	GLN	Peptide
2	M	79	VAL	Mainchain
2	N	316	MET	Mainchain
2	N	427	GLN	Peptide
2	N	79	VAL	Mainchain
4	P	39	ARG	Peptide
4	P	82	GLN	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2752	0	1302	90	0
1	B	2752	0	1303	75	0
1	C	2752	0	1303	102	0
1	I	2752	0	1301	138	0
1	J	2752	0	1303	54	3
1	K	2752	0	1303	94	0
2	D	2212	0	1009	74	0
2	E	2212	0	1009	57	0
2	F	2212	0	1009	80	0
2	L	2212	0	1009	92	0
2	M	2212	0	1009	52	3
2	N	2212	0	1009	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	639	0	299	141	0
3	O	639	0	299	144	0
4	H	509	0	255	24	0
4	P	509	0	254	20	0
All	All	32080	0	14976	1049	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (1049) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:142:ASN:CB	3:O:142:ASN:CA	1.75	1.64
3:O:189:GLU:CB	3:O:189:GLU:CA	1.76	1.64
3:G:205:GLU:CB	3:G:205:GLU:CA	1.78	1.62
3:O:163:ALA:C	3:O:163:ALA:CA	1.74	1.59
1:K:52:TYR:CA	1:K:295:PRO:CB	1.79	1.59
3:G:163:ALA:C	3:G:163:ALA:CA	1.74	1.59
3:O:52:ALA:CB	3:O:52:ALA:CA	1.76	1.59
1:B:24:MET:CB	2:E:66:LEU:CA	1.74	1.58
3:G:189:GLU:CA	3:G:189:GLU:CB	1.76	1.57
3:O:205:GLU:CA	3:O:205:GLU:CB	1.78	1.57
1:B:471:VAL:CB	4:H:98:ILE:CB	1.79	1.57
1:I:43:ASP:C	2:L:69:ALA:CB	1.76	1.57
3:G:52:ALA:CB	3:G:52:ALA:CA	1.75	1.57
2:D:359:SER:CB	2:D:362:MET:CB	1.78	1.56
3:G:194:LEU:C	3:G:194:LEU:CA	1.75	1.56
3:O:4:VAL:C	3:O:4:VAL:CA	1.78	1.55
3:G:4:VAL:C	3:G:4:VAL:CA	1.78	1.54
3:O:194:LEU:C	3:O:194:LEU:CA	1.74	1.54
3:G:142:ASN:CB	3:G:142:ASN:CA	1.75	1.54
1:I:71:LEU:CB	1:I:188:PRO:HA	1.31	1.54
1:C:52:TYR:HA	1:C:295:PRO:CB	1.16	1.54
2:N:140:VAL:CB	2:N:435:SER:CB	1.76	1.54
3:G:7:THR:CB	3:G:7:THR:CA	1.86	1.54
3:O:31:LYS:N	3:O:31:LYS:CA	1.71	1.54
1:C:52:TYR:CA	1:C:295:PRO:CB	1.85	1.53
3:O:167:VAL:C	3:O:167:VAL:CA	1.81	1.53
1:A:71:LEU:CB	1:A:188:PRO:HA	1.35	1.52
3:G:167:VAL:C	3:G:167:VAL:CA	1.81	1.52
3:O:27:LEU:CB	3:O:27:LEU:CA	1.87	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:31:LYS:N	3:G:31:LYS:CA	1.70	1.51
3:O:7:THR:CA	3:O:7:THR:CB	1.86	1.51
3:G:27:LEU:CA	3:G:27:LEU:CB	1.87	1.50
3:O:196:ARG:CA	3:O:196:ARG:C	1.84	1.50
1:C:352:PRO:CB	2:F:269:GLU:HA	1.41	1.50
1:I:44:GLY:N	2:L:69:ALA:CB	1.70	1.48
1:I:25:TYR:N	2:L:66:LEU:H	1.12	1.47
3:G:196:ARG:C	3:G:196:ARG:CA	1.84	1.46
1:B:24:MET:CB	2:E:66:LEU:HA	0.97	1.44
1:I:43:ASP:C	2:L:69:ALA:HB2	1.33	1.42
4:H:65:GLY:HA3	4:H:66:ARG:CB	1.16	1.41
1:B:9:ILE:CB	2:D:50:VAL:O	1.66	1.40
2:L:359:SER:CB	2:L:362:MET:CB	1.97	1.39
1:C:25:TYR:CB	2:F:65:GLY:HA2	1.55	1.37
1:I:25:TYR:H	2:L:66:LEU:N	1.23	1.37
3:G:44:ARG:O	3:G:47:MET:CB	1.71	1.36
1:I:266:LEU:C	2:N:124:ARG:CB	1.99	1.35
1:A:11:GLY:HA3	2:F:50:VAL:O	1.17	1.34
1:C:419:PHE:O	1:C:496:GLN:CA	1.73	1.34
3:O:44:ARG:O	3:O:47:MET:CB	1.72	1.34
1:K:52:TYR:HA	1:K:295:PRO:CB	0.87	1.34
1:K:259:GLY:O	2:M:296:GLU:C	1.67	1.34
1:I:11:GLY:CA	2:N:50:VAL:H	1.42	1.33
1:J:9:ILE:CB	2:L:50:VAL:O	1.78	1.32
1:I:11:GLY:HA3	2:N:50:VAL:C	1.55	1.30
1:C:419:PHE:O	1:C:496:GLN:HA	1.25	1.30
1:C:52:TYR:CB	1:C:295:PRO:CB	2.10	1.29
1:K:419:PHE:O	1:K:496:GLN:CA	1.79	1.28
1:I:267:VAL:N	2:N:124:ARG:CB	1.98	1.27
1:K:44:GLY:HA2	2:N:69:ALA:CB	1.63	1.27
1:I:44:GLY:CA	2:L:69:ALA:CB	2.12	1.26
1:I:224:ALA:CB	1:I:405:ALA:HB3	1.65	1.25
1:C:224:ALA:CB	1:C:405:ALA:HB3	1.65	1.25
1:I:24:MET:HA	2:L:66:LEU:CA	1.65	1.25
1:J:224:ALA:CB	1:J:405:ALA:HB3	1.65	1.24
1:B:224:ALA:CB	1:B:405:ALA:HB3	1.65	1.24
1:K:69:LEU:CB	1:K:72:ALA:HB3	1.66	1.24
1:A:224:ALA:CB	1:A:405:ALA:HB3	1.65	1.24
4:H:65:GLY:CA	4:H:66:ARG:CB	2.04	1.24
1:K:224:ALA:CB	1:K:405:ALA:HB3	1.66	1.23
2:M:140:VAL:CB	2:M:435:SER:CB	2.16	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:419:PHE:O	1:K:497:GLN:N	1.70	1.22
4:H:84:HIS:O	4:H:86:VAL:N	1.72	1.22
1:I:71:LEU:CB	1:I:188:PRO:CA	2.18	1.22
2:F:426:GLY:O	1:K:125:PRO:C	1.80	1.22
1:C:419:PHE:O	1:C:496:GLN:CB	1.86	1.21
1:I:11:GLY:CA	2:N:50:VAL:N	2.03	1.20
1:I:44:GLY:CA	2:L:69:ALA:HB1	1.68	1.20
1:I:11:GLY:HA3	2:N:50:VAL:O	1.40	1.20
1:K:419:PHE:O	1:K:496:GLN:HA	1.12	1.19
1:I:11:GLY:HA3	2:N:50:VAL:CA	1.72	1.17
1:B:10:ALA:O	2:D:50:VAL:N	1.77	1.16
1:C:352:PRO:CB	2:F:269:GLU:CA	2.23	1.16
1:B:11:GLY:HA3	2:D:49:GLU:CB	1.75	1.15
1:B:263:THR:CB	2:D:125:ARG:N	2.10	1.15
1:I:266:LEU:CB	2:N:124:ARG:CB	2.25	1.14
1:A:71:LEU:CB	1:A:188:PRO:CA	2.25	1.14
1:I:43:ASP:C	2:L:69:ALA:HB3	1.66	1.14
1:B:10:ALA:H	2:D:50:VAL:CB	1.60	1.12
1:A:10:ALA:O	2:F:50:VAL:CB	1.98	1.12
1:I:44:GLY:N	2:L:69:ALA:HB1	1.43	1.11
1:C:25:TYR:H	2:F:66:LEU:N	1.48	1.11
1:K:44:GLY:HA2	2:N:69:ALA:HB3	1.25	1.11
1:A:44:GLY:HA2	2:D:69:ALA:CB	1.80	1.10
1:A:266:LEU:CB	2:F:124:ARG:CB	2.29	1.10
1:I:11:GLY:HA3	2:N:50:VAL:N	1.65	1.10
1:I:44:GLY:HA2	2:L:69:ALA:CB	1.78	1.10
1:C:189:VAL:CB	1:C:305:VAL:HA	1.81	1.10
1:B:263:THR:CB	2:D:124:ARG:C	2.25	1.10
1:C:25:TYR:N	2:F:66:LEU:H	1.49	1.09
1:I:43:ASP:O	2:L:69:ALA:HB3	1.49	1.09
1:I:24:MET:CA	2:L:66:LEU:HA	1.81	1.09
1:C:44:GLY:HA2	2:F:69:ALA:CB	1.83	1.08
2:M:359:SER:CB	2:M:362:MET:CB	2.31	1.08
1:A:69:LEU:CB	1:A:71:LEU:C	2.26	1.08
4:H:62:LEU:O	4:H:63:MET:O	1.69	1.08
1:B:25:TYR:O	2:E:65:GLY:HA2	1.53	1.07
4:P:75:ALA:HB2	4:P:85:ASP:O	1.54	1.07
1:A:44:GLY:HA2	2:D:69:ALA:HB3	1.32	1.07
2:D:149:LYS:O	2:D:334:GLU:N	1.87	1.07
2:F:149:LYS:O	2:F:334:GLU:N	1.87	1.06
3:O:176:ILE:O	3:O:179:ILE:CB	2.03	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:176:ILE:O	3:G:179:ILE:CB	2.03	1.06
2:N:149:LYS:O	2:N:334:GLU:N	1.87	1.06
2:L:149:LYS:O	2:L:334:GLU:N	1.87	1.06
2:E:149:LYS:O	2:E:334:GLU:N	1.87	1.06
1:I:11:GLY:CA	2:N:50:VAL:O	2.02	1.06
1:K:259:GLY:C	2:M:296:GLU:C	2.22	1.06
1:I:259:GLY:N	2:N:296:GLU:CA	2.06	1.05
2:M:149:LYS:O	2:M:334:GLU:N	1.87	1.05
1:A:11:GLY:CA	2:F:50:VAL:O	2.05	1.04
1:B:9:ILE:HA	2:D:50:VAL:CB	1.87	1.04
3:O:7:THR:O	3:O:8:ARG:C	1.98	1.04
1:A:352:PRO:CB	2:D:272:ALA:HB3	1.88	1.04
1:A:44:GLY:CA	2:D:69:ALA:CB	2.35	1.03
1:C:419:PHE:C	1:C:496:GLN:HA	1.83	1.03
1:I:44:GLY:CA	2:L:69:ALA:HB3	1.83	1.03
1:B:11:GLY:HA3	2:D:49:GLU:CA	1.88	1.03
3:O:27:LEU:CB	3:O:163:ALA:HB2	1.87	1.03
1:A:44:GLY:N	2:D:69:ALA:CB	2.22	1.03
1:I:11:GLY:HA2	2:N:50:VAL:N	1.66	1.02
1:C:224:ALA:HB1	1:C:405:ALA:HB3	1.41	1.02
3:G:7:THR:O	3:G:8:ARG:C	1.98	1.02
1:A:224:ALA:HB1	1:A:405:ALA:HB3	1.41	1.01
1:B:9:ILE:CB	2:D:50:VAL:C	2.32	1.01
1:I:224:ALA:HB1	1:I:405:ALA:HB3	1.41	1.01
3:G:199:GLY:C	3:G:203:ALA:HB2	1.86	1.01
4:H:76:GLY:O	4:H:80:ALA:HB3	1.59	1.01
1:I:71:LEU:CB	1:I:189:VAL:H	1.74	1.01
1:K:44:GLY:CA	2:N:69:ALA:CB	2.39	1.00
1:K:224:ALA:HB1	1:K:405:ALA:HB3	1.41	1.00
1:K:259:GLY:O	2:M:296:GLU:O	1.78	1.00
1:A:11:GLY:HA3	2:F:50:VAL:C	1.86	1.00
1:K:52:TYR:CB	1:K:295:PRO:CB	2.38	1.00
1:K:419:PHE:O	1:K:496:GLN:C	2.03	1.00
4:P:62:LEU:O	4:P:63:MET:CB	2.07	0.99
3:O:199:GLY:C	3:O:203:ALA:HB2	1.86	0.99
1:B:224:ALA:HB2	1:B:405:ALA:HB3	1.45	0.99
1:J:224:ALA:HB1	1:J:405:ALA:HB3	1.41	0.99
1:C:24:MET:HA	2:F:66:LEU:HA	1.45	0.99
1:C:11:GLY:HA3	2:E:50:VAL:H	1.28	0.98
1:I:259:GLY:O	2:N:296:GLU:C	2.05	0.98
2:L:334:GLU:O	2:L:361:LEU:N	1.96	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:MET:CB	2:E:66:LEU:N	2.26	0.98
1:J:471:VAL:CB	4:P:98:ILE:O	2.12	0.98
1:B:224:ALA:HB1	1:B:405:ALA:HB3	1.42	0.97
1:I:259:GLY:N	2:N:296:GLU:HA	1.78	0.97
1:I:11:GLY:HA2	2:N:50:VAL:H	0.81	0.97
1:K:25:TYR:CB	2:N:65:GLY:HA2	1.94	0.97
3:G:199:GLY:O	3:G:203:ALA:HB2	1.63	0.97
4:P:77:LEU:O	4:P:78:LYS:C	1.88	0.97
1:C:224:ALA:HB2	1:C:405:ALA:HB3	1.46	0.97
1:I:43:ASP:CA	2:L:69:ALA:HB2	1.94	0.97
1:J:419:PHE:O	1:J:496:GLN:HA	1.63	0.96
1:A:69:LEU:CB	1:A:72:ALA:N	2.27	0.96
1:I:224:ALA:HB2	1:I:405:ALA:HB3	1.46	0.96
2:F:149:LYS:O	2:F:333:THR:HA	1.66	0.96
1:A:224:ALA:HB2	1:A:405:ALA:HB3	1.46	0.96
3:O:199:GLY:O	3:O:203:ALA:HB2	1.63	0.96
1:K:44:GLY:HA2	2:N:69:ALA:HB2	1.47	0.96
1:C:292:SER:CB	2:E:292:ALA:HB3	1.96	0.96
1:J:224:ALA:HB2	1:J:405:ALA:HB3	1.45	0.96
2:L:150:LEU:HA	2:L:335:GLY:O	1.66	0.96
2:F:150:LEU:HA	2:F:335:GLY:O	1.66	0.95
1:K:224:ALA:HB2	1:K:405:ALA:HB3	1.46	0.95
1:A:69:LEU:CB	1:A:71:LEU:O	2.14	0.95
2:D:150:LEU:HA	2:D:335:GLY:O	1.67	0.95
2:N:150:LEU:HA	2:N:335:GLY:O	1.66	0.95
3:G:148:LYS:O	3:G:152:GLU:CB	2.15	0.95
2:N:149:LYS:O	2:N:333:THR:HA	1.66	0.95
1:B:11:GLY:HA3	2:D:49:GLU:HA	1.49	0.94
3:O:47:MET:O	3:O:49:ALA:N	2.00	0.94
2:E:150:LEU:HA	2:E:335:GLY:O	1.66	0.94
1:I:25:TYR:CB	2:L:65:GLY:HA2	1.96	0.94
2:L:149:LYS:O	2:L:333:THR:HA	1.66	0.94
2:M:150:LEU:HA	2:M:335:GLY:O	1.67	0.94
2:N:134:GLY:O	2:N:429:ASN:HA	1.68	0.94
2:D:149:LYS:O	2:D:333:THR:HA	1.66	0.94
1:C:11:GLY:HA3	2:E:50:VAL:N	1.82	0.94
1:A:44:GLY:CA	2:D:69:ALA:HB3	1.96	0.93
3:O:148:LYS:O	3:O:152:GLU:CB	2.15	0.93
1:C:267:VAL:O	2:E:125:ARG:HA	1.62	0.93
2:F:426:GLY:O	1:K:125:PRO:O	1.86	0.93
3:G:47:MET:O	3:G:49:ALA:N	2.00	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:149:LYS:O	2:L:333:THR:CA	2.17	0.93
2:N:149:LYS:O	2:N:333:THR:CA	2.16	0.93
4:P:86:VAL:O	4:P:88:GLY:N	2.01	0.93
1:A:71:LEU:CB	1:A:72:ALA:HA	1.99	0.93
2:E:149:LYS:O	2:E:333:THR:HA	1.66	0.93
4:P:75:ALA:CB	4:P:85:ASP:O	2.17	0.93
2:F:149:LYS:O	2:F:333:THR:CA	2.16	0.93
2:M:149:LYS:O	2:M:333:THR:HA	1.66	0.93
2:D:149:LYS:O	2:D:333:THR:CA	2.16	0.93
2:E:149:LYS:O	2:E:333:THR:CA	2.17	0.92
1:J:24:MET:CB	2:M:66:LEU:HA	1.99	0.92
1:B:10:ALA:N	2:D:50:VAL:CB	2.31	0.92
1:I:71:LEU:CB	1:I:189:VAL:N	2.33	0.92
1:I:259:GLY:C	2:N:296:GLU:C	2.37	0.92
3:O:48:GLU:O	3:O:51:LYS:CB	2.18	0.92
3:G:48:GLU:O	3:G:51:LYS:CB	2.18	0.91
1:A:71:LEU:CB	1:A:189:VAL:H	1.83	0.91
1:C:11:GLY:CA	2:E:50:VAL:H	1.82	0.91
1:K:69:LEU:CB	1:K:72:ALA:CB	2.47	0.91
1:I:259:GLY:C	2:N:296:GLU:CA	2.44	0.91
2:M:149:LYS:O	2:M:333:THR:CA	2.17	0.91
1:K:419:PHE:C	1:K:496:GLN:HA	1.95	0.91
1:C:266:LEU:CB	2:E:124:ARG:HA	1.99	0.91
2:E:359:SER:CB	2:E:362:MET:CB	2.49	0.91
3:G:47:MET:O	3:G:48:GLU:C	2.09	0.91
4:P:84:HIS:O	4:P:86:VAL:N	2.03	0.90
3:G:174:ALA:O	3:G:175:GLN:C	2.09	0.90
1:I:43:ASP:O	2:L:69:ALA:CB	2.08	0.90
3:G:135:GLU:C	3:G:137:LEU:N	2.17	0.90
3:G:49:ALA:O	3:G:52:ALA:HB3	1.72	0.90
3:O:174:ALA:O	3:O:175:GLN:C	2.09	0.90
4:P:84:HIS:O	4:P:86:VAL:CB	2.19	0.90
1:C:266:LEU:C	2:E:124:ARG:CB	2.45	0.90
1:B:24:MET:CB	2:E:66:LEU:C	2.44	0.89
3:O:141:ALA:O	3:O:145:THR:CB	2.21	0.89
1:A:44:GLY:CA	2:D:69:ALA:HB1	2.02	0.89
1:K:44:GLY:CA	2:N:69:ALA:HB2	2.03	0.89
1:I:24:MET:C	2:L:66:LEU:H	1.79	0.89
1:B:10:ALA:C	2:D:50:VAL:H	1.79	0.89
4:H:76:GLY:O	4:H:80:ALA:CB	2.20	0.88
3:O:49:ALA:O	3:O:52:ALA:HB3	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:135:GLU:C	3:O:137:LEU:N	2.17	0.88
1:A:43:ASP:C	2:D:69:ALA:CB	2.46	0.88
3:G:141:ALA:O	3:G:145:THR:CB	2.21	0.88
2:F:295:TYR:CB	2:F:332:ILE:CB	2.53	0.87
2:E:140:VAL:CB	2:E:435:SER:CB	2.52	0.87
1:I:44:GLY:HA2	2:L:69:ALA:HB3	1.48	0.87
1:I:267:VAL:N	2:N:124:ARG:CA	2.24	0.87
2:M:295:TYR:CB	2:M:332:ILE:CB	2.52	0.87
2:N:295:TYR:CB	2:N:332:ILE:CB	2.53	0.87
2:F:359:SER:CB	2:F:362:MET:CB	2.53	0.86
1:K:10:ALA:O	2:M:50:VAL:CB	2.23	0.86
2:D:295:TYR:CB	2:D:332:ILE:CB	2.53	0.86
2:L:295:TYR:CB	2:L:332:ILE:CB	2.53	0.86
4:H:77:LEU:H	4:H:80:ALA:HB3	1.41	0.86
2:L:153:PHE:O	2:L:339:LEU:N	2.08	0.86
1:B:10:ALA:O	2:D:49:GLU:HA	1.74	0.86
2:D:134:GLY:HA2	2:D:430:ARG:O	1.76	0.86
1:I:12:PRO:N	2:N:49:GLU:CB	2.39	0.86
1:I:24:MET:HA	2:L:66:LEU:HA	0.86	0.86
2:L:150:LEU:CA	2:L:335:GLY:O	2.24	0.86
2:F:153:PHE:O	2:F:339:LEU:N	2.09	0.86
2:M:153:PHE:O	2:M:339:LEU:N	2.09	0.86
1:J:263:THR:CB	2:L:125:ARG:N	2.38	0.86
2:E:295:TYR:CB	2:E:332:ILE:CB	2.53	0.86
2:F:150:LEU:CA	2:F:335:GLY:O	2.24	0.85
2:M:150:LEU:CA	2:M:335:GLY:O	2.24	0.85
1:C:260:ASN:CB	2:E:298:ALA:HB3	2.06	0.85
2:N:153:PHE:O	2:N:339:LEU:N	2.09	0.85
4:H:77:LEU:N	4:H:80:ALA:HB3	1.91	0.85
2:D:150:LEU:CA	2:D:335:GLY:O	2.24	0.85
2:E:150:LEU:CA	2:E:335:GLY:O	2.24	0.85
1:A:43:ASP:C	2:D:69:ALA:HB2	2.02	0.85
1:I:11:GLY:CA	2:N:50:VAL:CA	2.50	0.85
3:O:47:MET:O	3:O:48:GLU:C	2.09	0.85
4:H:76:GLY:C	4:H:80:ALA:HB3	2.00	0.84
1:I:52:TYR:CB	1:I:297:ALA:HB3	2.08	0.84
2:D:153:PHE:O	2:D:339:LEU:N	2.09	0.84
3:O:199:GLY:O	3:O:203:ALA:CB	2.26	0.84
2:N:150:LEU:CA	2:N:335:GLY:O	2.24	0.84
1:C:208:GLY:HA2	1:C:507:CYS:O	1.78	0.84
1:I:25:TYR:N	2:L:66:LEU:N	1.94	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:24:MET:CA	2:L:66:LEU:CA	2.50	0.83
1:K:419:PHE:C	1:K:497:GLN:H	1.86	0.83
2:E:153:PHE:O	2:E:339:LEU:N	2.09	0.83
3:O:158:THR:O	3:O:161:VAL:CB	2.27	0.83
3:G:158:THR:O	3:G:161:VAL:CB	2.27	0.82
1:C:18:GLY:O	1:C:19:MET:CB	2.28	0.82
1:C:266:LEU:C	2:E:124:ARG:CA	2.50	0.82
1:I:25:TYR:CA	2:L:65:GLY:HA2	2.09	0.82
3:O:167:VAL:O	3:O:168:VAL:C	2.19	0.82
3:G:199:GLY:O	3:G:203:ALA:CB	2.25	0.82
3:O:163:ALA:C	3:O:163:ALA:HA	2.04	0.82
1:C:208:GLY:O	1:C:507:CYS:CB	2.28	0.82
1:I:18:GLY:O	1:I:19:MET:CB	2.27	0.82
3:O:196:ARG:C	3:O:196:ARG:HA	2.05	0.82
1:C:189:VAL:CB	1:C:305:VAL:CA	2.58	0.81
1:I:56:SER:CB	2:N:30:GLY:N	2.43	0.81
2:L:359:SER:C	2:L:361:LEU:H	1.86	0.81
2:L:359:SER:C	2:L:361:LEU:N	2.26	0.81
1:C:259:GLY:O	2:E:296:GLU:C	2.24	0.81
1:B:263:THR:CB	2:D:125:ARG:CA	2.59	0.81
1:C:344:MET:CB	2:F:272:ALA:HB1	2.11	0.81
1:J:263:THR:CB	2:L:125:ARG:C	2.54	0.80
2:F:427:GLN:CB	1:K:126:GLY:HA3	2.12	0.80
1:I:259:GLY:C	2:N:296:GLU:HA	2.04	0.80
1:K:18:GLY:O	1:K:19:MET:CB	2.28	0.80
3:O:167:VAL:O	3:O:169:ILE:N	2.14	0.80
1:A:259:GLY:N	2:F:296:GLU:HA	1.96	0.80
1:B:9:ILE:CA	2:D:50:VAL:CB	2.60	0.80
3:G:167:VAL:O	3:G:168:VAL:C	2.19	0.80
1:J:18:GLY:O	1:J:19:MET:CB	2.28	0.80
1:I:266:LEU:CA	2:N:124:ARG:CB	2.59	0.80
1:J:224:ALA:HB1	1:J:405:ALA:CB	2.12	0.80
1:A:224:ALA:HB1	1:A:405:ALA:CB	2.12	0.79
1:B:18:GLY:O	1:B:19:MET:CB	2.28	0.79
3:G:167:VAL:O	3:G:169:ILE:N	2.14	0.79
1:I:24:MET:CA	2:L:66:LEU:N	2.46	0.79
1:B:224:ALA:HB1	1:B:405:ALA:CB	2.12	0.79
1:C:224:ALA:HB1	1:C:405:ALA:CB	2.12	0.79
1:I:260:ASN:CB	2:N:298:ALA:O	2.30	0.79
3:O:194:LEU:C	3:O:194:LEU:HA	2.04	0.79
3:G:199:GLY:C	3:G:203:ALA:CB	2.56	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:132:ARG:C	3:G:134:ALA:N	2.37	0.79
3:G:132:ARG:N	3:G:134:ALA:HB3	1.98	0.79
3:G:194:LEU:C	3:G:194:LEU:HA	2.04	0.79
1:I:224:ALA:HB1	1:I:405:ALA:CB	2.12	0.79
1:K:224:ALA:HB1	1:K:405:ALA:CB	2.13	0.79
3:O:199:GLY:C	3:O:203:ALA:CB	2.56	0.78
3:O:132:ARG:C	3:O:134:ALA:N	2.37	0.78
1:A:71:LEU:CB	1:A:189:VAL:N	2.45	0.78
3:G:4:VAL:C	3:G:4:VAL:HA	2.07	0.78
2:L:334:GLU:CB	2:L:361:LEU:CB	2.60	0.78
1:C:201:PRO:O	1:C:434:ALA:HB1	1.84	0.78
3:O:132:ARG:N	3:O:134:ALA:HB3	1.98	0.78
1:A:18:GLY:O	1:A:19:MET:CB	2.28	0.78
1:B:11:GLY:CA	2:D:49:GLU:HA	2.13	0.78
3:O:45:GLU:O	3:O:46:ALA:C	2.27	0.78
1:C:259:GLY:O	2:E:297:ARG:N	2.16	0.77
3:G:45:GLU:O	3:G:46:ALA:C	2.27	0.77
1:B:263:THR:CB	2:D:125:ARG:C	2.58	0.77
3:G:196:ARG:C	3:G:196:ARG:HA	2.05	0.77
3:G:28:LEU:O	3:G:31:LYS:CB	2.32	0.77
3:O:28:LEU:O	3:O:31:LYS:CB	2.32	0.77
2:D:334:GLU:O	2:D:361:LEU:N	2.17	0.77
1:I:419:PHE:CB	1:I:497:GLN:O	2.32	0.77
2:F:51:SER:O	2:F:52:GLU:CB	2.33	0.77
2:M:51:SER:O	2:M:52:GLU:CB	2.33	0.77
1:B:10:ALA:O	2:D:49:GLU:CA	2.33	0.76
1:C:44:GLY:HA2	2:F:69:ALA:HB1	1.67	0.76
1:C:224:ALA:CB	1:C:405:ALA:CB	2.58	0.76
3:O:135:GLU:O	3:O:136:ALA:C	2.28	0.76
1:A:11:GLY:HA2	2:F:50:VAL:H	1.47	0.76
2:D:51:SER:O	2:D:52:GLU:CB	2.33	0.76
2:L:51:SER:O	2:L:52:GLU:CB	2.33	0.76
3:G:135:GLU:O	3:G:136:ALA:C	2.28	0.76
1:B:10:ALA:O	2:D:49:GLU:C	2.29	0.75
1:J:419:PHE:O	1:J:496:GLN:CA	2.35	0.75
2:N:51:SER:O	2:N:52:GLU:CB	2.33	0.75
1:I:224:ALA:CB	1:I:405:ALA:CB	2.58	0.75
1:I:71:LEU:CB	1:I:72:ALA:HA	2.17	0.75
2:E:149:LYS:CB	2:E:332:ILE:O	2.35	0.75
1:C:25:TYR:CB	2:F:65:GLY:CA	2.51	0.75
2:E:51:SER:O	2:E:52:GLU:CB	2.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:149:LYS:CB	2:F:332:ILE:O	2.35	0.75
2:L:149:LYS:CB	2:L:332:ILE:O	2.35	0.75
1:B:224:ALA:CB	1:B:405:ALA:CB	2.58	0.74
3:G:163:ALA:C	3:G:163:ALA:HA	2.04	0.74
1:B:419:PHE:O	1:B:496:GLN:HA	1.87	0.74
1:I:56:SER:CB	2:N:30:GLY:O	2.35	0.74
3:O:140:VAL:O	3:O:144:GLU:CB	2.35	0.74
3:G:140:VAL:O	3:G:144:GLU:CB	2.35	0.73
2:M:149:LYS:CB	2:M:332:ILE:O	2.35	0.73
2:N:69:ALA:O	2:N:70:THR:CB	2.36	0.73
3:O:142:ASN:O	3:O:146:ARG:CB	2.36	0.73
3:G:142:ASN:O	3:G:146:ARG:CB	2.36	0.73
3:O:48:GLU:C	3:O:51:LYS:H	1.97	0.73
2:N:149:LYS:CB	2:N:332:ILE:O	2.35	0.73
2:D:149:LYS:CB	2:D:332:ILE:O	2.35	0.73
2:L:69:ALA:O	2:L:70:THR:CB	2.36	0.73
1:A:224:ALA:CB	1:A:405:ALA:CB	2.58	0.73
1:C:292:SER:CB	2:E:292:ALA:CB	2.67	0.73
2:F:69:ALA:O	2:F:70:THR:CB	2.37	0.73
1:I:24:MET:HA	2:L:66:LEU:N	2.04	0.72
3:G:48:GLU:C	3:G:51:LYS:H	1.97	0.72
2:E:69:ALA:O	2:E:70:THR:CB	2.37	0.72
3:O:150:ILE:O	3:O:151:GLY:O	2.07	0.72
3:G:150:ILE:O	3:G:151:GLY:O	2.08	0.72
3:O:4:VAL:C	3:O:4:VAL:HA	2.07	0.72
4:H:74:ILE:O	4:H:75:ALA:O	2.07	0.72
2:D:69:ALA:O	2:D:70:THR:CB	2.36	0.72
2:M:69:ALA:O	2:M:70:THR:CB	2.37	0.72
2:N:65:GLY:O	2:N:66:LEU:CB	2.38	0.72
1:A:69:LEU:CB	1:A:72:ALA:H	1.99	0.71
1:A:44:GLY:HA2	2:D:69:ALA:HB1	1.63	0.71
2:N:359:SER:CB	2:N:362:MET:CB	2.68	0.71
1:C:352:PRO:CB	2:F:269:GLU:C	2.63	0.71
2:F:65:GLY:O	2:F:66:LEU:CB	2.39	0.70
2:E:65:GLY:O	2:E:66:LEU:CB	2.38	0.70
1:I:225:ALA:N	1:I:405:ALA:O	2.25	0.70
1:A:225:ALA:N	1:A:405:ALA:O	2.25	0.70
2:L:274:ARG:O	2:L:275:GLU:CB	2.37	0.70
2:M:65:GLY:O	2:M:66:LEU:CB	2.38	0.70
4:H:62:LEU:O	4:H:63:MET:C	2.34	0.70
1:I:132:GLY:HA3	1:I:371:LEU:CB	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:VAL:CB	4:H:98:ILE:CA	2.69	0.70
1:K:225:ALA:N	1:K:405:ALA:O	2.25	0.70
2:M:149:LYS:O	2:M:333:THR:C	2.35	0.70
2:F:274:ARG:O	2:F:275:GLU:CB	2.37	0.69
1:A:259:GLY:CA	2:F:296:GLU:HA	2.21	0.69
2:N:149:LYS:O	2:N:333:THR:C	2.35	0.69
2:N:274:ARG:O	2:N:275:GLU:CB	2.37	0.69
2:D:359:SER:C	2:D:361:LEU:N	2.41	0.69
2:D:65:GLY:O	2:D:66:LEU:CB	2.38	0.69
2:E:149:LYS:O	2:E:333:THR:C	2.35	0.69
2:F:149:LYS:O	2:F:333:THR:C	2.35	0.69
1:C:225:ALA:N	1:C:405:ALA:O	2.25	0.69
1:J:225:ALA:N	1:J:405:ALA:O	2.25	0.69
1:I:71:LEU:CB	1:I:188:PRO:C	2.64	0.69
2:L:149:LYS:O	2:L:333:THR:C	2.35	0.69
1:B:225:ALA:N	1:B:405:ALA:O	2.25	0.69
1:J:263:THR:CB	2:L:124:ARG:C	2.65	0.69
2:M:274:ARG:O	2:M:275:GLU:CB	2.37	0.69
3:O:31:LYS:N	3:O:31:LYS:HA	2.02	0.69
3:O:156:LYS:C	3:O:158:THR:N	2.44	0.69
3:G:156:LYS:C	3:G:158:THR:N	2.44	0.69
2:L:65:GLY:O	2:L:66:LEU:CB	2.39	0.69
1:C:266:LEU:O	2:E:124:ARG:CB	2.40	0.68
3:O:156:LYS:O	3:O:157:THR:C	2.33	0.68
3:O:197:ILE:O	3:O:200:LYS:CB	2.41	0.68
2:D:149:LYS:O	2:D:333:THR:C	2.35	0.68
3:G:197:ILE:O	3:G:200:LYS:CB	2.40	0.68
1:A:5:VAL:CB	1:A:18:GLY:O	2.42	0.68
1:J:5:VAL:CB	1:J:18:GLY:O	2.42	0.68
1:K:5:VAL:CB	1:K:18:GLY:O	2.42	0.68
1:B:24:MET:CB	2:E:66:LEU:H	2.06	0.68
3:G:151:GLY:O	3:G:152:GLU:C	2.36	0.68
1:I:5:VAL:CB	1:I:18:GLY:O	2.42	0.68
2:F:427:GLN:CB	1:K:126:GLY:CA	2.72	0.68
3:O:151:GLY:O	3:O:152:GLU:C	2.37	0.68
1:J:224:ALA:CB	1:J:405:ALA:CB	2.58	0.68
1:K:224:ALA:CB	1:K:405:ALA:CB	2.58	0.68
2:E:274:ARG:O	2:E:275:GLU:CB	2.37	0.67
1:C:5:VAL:CB	1:C:18:GLY:O	2.42	0.67
2:F:61:GLU:HA	2:F:229:ILE:CB	2.25	0.67
3:G:156:LYS:O	3:G:157:THR:C	2.33	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:292:SER:CB	2:N:292:ALA:HB3	2.24	0.67
1:B:5:VAL:CB	1:B:18:GLY:O	2.42	0.67
3:G:151:GLY:HA2	3:G:155:LYS:CB	2.25	0.67
2:D:274:ARG:O	2:D:275:GLU:CB	2.37	0.67
3:G:31:LYS:N	3:G:31:LYS:HA	2.02	0.67
3:O:135:GLU:C	3:O:137:LEU:H	2.03	0.67
3:O:151:GLY:HA2	3:O:155:LYS:CB	2.26	0.66
3:G:3:GLN:O	3:G:5:SER:N	2.29	0.66
3:O:41:GLY:O	3:O:42:LEU:C	2.38	0.66
3:G:41:GLY:O	3:G:42:LEU:C	2.38	0.66
4:P:86:VAL:O	4:P:89:TYR:N	2.29	0.66
1:A:69:LEU:C	1:A:71:LEU:O	2.37	0.66
1:A:71:LEU:CB	1:A:72:ALA:CA	2.74	0.66
1:B:24:MET:HA	2:E:67:ASP:O	1.96	0.66
3:O:141:ALA:HA	3:O:144:GLU:CB	2.26	0.66
3:O:3:GLN:O	3:O:5:SER:N	2.29	0.66
1:C:260:ASN:N	2:E:296:GLU:HA	2.09	0.66
3:G:135:GLU:C	3:G:137:LEU:H	2.03	0.66
1:K:189:VAL:O	1:K:304:TYR:CB	2.44	0.66
3:G:141:ALA:HA	3:G:144:GLU:CB	2.26	0.66
1:K:266:LEU:CB	2:M:124:ARG:CB	2.74	0.66
1:C:352:PRO:CB	2:F:269:GLU:O	2.44	0.65
2:D:359:SER:C	2:D:361:LEU:H	2.04	0.65
4:H:84:HIS:C	4:H:86:VAL:N	2.53	0.65
1:A:11:GLY:CA	2:F:50:VAL:H	2.10	0.65
2:M:61:GLU:O	2:M:227:PRO:CB	2.44	0.65
3:O:158:THR:C	3:O:161:VAL:CB	2.70	0.65
3:G:158:THR:C	3:G:161:VAL:CB	2.70	0.65
1:A:292:SER:CB	2:F:292:ALA:HB1	2.26	0.65
1:K:26:ASP:O	1:K:71:LEU:N	2.30	0.65
2:L:334:GLU:O	2:L:361:LEU:CB	2.44	0.65
1:K:132:GLY:HA3	1:K:371:LEU:CB	2.27	0.65
3:O:172:ILE:O	3:O:176:ILE:CB	2.45	0.64
1:I:44:GLY:HA2	2:L:69:ALA:HB1	1.53	0.64
2:F:426:GLY:O	1:K:125:PRO:CB	2.46	0.64
3:O:150:ILE:C	3:O:151:GLY:O	2.39	0.64
3:G:141:ALA:HA	3:G:145:THR:H	1.62	0.64
1:B:11:GLY:CA	2:D:49:GLU:CB	2.66	0.64
1:K:11:GLY:HA3	2:M:49:GLU:CA	2.28	0.64
1:A:43:ASP:C	2:D:69:ALA:HB3	2.22	0.64
3:G:172:ILE:O	3:G:176:ILE:CB	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:25:TYR:O	2:L:65:GLY:HA2	1.97	0.64
1:A:259:GLY:CA	2:F:296:GLU:CA	2.73	0.63
3:O:141:ALA:HA	3:O:145:THR:H	1.62	0.63
1:I:346:ALA:HB2	2:L:272:ALA:HB1	1.80	0.63
1:K:11:GLY:CA	2:M:49:GLU:HA	2.29	0.63
2:E:134:GLY:O	2:E:429:ASN:HA	1.97	0.63
1:K:56:SER:CB	2:M:30:GLY:O	2.47	0.63
1:A:259:GLY:N	2:F:296:GLU:CA	2.62	0.63
1:A:259:GLY:H	2:F:296:GLU:CA	2.11	0.63
1:B:71:LEU:O	1:B:72:ALA:HB2	1.98	0.63
3:G:150:ILE:C	3:G:151:GLY:O	2.39	0.63
1:I:346:ALA:HB2	2:L:272:ALA:CB	2.29	0.63
2:N:76:VAL:O	2:N:77:GLU:CB	2.47	0.63
3:G:18:LEU:O	3:G:21:ALA:HB3	1.99	0.63
1:I:70:PRO:CB	1:I:190:ARG:CB	2.77	0.63
3:O:156:LYS:HA	3:O:159:ARG:H	1.64	0.63
2:F:76:VAL:O	2:F:77:GLU:CB	2.47	0.63
1:B:25:TYR:O	2:E:65:GLY:CA	2.40	0.62
3:O:148:LYS:O	3:O:149:LYS:O	2.17	0.62
2:E:76:VAL:O	2:E:77:GLU:CB	2.47	0.62
2:L:76:VAL:O	2:L:77:GLU:CB	2.47	0.62
1:C:52:TYR:C	1:C:295:PRO:CB	2.69	0.62
1:C:259:GLY:C	2:E:296:GLU:C	2.65	0.62
3:G:47:MET:C	3:G:49:ALA:N	2.57	0.62
3:G:156:LYS:HA	3:G:159:ARG:H	1.64	0.62
4:H:84:HIS:C	4:H:86:VAL:H	2.06	0.62
1:I:267:VAL:H	2:N:124:ARG:CA	1.97	0.62
1:I:267:VAL:CA	2:N:124:ARG:CB	2.74	0.62
3:O:18:LEU:O	3:O:21:ALA:HB3	1.99	0.62
3:G:47:MET:C	3:G:49:ALA:H	2.08	0.62
1:K:25:TYR:CB	2:N:65:GLY:CA	2.74	0.62
1:I:259:GLY:O	2:N:296:GLU:O	2.18	0.62
1:J:10:ALA:O	2:L:49:GLU:HA	1.99	0.61
1:K:11:GLY:HA3	2:M:49:GLU:CB	2.30	0.61
2:D:76:VAL:O	2:D:77:GLU:CB	2.47	0.61
3:O:27:LEU:CB	3:O:163:ALA:CB	2.73	0.61
3:G:148:LYS:O	3:G:149:LYS:O	2.17	0.61
2:E:61:GLU:O	2:E:227:PRO:CB	2.48	0.61
4:H:77:LEU:H	4:H:80:ALA:CB	2.12	0.61
3:O:44:ARG:C	3:O:47:MET:CB	2.72	0.61
1:A:259:GLY:H	2:F:296:GLU:N	1.97	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:24:MET:CA	2:L:66:LEU:H	2.08	0.61
1:I:419:PHE:HA	1:I:420:PRO:C	2.25	0.61
3:O:47:MET:C	3:O:49:ALA:H	2.09	0.61
1:I:11:GLY:CA	2:N:50:VAL:CB	2.78	0.61
3:O:132:ARG:O	3:O:133:TYR:C	2.38	0.61
2:M:76:VAL:O	2:M:77:GLU:CB	2.47	0.61
3:O:47:MET:C	3:O:49:ALA:N	2.57	0.61
3:O:170:PRO:O	3:O:174:ALA:HB2	2.00	0.61
1:I:25:TYR:CB	2:L:64:THR:O	2.49	0.61
1:A:11:GLY:HA3	2:F:50:VAL:CA	2.31	0.61
3:G:170:PRO:O	3:G:174:ALA:HB2	2.00	0.61
4:P:86:VAL:O	4:P:87:GLU:C	2.44	0.61
1:B:10:ALA:H	2:D:50:VAL:CA	2.14	0.60
1:C:44:GLY:HA2	2:F:69:ALA:HB2	1.77	0.60
1:C:419:PHE:HA	1:C:420:PRO:C	2.25	0.60
3:G:135:GLU:O	3:G:137:LEU:N	2.33	0.60
1:B:419:PHE:HA	1:B:420:PRO:C	2.25	0.60
1:C:12:PRO:N	2:E:49:GLU:CB	2.64	0.60
1:I:25:TYR:O	2:L:65:GLY:CA	2.49	0.60
3:O:45:GLU:C	3:O:47:MET:N	2.58	0.60
1:I:25:TYR:H	2:L:65:GLY:C	2.04	0.60
1:K:419:PHE:HA	1:K:420:PRO:C	2.25	0.60
4:P:84:HIS:O	4:P:86:VAL:CA	2.48	0.60
1:C:12:PRO:O	1:C:13:ALA:HB3	2.02	0.60
1:I:12:PRO:O	1:I:13:ALA:HB3	2.01	0.60
1:A:12:PRO:O	1:A:13:ALA:HB3	2.01	0.60
3:G:160:ARG:O	3:G:164:LEU:CB	2.50	0.60
3:G:132:ARG:O	3:G:133:TYR:C	2.37	0.60
1:K:11:GLY:HA3	2:M:50:VAL:H	1.66	0.60
1:I:25:TYR:C	2:L:65:GLY:HA2	2.26	0.60
3:G:44:ARG:C	3:G:47:MET:CB	2.72	0.59
1:J:12:PRO:O	1:J:13:ALA:HB3	2.02	0.59
1:J:419:PHE:HA	1:J:420:PRO:C	2.25	0.59
1:K:12:PRO:O	1:K:13:ALA:HB3	2.02	0.59
1:I:241:LEU:O	1:I:245:SER:N	2.33	0.59
1:K:27:ILE:HA	1:K:71:LEU:H	1.68	0.59
2:D:334:GLU:CB	2:D:361:LEU:CB	2.80	0.59
1:I:25:TYR:H	2:L:66:LEU:H	0.61	0.59
1:A:419:PHE:HA	1:A:420:PRO:C	2.25	0.59
3:G:135:GLU:HA	3:G:138:ILE:N	2.17	0.59
1:I:56:SER:CB	2:N:30:GLY:CA	2.81	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLY:N	2:D:69:ALA:HB1	2.08	0.59
1:B:12:PRO:O	1:B:13:ALA:HB3	2.01	0.59
3:O:135:GLU:HA	3:O:138:ILE:N	2.17	0.59
1:K:70:PRO:CB	1:K:71:LEU:O	2.50	0.59
3:O:135:GLU:O	3:O:137:LEU:N	2.33	0.59
3:O:160:ARG:O	3:O:164:LEU:CB	2.50	0.59
1:J:263:THR:CB	2:L:125:ARG:CA	2.80	0.59
1:A:71:LEU:CB	1:A:188:PRO:C	2.76	0.59
1:B:9:ILE:CB	2:D:52:GLU:N	2.66	0.59
1:I:292:SER:CB	2:N:292:ALA:CB	2.81	0.58
3:G:167:VAL:C	3:G:169:ILE:N	2.61	0.58
1:C:197:ARG:O	1:C:368:VAL:HA	2.04	0.58
1:I:208:GLY:O	1:I:507:CYS:O	2.21	0.58
1:J:24:MET:HA	2:M:67:ASP:O	2.04	0.58
4:P:86:VAL:C	4:P:88:GLY:N	2.62	0.58
1:C:430:LEU:C	1:C:432:THR:H	2.12	0.58
1:I:132:GLY:HA3	1:I:371:LEU:C	2.28	0.58
2:L:134:GLY:HA2	2:L:430:ARG:O	2.04	0.58
1:C:189:VAL:O	1:C:304:TYR:O	2.22	0.57
1:C:344:MET:CB	2:F:272:ALA:CB	2.81	0.57
1:A:267:VAL:CB	2:F:125:ARG:HA	2.34	0.57
3:O:167:VAL:C	3:O:167:VAL:HA	2.16	0.57
1:A:419:PHE:C	1:A:497:GLN:O	2.47	0.57
1:I:11:GLY:N	2:N:50:VAL:O	2.38	0.57
3:O:186:ARG:O	3:O:190:ASP:CB	2.53	0.57
3:G:45:GLU:C	3:G:47:MET:N	2.58	0.57
3:G:165:GLU:O	3:G:166:GLN:C	2.47	0.57
1:J:241:LEU:O	1:J:245:SER:N	2.33	0.57
1:C:420:PRO:N	1:C:496:GLN:HA	2.19	0.57
1:K:259:GLY:O	2:M:297:ARG:N	2.34	0.57
1:K:241:LEU:O	1:K:245:SER:N	2.32	0.56
1:C:241:LEU:O	1:C:245:SER:N	2.31	0.56
1:C:266:LEU:C	2:E:124:ARG:HA	2.30	0.56
1:I:352:PRO:CB	2:L:269:GLU:O	2.53	0.56
3:O:167:VAL:C	3:O:169:ILE:N	2.61	0.56
3:G:186:ARG:O	3:G:190:ASP:CB	2.53	0.56
1:I:25:TYR:N	2:L:65:GLY:HA2	2.19	0.56
2:M:334:GLU:O	2:M:360:ARG:N	2.37	0.56
3:O:48:GLU:O	3:O:51:LYS:N	2.38	0.56
1:A:241:LEU:O	1:A:245:SER:CB	2.54	0.56
1:J:263:THR:CB	2:L:125:ARG:O	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:25:TYR:CB	2:L:65:GLY:CA	2.79	0.56
2:N:136:SER:CB	2:N:430:ARG:CB	2.84	0.56
3:G:52:ALA:CB	3:G:52:ALA:C	2.74	0.56
3:G:137:LEU:O	3:G:140:VAL:CB	2.54	0.56
3:G:189:GLU:CB	3:G:189:GLU:HA	2.18	0.56
3:O:165:GLU:O	3:O:166:GLN:C	2.47	0.56
1:C:430:LEU:O	1:C:432:THR:N	2.38	0.56
1:C:344:MET:CB	2:F:272:ALA:CA	2.84	0.56
2:F:426:GLY:C	1:K:125:PRO:O	2.48	0.56
3:G:132:ARG:N	3:G:134:ALA:CB	2.68	0.56
1:I:266:LEU:CB	2:N:124:ARG:CA	2.82	0.56
3:O:52:ALA:CB	3:O:52:ALA:C	2.74	0.55
3:O:138:ILE:C	3:O:139:ARG:O	2.45	0.55
3:O:137:LEU:O	3:O:140:VAL:CB	2.54	0.55
3:O:158:THR:HA	3:O:161:VAL:CB	2.37	0.55
3:G:142:ASN:CB	3:G:142:ASN:HA	2.17	0.55
2:L:359:SER:CB	2:L:362:MET:H	2.18	0.55
1:C:266:LEU:CB	2:E:124:ARG:CA	2.80	0.55
3:G:138:ILE:C	3:G:139:ARG:O	2.45	0.55
3:O:142:ASN:CB	3:O:142:ASN:HA	2.16	0.55
3:G:48:GLU:O	3:G:51:LYS:N	2.39	0.55
1:K:11:GLY:HA2	2:M:49:GLU:HA	1.88	0.55
4:P:84:HIS:O	4:P:85:ASP:C	2.47	0.55
1:K:10:ALA:O	2:M:50:VAL:N	2.39	0.55
3:G:194:LEU:C	3:G:194:LEU:CB	2.73	0.55
3:O:136:ALA:O	3:O:140:VAL:CB	2.55	0.54
3:O:137:LEU:O	3:O:140:VAL:N	2.40	0.54
1:B:241:LEU:O	1:B:245:SER:N	2.31	0.54
3:G:146:ARG:O	3:G:147:LEU:C	2.50	0.54
3:G:132:ARG:C	3:G:134:ALA:H	2.13	0.54
3:G:158:THR:HA	3:G:161:VAL:CB	2.37	0.54
1:I:56:SER:CB	2:N:30:GLY:H	2.20	0.54
1:K:189:VAL:CB	1:K:304:TYR:CB	2.85	0.54
1:A:25:TYR:H	2:D:66:LEU:H	1.56	0.54
3:G:137:LEU:O	3:G:140:VAL:N	2.40	0.54
1:A:557:GLU:C	1:A:559:PHE:N	2.66	0.54
1:J:24:MET:CB	2:M:66:LEU:CA	2.80	0.54
1:J:557:GLU:C	1:J:559:PHE:N	2.66	0.54
3:G:136:ALA:O	3:G:140:VAL:CB	2.55	0.54
3:G:43:VAL:O	3:G:44:ARG:C	2.51	0.54
1:I:225:ALA:O	1:I:406:PHE:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:225:ALA:O	1:K:406:PHE:HA	2.07	0.54
3:O:7:THR:O	3:O:9:MET:N	2.41	0.54
3:O:132:ARG:C	3:O:134:ALA:H	2.13	0.54
1:A:292:SER:CB	2:F:292:ALA:CB	2.86	0.53
1:A:296:VAL:HA	1:A:333:ALA:HB1	1.90	0.53
2:E:153:PHE:CB	2:E:338:GLN:HA	2.38	0.53
3:O:132:ARG:N	3:O:134:ALA:CB	2.68	0.53
3:O:146:ARG:O	3:O:147:LEU:C	2.50	0.53
1:A:225:ALA:O	1:A:406:PHE:HA	2.08	0.53
1:B:225:ALA:O	1:B:406:PHE:HA	2.08	0.53
1:C:225:ALA:O	1:C:406:PHE:HA	2.08	0.53
4:H:84:HIS:O	4:H:85:ASP:C	2.43	0.53
1:B:224:ALA:CA	1:B:405:ALA:HB3	2.37	0.53
1:I:259:GLY:O	2:N:297:ARG:N	2.42	0.53
1:J:227:PRO:HA	1:J:384:VAL:CB	2.39	0.53
1:J:296:VAL:HA	1:J:333:ALA:HB1	1.90	0.53
1:K:224:ALA:CA	1:K:405:ALA:HB3	2.37	0.53
3:G:138:ILE:O	3:G:139:ARG:O	2.27	0.53
1:K:44:GLY:CA	2:N:69:ALA:HB3	2.14	0.53
4:P:77:LEU:O	4:P:78:LYS:O	2.23	0.53
1:B:296:VAL:HA	1:B:333:ALA:HB1	1.90	0.53
1:B:557:GLU:C	1:B:559:PHE:N	2.66	0.53
2:L:153:PHE:CB	2:L:338:GLN:HA	2.39	0.53
2:F:426:GLY:O	1:K:125:PRO:CA	2.57	0.53
4:H:76:GLY:O	4:H:80:ALA:HB1	2.06	0.53
1:I:557:GLU:C	1:I:559:PHE:N	2.66	0.53
2:M:153:PHE:CB	2:M:338:GLN:HA	2.39	0.53
3:O:42:LEU:O	3:O:45:GLU:CB	2.57	0.53
3:O:145:THR:O	3:O:149:LYS:CB	2.57	0.53
3:O:198:LYS:O	3:O:199:GLY:C	2.52	0.53
1:A:227:PRO:HA	1:A:384:VAL:CB	2.39	0.53
1:C:557:GLU:C	1:C:559:PHE:N	2.66	0.53
2:D:153:PHE:CB	2:D:338:GLN:HA	2.39	0.53
3:G:166:GLN:O	3:G:169:ILE:CB	2.57	0.53
1:A:224:ALA:CA	1:A:405:ALA:HB3	2.37	0.53
1:C:296:VAL:HA	1:C:333:ALA:HB1	1.91	0.53
2:F:153:PHE:CB	2:F:338:GLN:HA	2.39	0.53
1:I:43:ASP:HA	2:L:69:ALA:HB2	1.88	0.53
1:I:227:PRO:HA	1:I:384:VAL:CB	2.39	0.53
1:I:260:ASN:N	2:N:296:GLU:HA	2.23	0.53
1:K:557:GLU:C	1:K:559:PHE:N	2.66	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:153:PHE:CB	2:N:338:GLN:HA	2.39	0.53
3:O:138:ILE:O	3:O:139:ARG:O	2.27	0.53
1:A:419:PHE:CB	1:A:497:GLN:O	2.56	0.53
3:G:39:PHE:O	3:G:42:LEU:CB	2.57	0.53
1:B:227:PRO:HA	1:B:384:VAL:CB	2.39	0.52
1:C:227:PRO:HA	1:C:384:VAL:CB	2.39	0.52
3:G:145:THR:O	3:G:149:LYS:CB	2.57	0.52
3:G:198:LYS:O	3:G:199:GLY:C	2.52	0.52
1:A:81:ASN:HA	1:A:282:MET:O	2.10	0.52
1:I:189:VAL:HA	1:I:308:THR:CB	2.39	0.52
1:I:296:VAL:HA	1:I:333:ALA:HB1	1.91	0.52
3:G:141:ALA:CA	3:G:145:THR:H	2.22	0.52
1:J:225:ALA:O	1:J:406:PHE:HA	2.08	0.52
3:O:173:ARG:O	3:O:177:ARG:CB	2.58	0.52
1:K:227:PRO:HA	1:K:384:VAL:CB	2.39	0.52
2:N:334:GLU:O	2:N:360:ARG:N	2.43	0.52
3:O:43:VAL:O	3:O:44:ARG:C	2.51	0.52
3:O:166:GLN:O	3:O:169:ILE:CB	2.57	0.52
2:L:359:SER:CA	2:L:362:MET:H	2.23	0.52
1:A:52:TYR:O	1:A:53:GLU:CB	2.58	0.52
2:E:150:LEU:C	2:E:335:GLY:O	2.53	0.52
3:G:42:LEU:O	3:G:45:GLU:CB	2.57	0.52
1:I:44:GLY:N	2:L:69:ALA:HB2	1.76	0.52
3:O:167:VAL:C	3:O:169:ILE:H	2.18	0.52
1:C:52:TYR:O	1:C:53:GLU:CB	2.58	0.52
2:F:150:LEU:C	2:F:335:GLY:O	2.53	0.52
1:K:11:GLY:HA3	2:M:49:GLU:HA	1.90	0.52
3:O:194:LEU:C	3:O:194:LEU:CB	2.73	0.52
1:I:52:TYR:O	1:I:53:GLU:CB	2.58	0.52
1:I:259:GLY:O	2:N:298:ALA:N	2.43	0.52
1:K:52:TYR:C	1:K:295:PRO:CB	2.77	0.52
2:M:150:LEU:C	2:M:335:GLY:O	2.53	0.52
1:K:52:TYR:O	1:K:53:GLU:CB	2.58	0.51
1:J:69:LEU:C	1:J:70:PRO:O	2.47	0.51
1:I:224:ALA:CA	1:I:405:ALA:HB3	2.37	0.51
2:L:150:LEU:C	2:L:335:GLY:O	2.52	0.51
1:B:52:TYR:O	1:B:53:GLU:CB	2.58	0.51
1:B:224:ALA:HB2	1:B:405:ALA:CB	2.31	0.51
2:D:150:LEU:C	2:D:335:GLY:O	2.53	0.51
1:I:204:PRO:CB	1:I:435:LEU:CB	2.89	0.51
1:K:296:VAL:HA	1:K:333:ALA:HB1	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:205:GLU:CB	3:O:205:GLU:N	2.67	0.51
3:O:141:ALA:CA	3:O:145:THR:H	2.22	0.51
1:C:202:ASN:HA	1:C:434:ALA:O	2.11	0.51
3:G:7:THR:O	3:G:9:MET:N	2.42	0.51
3:G:171:GLY:O	3:G:174:ALA:HB3	2.11	0.51
3:G:173:ARG:O	3:G:177:ARG:CB	2.58	0.51
3:O:171:GLY:O	3:O:174:ALA:HB3	2.11	0.51
1:I:266:LEU:CB	2:N:124:ARG:HA	2.41	0.51
2:N:150:LEU:C	2:N:335:GLY:O	2.53	0.51
3:G:183:LEU:O	3:G:186:ARG:CB	2.59	0.51
3:G:167:VAL:C	3:G:169:ILE:H	2.18	0.50
1:J:71:LEU:O	1:J:188:PRO:HA	2.10	0.50
3:O:183:LEU:O	3:O:186:ARG:CB	2.60	0.50
1:A:69:LEU:O	1:A:71:LEU:O	2.29	0.50
1:C:73:VAL:O	1:C:186:THR:HA	2.12	0.50
1:J:52:TYR:O	1:J:53:GLU:CB	2.58	0.50
1:K:11:GLY:HA3	2:M:50:VAL:N	2.27	0.50
1:A:73:VAL:O	1:A:186:THR:HA	2.12	0.50
1:A:266:LEU:CB	2:F:124:ARG:CA	2.89	0.50
3:O:148:LYS:O	3:O:152:GLU:CA	2.59	0.50
1:A:43:ASP:O	2:D:69:ALA:HB3	2.12	0.50
4:H:77:LEU:O	4:H:78:LYS:C	2.32	0.50
1:J:224:ALA:CA	1:J:405:ALA:HB3	2.37	0.50
1:K:216:PHE:HA	1:K:429:SER:CB	2.42	0.50
1:B:73:VAL:O	1:B:186:THR:HA	2.12	0.49
2:L:150:LEU:CB	2:L:335:GLY:O	2.60	0.49
2:N:149:LYS:O	2:N:333:THR:CB	2.59	0.49
1:C:352:PRO:O	2:F:269:GLU:CB	2.60	0.49
1:J:73:VAL:O	1:J:186:THR:HA	2.11	0.49
1:J:224:ALA:HB2	1:J:405:ALA:CB	2.31	0.49
1:K:73:VAL:O	1:K:186:THR:HA	2.12	0.49
3:O:142:ASN:CB	3:O:142:ASN:N	2.67	0.49
1:A:11:GLY:CA	2:F:50:VAL:N	2.73	0.49
2:E:149:LYS:O	2:E:333:THR:CB	2.59	0.49
2:F:149:LYS:O	2:F:333:THR:CB	2.59	0.49
3:G:205:GLU:CB	3:G:205:GLU:N	2.66	0.49
1:J:9:ILE:CA	2:L:50:VAL:O	2.57	0.49
1:K:189:VAL:C	1:K:304:TYR:CB	2.85	0.49
1:C:344:MET:CB	2:F:272:ALA:HA	2.42	0.49
2:D:149:LYS:O	2:D:333:THR:CB	2.59	0.49
3:G:146:ARG:O	3:G:149:LYS:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:148:LYS:O	3:G:152:GLU:CA	2.59	0.49
3:O:146:ARG:O	3:O:149:LYS:N	2.45	0.49
2:N:61:GLU:HA	2:N:229:ILE:CB	2.42	0.49
3:O:49:ALA:O	3:O:52:ALA:CB	2.53	0.49
2:E:150:LEU:CB	2:E:335:GLY:O	2.61	0.49
1:J:9:ILE:HA	2:L:50:VAL:CB	2.42	0.49
2:M:150:LEU:CB	2:M:335:GLY:O	2.61	0.49
2:N:150:LEU:CB	2:N:335:GLY:O	2.61	0.49
1:A:259:GLY:H	2:F:296:GLU:HA	1.68	0.49
2:D:150:LEU:CB	2:D:335:GLY:O	2.60	0.49
2:L:149:LYS:O	2:L:333:THR:CB	2.59	0.49
3:O:198:LYS:O	3:O:199:GLY:O	2.31	0.49
2:M:149:LYS:O	2:M:333:THR:CB	2.60	0.49
3:O:134:ALA:O	3:O:137:LEU:CB	2.61	0.48
3:O:179:ILE:O	3:O:180:GLN:C	2.55	0.48
1:B:9:ILE:C	2:D:50:VAL:CB	2.86	0.48
3:G:198:LYS:O	3:G:199:GLY:O	2.31	0.48
1:I:24:MET:CB	2:L:66:LEU:N	2.76	0.48
1:I:73:VAL:O	1:I:186:THR:HA	2.12	0.48
3:O:3:GLN:O	3:O:6:PRO:N	2.46	0.48
1:C:44:GLY:HA2	2:F:69:ALA:HB3	1.84	0.48
1:C:224:ALA:CA	1:C:405:ALA:HB3	2.37	0.48
3:G:3:GLN:O	3:G:6:PRO:N	2.47	0.48
3:G:134:ALA:O	3:G:137:LEU:CB	2.62	0.48
1:I:440:ARG:HA	1:I:444:ALA:O	2.14	0.48
1:J:440:ARG:HA	1:J:444:ALA:O	2.14	0.48
2:N:349:TYR:HA	2:N:350:PRO:C	2.38	0.48
3:O:163:ALA:C	3:O:163:ALA:CB	2.79	0.48
3:O:200:LYS:HA	3:O:203:ALA:HB3	1.96	0.48
4:P:86:VAL:C	4:P:88:GLY:H	2.19	0.48
3:O:138:ILE:O	3:O:142:ASN:CB	2.62	0.48
1:C:189:VAL:HA	1:C:308:THR:CB	2.43	0.48
3:O:48:GLU:CB	3:O:51:LYS:CB	2.92	0.48
2:F:150:LEU:CB	2:F:335:GLY:O	2.61	0.48
1:B:263:THR:CA	2:D:124:ARG:C	2.86	0.48
3:G:135:GLU:HA	3:G:138:ILE:H	1.79	0.48
2:M:349:TYR:HA	2:M:350:PRO:C	2.39	0.48
2:D:349:TYR:HA	2:D:350:PRO:C	2.38	0.48
2:F:349:TYR:HA	2:F:350:PRO:C	2.39	0.48
1:K:260:ASN:N	2:M:296:GLU:HA	1.95	0.48
2:L:349:TYR:HA	2:L:350:PRO:C	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:4:VAL:CA	3:G:5:SER:N	2.68	0.47
3:O:153:GLU:O	3:O:154:ILE:O	2.32	0.47
1:B:11:GLY:HA2	2:D:48:ILE:O	2.14	0.47
3:G:153:GLU:O	3:G:154:ILE:O	2.32	0.47
1:A:440:ARG:HA	1:A:444:ALA:O	2.14	0.47
4:P:65:GLY:CA	4:P:66:ARG:CB	2.93	0.47
1:C:24:MET:CA	2:F:66:LEU:HA	2.31	0.47
3:G:48:GLU:CB	3:G:51:LYS:CB	2.92	0.47
1:K:44:GLY:HA3	2:N:69:ALA:CB	2.40	0.47
3:G:138:ILE:O	3:G:142:ASN:CB	2.62	0.47
3:G:4:VAL:C	3:G:6:PRO:N	2.71	0.47
1:K:267:VAL:N	2:M:124:ARG:CB	2.78	0.47
1:K:440:ARG:HA	1:K:444:ALA:O	2.14	0.47
3:G:167:VAL:C	3:G:167:VAL:HA	2.16	0.47
3:G:200:LYS:HA	3:G:203:ALA:HB3	1.96	0.47
3:O:135:GLU:HA	3:O:138:ILE:H	1.80	0.47
1:C:440:ARG:HA	1:C:444:ALA:O	2.14	0.47
2:E:349:TYR:HA	2:E:350:PRO:C	2.39	0.47
1:B:9:ILE:CA	2:D:50:VAL:O	2.53	0.46
1:B:440:ARG:HA	1:B:444:ALA:O	2.14	0.46
1:J:429:SER:C	1:J:431:PHE:H	2.23	0.46
1:C:430:LEU:C	1:C:432:THR:N	2.73	0.46
1:K:11:GLY:CA	2:M:49:GLU:CB	2.93	0.46
3:O:200:LYS:CA	3:O:203:ALA:HB3	2.45	0.46
1:C:189:VAL:CB	1:C:305:VAL:N	2.78	0.46
1:J:86:GLY:HA2	1:J:302:SER:CB	2.46	0.46
1:J:419:PHE:O	1:J:496:GLN:CB	2.63	0.46
1:B:475:ALA:O	4:H:102:ILE:CB	2.63	0.46
3:G:49:ALA:O	3:G:52:ALA:CB	2.53	0.46
2:M:134:GLY:O	2:M:429:ASN:HA	2.14	0.46
1:I:71:LEU:CB	1:I:72:ALA:CA	2.92	0.46
1:A:224:ALA:HB2	1:A:405:ALA:CB	2.31	0.46
1:C:25:TYR:CA	2:F:65:GLY:HA2	2.36	0.46
2:D:359:SER:CB	2:D:362:MET:H	2.28	0.46
3:G:200:LYS:CA	3:G:203:ALA:HB3	2.45	0.46
3:G:27:LEU:CB	3:G:27:LEU:C	2.79	0.46
3:G:40:PHE:O	3:G:43:VAL:N	2.49	0.45
3:G:138:ILE:CB	4:H:16:ALA:CB	2.94	0.45
1:I:352:PRO:CB	2:L:272:ALA:HB3	2.47	0.45
1:I:11:GLY:HA3	2:N:50:VAL:CB	2.38	0.45
2:L:334:GLU:CA	2:L:361:LEU:CB	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:7:THR:O	3:G:8:ARG:O	2.30	0.45
3:G:179:ILE:O	3:G:180:GLN:C	2.56	0.45
1:I:475:ALA:HB1	2:L:398:ILE:O	2.16	0.45
3:O:52:ALA:O	3:O:55:GLN:O	2.34	0.45
3:G:35:LEU:O	3:G:38:GLU:CB	2.65	0.45
1:I:241:LEU:O	1:I:245:SER:CB	2.64	0.45
1:K:70:PRO:N	1:K:72:ALA:HB2	2.32	0.45
3:O:35:LEU:O	3:O:38:GLU:CB	2.65	0.45
1:C:266:LEU:CB	2:E:124:ARG:CB	2.94	0.45
3:G:52:ALA:O	3:G:55:GLN:O	2.34	0.45
1:J:241:LEU:O	1:J:245:SER:CB	2.64	0.45
1:K:241:LEU:O	1:K:245:SER:CB	2.64	0.45
2:L:334:GLU:O	2:L:361:LEU:CA	2.63	0.45
1:A:259:GLY:C	2:F:296:GLU:HA	2.41	0.45
1:C:268:GLU:CB	2:E:126:LYS:CB	2.94	0.45
3:G:148:LYS:C	3:G:149:LYS:O	2.60	0.45
3:G:151:GLY:O	3:G:152:GLU:O	2.35	0.45
3:O:7:THR:O	3:O:8:ARG:O	2.30	0.45
4:P:94:VAL:O	4:P:95:ARG:C	2.58	0.45
1:I:132:GLY:HA3	1:I:371:LEU:O	2.17	0.45
1:K:296:VAL:CA	1:K:333:ALA:HB1	2.47	0.45
1:B:9:ILE:CB	2:D:51:SER:C	2.89	0.45
2:L:334:GLU:O	2:L:360:ARG:C	2.56	0.45
1:A:352:PRO:CB	2:D:269:GLU:O	2.64	0.45
1:C:131:GLY:O	1:C:371:LEU:CB	2.65	0.45
1:C:388:GLY:C	1:C:390:ASP:H	2.25	0.45
3:G:163:ALA:C	3:G:163:ALA:CB	2.79	0.45
1:A:11:GLY:HA3	2:F:50:VAL:N	2.32	0.44
1:C:296:VAL:CA	1:C:333:ALA:HB1	2.47	0.44
3:G:142:ASN:CB	3:G:142:ASN:N	2.67	0.44
3:G:189:GLU:CB	3:G:189:GLU:N	2.69	0.44
3:G:141:ALA:HB1	3:G:145:THR:CB	2.47	0.44
1:J:296:VAL:CA	1:J:333:ALA:HB1	2.47	0.44
1:K:259:GLY:H	2:M:296:GLU:CB	2.20	0.44
3:O:4:VAL:C	3:O:6:PRO:N	2.71	0.44
3:O:27:LEU:CB	3:O:27:LEU:C	2.80	0.44
1:A:388:GLY:C	1:A:390:ASP:H	2.25	0.44
1:B:388:GLY:C	1:B:390:ASP:H	2.25	0.44
1:C:81:ASN:N	1:C:282:MET:O	2.46	0.44
1:C:314:ARG:HA	1:C:318:PHE:O	2.18	0.44
2:D:153:PHE:O	2:D:338:GLN:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:388:GLY:C	1:K:390:ASP:H	2.26	0.44
3:O:141:ALA:HB1	3:O:145:THR:CB	2.47	0.44
1:B:296:VAL:CA	1:B:333:ALA:HB1	2.47	0.44
3:G:45:GLU:O	3:G:47:MET:N	2.50	0.44
1:J:314:ARG:HA	1:J:318:PHE:O	2.17	0.44
1:A:296:VAL:CA	1:A:333:ALA:HB1	2.47	0.44
1:A:419:PHE:C	1:A:496:GLN:HA	2.41	0.44
3:G:175:GLN:O	3:G:177:ARG:N	2.51	0.44
1:K:11:GLY:CA	2:M:49:GLU:CA	2.92	0.44
3:O:175:GLN:O	3:O:177:ARG:N	2.51	0.44
1:A:314:ARG:HA	1:A:318:PHE:O	2.18	0.44
1:B:314:ARG:HA	1:B:318:PHE:O	2.18	0.44
3:O:151:GLY:O	3:O:152:GLU:O	2.35	0.44
2:E:153:PHE:O	2:E:338:GLN:HA	2.18	0.44
1:I:56:SER:CB	2:N:30:GLY:C	2.91	0.44
1:I:296:VAL:CA	1:I:333:ALA:HB1	2.47	0.44
1:K:314:ARG:HA	1:K:318:PHE:O	2.18	0.44
2:L:153:PHE:O	2:L:338:GLN:HA	2.18	0.44
3:O:177:ARG:C	3:O:179:ILE:N	2.72	0.44
1:B:80:LEU:C	1:B:82:GLY:H	2.26	0.43
1:J:388:GLY:C	1:J:390:ASP:H	2.26	0.43
1:A:44:GLY:N	2:D:69:ALA:HB3	2.12	0.43
1:A:71:LEU:CA	1:A:189:VAL:H	2.27	0.43
1:I:314:ARG:HA	1:I:318:PHE:O	2.18	0.43
1:K:259:GLY:C	2:M:296:GLU:O	2.50	0.43
2:N:153:PHE:O	2:N:338:GLN:HA	2.18	0.43
1:B:471:VAL:CB	4:H:98:ILE:HA	2.48	0.43
1:C:80:LEU:C	1:C:82:GLY:H	2.26	0.43
1:K:208:GLY:O	1:K:507:CYS:O	2.35	0.43
1:K:224:ALA:HB2	1:K:405:ALA:CB	2.32	0.43
2:M:153:PHE:O	2:M:338:GLN:HA	2.18	0.43
1:K:69:LEU:CA	1:K:72:ALA:CB	2.97	0.43
4:P:59:VAL:O	4:P:60:GLU:C	2.61	0.43
1:A:80:LEU:C	1:A:82:GLY:H	2.27	0.43
1:I:69:LEU:CB	1:I:71:LEU:N	2.82	0.43
1:I:255:CYS:HA	1:I:290:ASN:CB	2.49	0.43
1:J:75:LEU:O	1:J:184:TYR:HA	2.19	0.43
2:F:258:THR:HA	2:F:259:ASP:HA	1.85	0.43
3:G:177:ARG:C	3:G:179:ILE:N	2.72	0.43
4:H:59:VAL:O	4:H:60:GLU:C	2.61	0.43
3:O:189:GLU:CB	3:O:189:GLU:N	2.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:75:LEU:O	1:K:184:TYR:HA	2.19	0.43
3:O:40:PHE:O	3:O:43:VAL:CB	2.67	0.43
3:O:140:VAL:O	3:O:144:GLU:N	2.47	0.43
3:O:159:ARG:C	3:O:161:VAL:N	2.77	0.43
3:O:189:GLU:CB	3:O:189:GLU:HA	2.18	0.43
3:O:189:GLU:O	3:O:190:ASP:C	2.62	0.43
1:A:255:CYS:HA	1:A:290:ASN:CB	2.49	0.43
1:B:241:LEU:O	1:B:245:SER:CB	2.67	0.43
2:E:258:THR:HA	2:E:259:ASP:HA	1.85	0.43
2:F:427:GLN:CB	1:K:126:GLY:HA2	2.46	0.43
3:O:45:GLU:O	3:O:47:MET:N	2.50	0.43
1:A:259:GLY:O	2:F:296:GLU:C	2.62	0.43
3:G:135:GLU:O	3:G:139:ARG:CB	2.67	0.43
3:G:175:GLN:O	3:G:178:PHE:N	2.51	0.43
1:I:388:GLY:C	1:I:390:ASP:H	2.25	0.43
3:O:135:GLU:O	3:O:139:ARG:CB	2.67	0.43
4:P:64:ARG:C	4:P:65:GLY:O	2.56	0.43
1:J:80:LEU:C	1:J:82:GLY:H	2.26	0.42
1:K:255:CYS:HA	1:K:290:ASN:CB	2.49	0.42
1:B:255:CYS:HA	1:B:290:ASN:CB	2.49	0.42
1:I:258:ARG:C	2:N:296:GLU:HA	2.41	0.42
1:J:266:LEU:CB	2:L:124:ARG:CB	2.97	0.42
1:C:241:LEU:O	1:C:245:SER:CB	2.67	0.42
2:F:153:PHE:O	2:F:338:GLN:HA	2.18	0.42
1:I:11:GLY:C	2:N:50:VAL:O	2.59	0.42
3:O:174:ALA:O	3:O:175:GLN:O	2.37	0.42
1:B:75:LEU:O	1:B:184:TYR:HA	2.19	0.42
2:D:189:VAL:O	2:D:217:SER:HA	2.19	0.42
3:G:40:PHE:O	3:G:43:VAL:CB	2.67	0.42
1:I:25:TYR:O	2:L:65:GLY:HA3	2.16	0.42
1:I:346:ALA:HB2	2:L:272:ALA:HB2	2.01	0.42
3:O:148:LYS:C	3:O:149:LYS:O	2.59	0.42
1:C:75:LEU:O	1:C:184:TYR:HA	2.19	0.42
2:E:189:VAL:O	2:E:217:SER:HA	2.20	0.42
1:I:25:TYR:N	2:L:65:GLY:CA	2.82	0.42
1:J:255:CYS:HA	1:J:290:ASN:CB	2.49	0.42
2:L:189:VAL:O	2:L:217:SER:HA	2.20	0.42
3:O:4:VAL:CA	3:O:5:SER:N	2.68	0.42
1:B:70:PRO:O	1:B:71:LEU:CB	2.68	0.42
2:D:149:LYS:C	2:D:334:GLU:H	2.14	0.42
1:A:241:LEU:O	1:A:244:TRP:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:75:LEU:O	1:I:184:TYR:HA	2.18	0.42
1:K:69:LEU:CA	1:K:72:ALA:HB2	2.49	0.42
1:A:133:MET:O	1:A:148:LEU:HA	2.20	0.42
2:F:189:VAL:O	2:F:217:SER:HA	2.20	0.42
4:H:94:VAL:O	4:H:95:ARG:C	2.58	0.42
3:O:3:GLN:O	3:O:4:VAL:C	2.63	0.42
1:B:10:ALA:C	2:D:49:GLU:HA	2.43	0.42
3:G:189:GLU:O	3:G:190:ASP:C	2.62	0.42
1:A:221:GLY:O	1:A:366:GLY:HA2	2.21	0.41
1:C:260:ASN:HA	2:E:296:GLU:O	2.20	0.41
1:I:80:LEU:C	1:I:82:GLY:H	2.27	0.41
1:J:133:MET:O	1:J:148:LEU:HA	2.20	0.41
1:K:80:LEU:C	1:K:82:GLY:H	2.27	0.41
3:O:175:GLN:O	3:O:178:PHE:N	2.51	0.41
1:A:75:LEU:O	1:A:184:TYR:HA	2.19	0.41
1:B:227:PRO:CB	1:B:384:VAL:CB	2.98	0.41
1:C:81:ASN:HA	1:C:282:MET:C	2.45	0.41
3:G:48:GLU:C	3:G:51:LYS:CB	2.92	0.41
1:K:227:PRO:CB	1:K:384:VAL:CB	2.99	0.41
2:M:189:VAL:O	2:M:217:SER:HA	2.20	0.41
3:O:48:GLU:O	3:O:51:LYS:CA	2.67	0.41
1:C:202:ASN:O	1:C:435:LEU:HA	2.20	0.41
3:O:134:ALA:O	4:P:16:ALA:HB2	2.19	0.41
1:B:221:GLY:O	1:B:366:GLY:HA2	2.21	0.41
1:C:25:TYR:N	2:F:66:LEU:N	2.31	0.41
1:C:133:MET:O	1:C:148:LEU:HA	2.20	0.41
1:C:255:CYS:HA	1:C:290:ASN:CB	2.49	0.41
3:G:43:VAL:O	3:G:45:GLU:N	2.54	0.41
2:N:189:VAL:O	2:N:217:SER:HA	2.20	0.41
3:O:11:LEU:O	3:O:12:LEU:C	2.64	0.41
1:B:133:MET:O	1:B:148:LEU:HA	2.20	0.41
2:D:149:LYS:CB	2:D:333:THR:HA	2.51	0.41
3:G:3:GLN:O	3:G:4:VAL:C	2.63	0.41
3:G:149:LYS:O	3:G:150:ILE:C	2.63	0.41
1:K:133:MET:O	1:K:148:LEU:HA	2.21	0.41
1:C:419:PHE:O	1:C:496:GLN:C	2.56	0.41
2:F:149:LYS:CB	2:F:333:THR:HA	2.51	0.41
3:O:20:LEU:O	3:O:21:ALA:C	2.64	0.41
1:A:56:SER:CB	2:F:30:GLY:H	2.34	0.41
1:B:141:PHE:O	1:B:143:PHE:O	2.39	0.41
1:C:11:GLY:CA	2:E:50:VAL:N	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:133:MET:O	1:I:148:LEU:HA	2.21	0.41
1:K:221:GLY:O	1:K:366:GLY:HA2	2.21	0.41
1:B:24:MET:CA	2:E:66:LEU:C	2.92	0.41
1:K:141:PHE:O	1:K:143:PHE:O	2.39	0.41
1:A:227:PRO:CB	1:A:384:VAL:CB	2.99	0.41
1:C:141:PHE:O	1:C:143:PHE:O	2.39	0.41
1:C:221:GLY:O	1:C:366:GLY:HA2	2.21	0.41
2:F:149:LYS:C	2:F:334:GLU:H	2.14	0.41
1:I:227:PRO:CB	1:I:384:VAL:CB	2.99	0.41
1:J:221:GLY:O	1:J:366:GLY:HA2	2.20	0.41
2:M:149:LYS:C	2:M:334:GLU:H	2.14	0.41
2:N:149:LYS:CB	2:N:333:THR:HA	2.51	0.41
3:O:43:VAL:O	3:O:45:GLU:N	2.54	0.41
1:C:81:ASN:HA	1:C:282:MET:O	2.21	0.41
3:G:48:GLU:O	3:G:51:LYS:CA	2.68	0.41
3:G:146:ARG:O	3:G:149:LYS:CB	2.68	0.41
1:J:208:GLY:O	1:J:507:CYS:N	2.53	0.41
2:L:359:SER:CB	2:L:362:MET:N	2.83	0.41
1:C:227:PRO:CB	1:C:384:VAL:CB	2.99	0.40
3:G:174:ALA:O	3:G:175:GLN:O	2.36	0.40
1:I:221:GLY:O	1:I:366:GLY:HA2	2.21	0.40
1:A:226:ILE:O	1:A:384:VAL:N	2.55	0.40
1:I:226:ILE:O	1:I:384:VAL:N	2.55	0.40
2:M:149:LYS:CB	2:M:333:THR:HA	2.51	0.40
3:O:146:ARG:O	3:O:149:LYS:CB	2.69	0.40
1:I:24:MET:CB	2:L:66:LEU:CA	2.99	0.40
1:J:141:PHE:O	1:J:143:PHE:O	2.39	0.40
1:K:27:ILE:HA	1:K:71:LEU:N	2.33	0.40
2:L:149:LYS:CB	2:L:333:THR:HA	2.51	0.40
2:N:258:THR:HA	2:N:259:ASP:HA	1.85	0.40
3:O:149:LYS:O	3:O:150:ILE:C	2.64	0.40
1:A:259:GLY:O	2:F:296:GLU:O	2.39	0.40
1:C:226:ILE:O	1:C:384:VAL:N	2.55	0.40
1:I:141:PHE:O	1:I:143:PHE:O	2.39	0.40
1:J:226:ILE:O	1:J:384:VAL:N	2.55	0.40
1:J:227:PRO:CB	1:J:384:VAL:CB	2.99	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:6:ILE:CB	2:M:24:ALA:O[5_555]	1.43	0.77
1:J:1:MET:N	2:M:9:THR:CA[5_555]	1.83	0.37
1:J:5:VAL:CA	2:M:24:ALA:CB[5_555]	1.92	0.28

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	557/578 (96%)	488 (88%)	52 (9%)	17 (3%)	3	21
1	B	557/578 (96%)	493 (88%)	48 (9%)	16 (3%)	3	23
1	C	557/578 (96%)	491 (88%)	48 (9%)	18 (3%)	3	21
1	I	557/578 (96%)	491 (88%)	50 (9%)	16 (3%)	3	23
1	J	557/578 (96%)	492 (88%)	48 (9%)	17 (3%)	3	21
1	K	557/578 (96%)	493 (88%)	47 (8%)	17 (3%)	3	21
2	D	446/478 (93%)	420 (94%)	17 (4%)	9 (2%)	6	31
2	E	446/478 (93%)	421 (94%)	16 (4%)	9 (2%)	6	31
2	F	446/478 (93%)	421 (94%)	16 (4%)	9 (2%)	6	31
2	L	446/478 (93%)	419 (94%)	17 (4%)	10 (2%)	5	28
2	M	446/478 (93%)	422 (95%)	15 (3%)	9 (2%)	6	31
2	N	446/478 (93%)	422 (95%)	15 (3%)	9 (2%)	6	31
3	G	125/223 (56%)	76 (61%)	20 (16%)	29 (23%)	0	1
3	O	125/223 (56%)	76 (61%)	20 (16%)	29 (23%)	0	1
4	H	102/104 (98%)	87 (85%)	9 (9%)	6 (6%)	1	13
4	P	102/104 (98%)	86 (84%)	11 (11%)	5 (5%)	1	16
All	All	6472/6990 (93%)	5798 (90%)	449 (7%)	225 (4%)	3	20

All (225) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	PRO
1	A	19	MET
1	A	53	GLU
1	A	143	PHE
1	A	227	PRO
1	A	256	GLY
1	A	260	ASN
1	A	325	ASP
1	A	394	PRO
1	A	395	VAL
1	A	558	GLU
1	B	12	PRO
1	B	19	MET
1	B	53	GLU
1	B	143	PHE
1	B	227	PRO
1	B	256	GLY
1	B	260	ASN
1	B	325	ASP
1	B	394	PRO
1	B	395	VAL
1	B	558	GLU
1	C	12	PRO
1	C	19	MET
1	C	53	GLU
1	C	143	PHE
1	C	227	PRO
1	C	256	GLY
1	C	260	ASN
1	C	325	ASP
1	C	394	PRO
1	C	395	VAL
1	C	431	PHE
1	C	558	GLU
2	D	52	GLU
2	D	79	VAL
2	D	316	MET
2	D	356	PRO
2	D	427	GLN
2	E	52	GLU
2	E	79	VAL
2	E	316	MET
2	E	356	PRO

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Mol	Chain	Res	Type
2	E	427	GLN
2	F	52	GLU
2	F	316	MET
2	F	356	PRO
2	F	427	GLN
3	G	3	GLN
3	G	4	VAL
3	G	43	VAL
3	G	47	MET
3	G	48	GLU
3	G	140	VAL
3	G	149	LYS
3	G	152	GLU
3	G	161	VAL
3	G	172	ILE
3	G	174	ALA
4	H	63	MET
4	H	66	ARG
4	H	75	ALA
4	H	85	ASP
4	H	100	PHE
1	I	12	PRO
1	I	19	MET
1	I	53	GLU
1	I	143	PHE
1	I	227	PRO
1	I	256	GLY
1	I	260	ASN
1	I	325	ASP
1	I	394	PRO
1	I	395	VAL
1	I	558	GLU
1	J	12	PRO
1	J	19	MET
1	J	53	GLU
1	J	143	PHE
1	J	227	PRO
1	J	256	GLY
1	J	260	ASN
1	J	325	ASP
1	J	394	PRO
1	J	395	VAL

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Mol	Chain	Res	Type
1	J	430	LEU
1	J	558	GLU
1	K	12	PRO
1	K	19	MET
1	K	53	GLU
1	K	143	PHE
1	K	227	PRO
1	K	256	GLY
1	K	260	ASN
1	K	325	ASP
1	K	394	PRO
1	K	395	VAL
1	K	558	GLU
2	L	52	GLU
2	L	79	VAL
2	L	81	ARG
2	L	316	MET
2	L	356	PRO
2	L	427	GLN
2	M	52	GLU
2	M	316	MET
2	M	356	PRO
2	M	427	GLN
2	N	52	GLU
2	N	316	MET
2	N	356	PRO
2	N	427	GLN
3	O	3	GLN
3	O	4	VAL
3	O	43	VAL
3	O	47	MET
3	O	48	GLU
3	O	140	VAL
3	O	149	LYS
3	O	152	GLU
3	O	161	VAL
3	O	172	ILE
3	O	174	ALA
3	O	200	LYS
4	P	63	MET
4	P	86	VAL
4	P	87	GLU

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Mol	Chain	Res	Type
4	P	100	PHE
1	A	88	GLN
1	A	255	CYS
1	B	88	GLN
1	B	255	CYS
1	C	88	GLN
1	C	199	LEU
1	C	255	CYS
2	D	26	ASP
2	D	428	GLN
2	E	26	ASP
2	E	428	GLN
2	F	26	ASP
2	F	428	GLN
3	G	2	SER
3	G	6	PRO
3	G	150	ILE
3	G	151	GLY
3	G	185	GLN
3	G	200	LYS
4	H	64	ARG
1	I	88	GLN
1	I	255	CYS
1	J	88	GLN
1	J	255	CYS
1	K	71	LEU
1	K	88	GLN
1	K	255	CYS
2	L	26	ASP
2	L	428	GLN
2	M	26	ASP
2	M	79	VAL
2	M	428	GLN
2	N	26	ASP
2	N	428	GLN
3	O	2	SER
3	O	6	PRO
3	O	13	GLN
3	O	150	ILE
3	O	151	GLY
3	O	185	GLN
1	A	109	HIS

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Mol	Chain	Res	Type
1	B	109	HIS
1	C	109	HIS
3	G	13	GLN
3	G	139	ARG
3	G	155	LYS
3	G	162	ASN
3	G	165	GLU
1	I	109	HIS
1	J	109	HIS
1	K	109	HIS
3	O	139	ARG
3	O	155	LYS
3	O	162	ASN
3	O	165	GLU
1	A	71	LEU
3	G	45	GLU
3	G	186	ARG
2	N	79	VAL
3	O	45	GLU
3	O	137	LEU
3	O	186	ARG
4	P	85	ASP
1	A	374	GLU
1	B	374	GLU
1	C	374	GLU
2	D	317	PRO
2	E	317	PRO
2	F	317	PRO
3	G	53	LEU
3	G	137	LEU
3	G	197	ILE
1	I	374	GLU
1	J	374	GLU
1	K	374	GLU
2	L	317	PRO
2	M	317	PRO
2	N	317	PRO
3	O	53	LEU
2	F	79	VAL
3	O	197	ILE
2	D	355	LEU
2	E	355	LEU

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Mol	Chain	Res	Type
2	F	355	LEU
2	L	355	LEU
2	M	355	LEU
2	N	355	LEU
1	A	388	GLY
1	B	388	GLY
1	C	388	GLY
3	G	179	ILE
1	I	388	GLY
1	J	388	GLY
1	K	388	GLY
3	O	179	ILE
3	G	168	VAL
3	O	168	VAL

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	561/578 (97%)	2.40	274 (48%) 0 2	168, 196, 399, 399	0
1	B	561/578 (97%)	1.37	137 (24%) 2 6	97, 98, 159, 159	0
1	C	561/578 (97%)	2.73	320 (57%) 0 1	208, 224, 414, 414	0
1	I	561/578 (97%)	2.73	312 (55%) 0 1	198, 211, 393, 393	0
1	J	561/578 (97%)	1.65	178 (31%) 1 4	90, 94, 161, 161	0
1	K	561/578 (97%)	2.99	343 (61%) 0 1	207, 219, 403, 403	0
2	D	450/478 (94%)	1.92	171 (38%) 1 3	138, 159, 262, 262	0
2	E	450/478 (94%)	2.05	179 (39%) 1 2	157, 157, 176, 176	0
2	F	450/478 (94%)	2.43	219 (48%) 0 2	155, 241, 275, 275	0
2	L	450/478 (94%)	2.19	189 (42%) 0 2	145, 154, 244, 244	0
2	M	450/478 (94%)	2.50	209 (46%) 0 2	151, 151, 191, 191	0
2	N	450/478 (94%)	2.60	240 (53%) 0 2	181, 256, 256, 256	0
3	G	129/223 (57%)	1.01	24 (18%) 3 8	71, 85, 85, 85	0
3	O	129/223 (57%)	0.69	18 (13%) 6 12	89, 89, 105, 105	0
4	H	104/104 (100%)	2.97	54 (51%) 0 2	159, 185, 185, 185	0
4	P	104/104 (100%)	2.32	40 (38%) 1 3	159, 167, 167, 167	0
All	All	6532/6990 (93%)	2.25	2907 (44%) 0 2	71, 176, 399, 414	0

All (2907) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	24	SER	34.7
1	I	78	GLY	29.0
2	M	302	GLU	25.7
2	L	121	PRO	22.1
2	L	122	VAL	21.2

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Mol	Chain	Res	Type	RSRZ
1	K	345	PRO	19.3
2	L	77	GLU	18.7
2	M	300	VAL	18.5
2	M	363	ASN	18.3
4	P	85	ASP	17.9
1	A	194	PRO	17.5
1	K	576	ALA	17.4
1	I	77	PRO	16.8
2	M	301	VAL	16.4
2	M	360	ARG	15.9
4	H	76	GLY	15.0
2	M	299	GLY	15.0
2	D	121	PRO	14.9
1	I	145	HIS	14.6
2	D	102	GLY	14.3
2	M	121	PRO	14.2
1	K	293	ASN	14.1
1	I	296	VAL	14.0
1	K	297	ALA	13.9
1	A	192	ALA	13.8
1	I	232	SER	13.5
2	L	20	PHE	13.1
2	M	122	VAL	12.9
2	E	150	LEU	12.9
1	K	349	GLY	12.9
1	C	292	SER	12.8
1	B	471	VAL	12.7
1	I	12	PRO	12.7
2	N	80	ALA	12.7
1	K	240	SER	12.6
1	C	165	GLU	12.6
1	K	195	VAL	12.4
2	M	365	GLY	12.2
1	J	471	VAL	12.2
4	H	38	GLU	12.1
1	K	394	PRO	12.1
2	E	172	THR	12.0
1	C	194	PRO	12.0
1	A	12	PRO	11.8
1	A	554	VAL	11.8
2	N	118	PRO	11.8
1	I	63	PRO	11.8

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Mol	Chain	Res	Type	RSRZ
1	A	201	PRO	11.7
1	B	387	PRO	11.7
2	E	120	ASN	11.7
1	J	266	LEU	11.6
1	K	194	PRO	11.5
1	A	193	ARG	11.5
1	C	1	MET	11.3
2	N	66	LEU	11.3
1	A	128	GLU	11.2
1	I	84	TYR	11.2
1	K	190	ARG	11.2
2	F	224	ALA	11.2
2	N	419	GLU	11.1
2	N	121	PRO	11.1
2	N	191	PHE	11.1
4	P	75	ALA	11.0
2	F	225	ASP	11.0
1	K	140	GLU	11.0
1	A	14	VAL	11.0
2	D	75	LEU	11.0
2	M	117	LEU	10.8
1	K	141	PHE	10.7
2	M	168	ALA	10.6
1	C	47	ALA	10.6
1	K	346	ALA	10.5
1	C	85	ASP	10.5
1	J	12	PRO	10.4
1	I	22	ALA	10.4
2	E	165	ALA	10.4
2	M	383	TYR	10.3
2	E	335	GLY	10.3
1	K	77	PRO	10.3
1	C	502	GLU	10.3
1	K	193	ARG	10.2
1	K	575	LYS	10.2
2	E	463	TYR	10.0
1	K	393	GLU	10.0
2	N	137	THR	10.0
1	C	36	VAL	10.0
1	I	424	TRP	9.9
1	A	167	THR	9.9
1	K	108	VAL	9.9

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Mol	Chain	Res	Type	RSRZ
2	F	221	LEU	9.9
1	C	270	PRO	9.8
2	E	119	LEU	9.8
2	M	359	SER	9.7
2	F	401	GLU	9.6
1	B	12	PRO	9.6
2	D	67	ASP	9.5
1	C	151	PRO	9.5
2	L	21	VAL	9.5
1	C	73	VAL	9.4
4	H	25	SER	9.3
2	M	362	MET	9.3
1	K	197	ARG	9.3
1	K	192	ALA	9.3
4	P	69	PRO	9.3
1	I	234	LYS	9.3
2	L	75	LEU	9.3
4	H	23	ALA	9.2
2	N	117	LEU	9.2
1	K	324	ALA	9.1
3	G	54	ASP	9.1
1	K	387	PRO	9.1
4	H	98	ILE	9.1
1	B	388	GLY	9.0
1	I	164	GLY	9.0
2	E	168	ALA	9.0
1	C	376	GLY	9.0
1	I	499	ALA	8.9
2	F	421	PHE	8.9
2	N	140	VAL	8.8
2	D	27	LEU	8.8
1	I	79	MET	8.8
2	F	86	LYS	8.7
2	N	359	SER	8.7
2	L	15	SER	8.7
2	F	201	LEU	8.7
2	M	80	ALA	8.7
2	D	450	GLU	8.7
4	H	29	ALA	8.6
1	A	173	VAL	8.6
2	F	141	MET	8.6
2	L	40	GLY	8.6

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Mol	Chain	Res	Type	RSRZ
1	C	445	GLU	8.5
1	K	142	GLY	8.5
2	F	402	ASP	8.5
2	N	79	VAL	8.5
2	E	173	VAL	8.4
1	K	451	ARG	8.4
2	L	302	GLU	8.4
2	N	122	VAL	8.4
1	A	140	GLU	8.3
1	I	1	MET	8.3
1	I	45	ASP	8.3
2	M	361	LEU	8.3
1	C	150	PRO	8.3
4	P	104	LEU	8.3
2	D	77	GLU	8.3
2	M	141	MET	8.2
2	N	141	MET	8.2
1	C	190	ARG	8.2
2	E	122	VAL	8.2
1	K	298	ALA	8.2
1	K	395	VAL	8.2
1	C	237	THR	8.2
2	F	21	VAL	8.2
2	N	193	ALA	8.2
1	K	198	LYS	8.1
2	D	302	GLU	8.1
2	E	141	MET	8.1
2	N	205	ILE	8.1
1	I	193	ARG	8.1
2	L	229	ILE	8.1
1	C	193	ARG	8.1
1	K	57	GLY	8.1
1	K	74	GLU	8.1
2	F	278	PRO	8.1
2	N	67	ASP	8.0
4	H	16	ALA	8.0
1	I	416	ARG	8.0
2	F	122	VAL	8.0
2	D	360	ARG	8.0
1	A	559	PHE	8.0
1	I	237	THR	7.9
2	D	117	LEU	7.9

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Mol	Chain	Res	Type	RSRZ
2	L	28	ALA	7.9
1	A	166	TYR	7.9
2	M	169	ARG	7.9
2	D	118	PRO	7.9
1	A	219	ALA	7.9
1	J	388	GLY	7.9
1	I	26	ASP	7.8
1	A	181	LEU	7.8
1	C	28	CYS	7.8
1	I	233	GLY	7.8
1	K	78	GLY	7.8
1	K	201	PRO	7.8
1	I	291	THR	7.8
2	L	137	THR	7.8
1	I	372	GLY	7.8
2	F	297	ARG	7.8
1	I	224	ALA	7.8
1	A	61	GLY	7.8
1	I	146	LYS	7.8
2	D	122	VAL	7.7
1	A	129	VAL	7.7
2	F	137	THR	7.7
2	F	24	ALA	7.7
1	C	243	LYS	7.6
1	I	55	THR	7.6
1	A	13	ALA	7.6
4	P	78	LYS	7.6
1	C	379	THR	7.6
1	I	138	VAL	7.6
1	C	549	GLY	7.6
2	M	11	ILE	7.5
1	K	538	GLU	7.5
1	A	200	ASP	7.5
1	J	345	PRO	7.5
1	A	296	VAL	7.5
2	M	402	ASP	7.5
2	M	235	PRO	7.5
1	C	192	ALA	7.5
1	C	274	ASP	7.5
1	A	155	GLY	7.4
1	A	345	PRO	7.4
2	L	56	VAL	7.4

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Mol	Chain	Res	Type	RSRZ
1	I	218	VAL	7.4
2	F	216	ARG	7.4
1	C	337	ILE	7.4
2	M	142	ASN	7.4
2	E	118	PRO	7.3
2	M	70	THR	7.3
1	J	478	ASP	7.3
2	M	171	ALA	7.3
2	D	101	ASP	7.3
1	C	369	ILE	7.3
2	E	164	ALA	7.3
2	M	225	ASP	7.2
2	M	408	ASP	7.2
4	P	98	ILE	7.2
1	A	218	VAL	7.2
1	C	112	ASP	7.2
2	N	192	ALA	7.2
1	C	169	GLU	7.2
1	J	416	ARG	7.2
1	J	493	ASP	7.1
4	H	101	ASP	7.1
2	N	334	GLU	7.1
1	A	210	ARG	7.1
2	N	358	LEU	7.0
1	C	273	THR	7.0
1	I	180	GLU	7.0
2	M	438	ILE	7.0
2	D	26	ASP	7.0
1	C	345	PRO	7.0
1	J	263	THR	7.0
1	K	510	LYS	7.0
1	C	10	ALA	7.0
1	K	382	GLY	7.0
1	A	134	VAL	7.0
1	I	140	GLU	7.0
1	J	2	ILE	6.9
1	K	383	ALA	6.9
1	B	194	PRO	6.9
1	I	402	ILE	6.9
2	N	78	ASP	6.9
2	M	86	LYS	6.9
1	K	256	GLY	6.9

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Mol	Chain	Res	Type	RSRZ
2	L	417	ALA	6.9
1	J	267	VAL	6.9
2	F	295	TYR	6.8
2	E	326	PRO	6.8
1	C	197	ARG	6.8
1	C	540	LEU	6.8
1	J	494	PHE	6.8
2	L	346	LYS	6.8
4	H	53	PRO	6.8
1	A	147	ILE	6.8
4	H	30	GLN	6.8
1	C	171	PRO	6.8
2	N	258	THR	6.7
2	L	215	SER	6.7
2	E	193	ALA	6.7
2	N	360	ARG	6.7
2	N	185	GLU	6.7
1	I	400	LEU	6.7
1	C	170	GLU	6.7
1	K	295	PRO	6.7
2	M	224	ALA	6.7
2	M	137	THR	6.7
1	K	416	ARG	6.7
2	N	184	GLU	6.7
1	C	531	LYS	6.7
1	I	163	ALA	6.6
2	L	260	MET	6.6
2	N	278	PRO	6.6
4	P	15	LEU	6.6
1	C	143	PHE	6.6
2	M	243	GLU	6.6
2	L	301	VAL	6.6
1	K	292	SER	6.5
2	L	97	GLY	6.5
1	A	45	ASP	6.5
1	A	150	PRO	6.5
1	A	422	ILE	6.5
2	D	371	THR	6.5
1	J	23	ARG	6.5
1	I	343	GLU	6.5
1	K	550	ARG	6.5
1	I	290	ASN	6.5

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Mol	Chain	Res	Type	RSRZ
1	K	91	LEU	6.5
1	K	360	ALA	6.5
1	A	403	VAL	6.5
1	C	368	VAL	6.5
1	K	251	VAL	6.5
1	B	367	LYS	6.5
1	A	50	GLN	6.5
2	E	174	ARG	6.5
2	F	119	LEU	6.4
1	K	117	TRP	6.4
1	I	371	LEU	6.4
2	D	119	LEU	6.4
2	N	312	PRO	6.4
2	E	325	ILE	6.4
2	M	201	LEU	6.4
2	M	442	LEU	6.4
2	N	261	THR	6.4
1	A	346	ALA	6.4
1	K	551	ALA	6.4
1	B	110	ALA	6.3
1	B	192	ALA	6.3
2	N	341	ARG	6.3
1	C	389	GLY	6.3
2	L	300	VAL	6.3
2	N	83	GLY	6.3
2	F	298	ALA	6.3
1	J	495	LEU	6.3
2	L	80	ALA	6.3
1	A	395	VAL	6.3
2	F	136	SER	6.3
2	F	365	GLY	6.3
2	F	189	VAL	6.3
2	L	296	GLU	6.3
2	F	274	ARG	6.3
2	F	294	ILE	6.2
1	C	139	PRO	6.2
2	E	449	GLY	6.2
2	F	193	ALA	6.2
1	C	77	PRO	6.2
1	I	54	ASP	6.2
1	K	186	THR	6.2
1	C	545	LEU	6.2

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Mol	Chain	Res	Type	RSRZ
1	C	144	THR	6.2
1	C	532	ARG	6.2
1	J	210	ARG	6.2
1	K	232	SER	6.2
2	N	310	GLN	6.2
1	C	35	LEU	6.2
1	I	13	ALA	6.1
1	I	118	ALA	6.1
1	K	237	THR	6.1
1	J	3	GLN	6.1
1	I	365	ALA	6.1
2	F	187	PHE	6.1
4	P	64	ARG	6.1
2	M	172	THR	6.1
1	J	387	PRO	6.1
2	N	161	ASN	6.1
2	L	29	TYR	6.1
2	L	52	GLU	6.1
1	I	472	GLY	6.1
4	P	89	TYR	6.1
2	F	173	VAL	6.1
1	A	209	MET	6.0
1	C	37	GLY	6.0
1	I	85	ASP	6.0
2	F	215	SER	6.0
2	F	332	ILE	6.0
1	C	275	PRO	6.0
1	J	474	ASP	6.0
4	P	82	GLN	6.0
2	N	335	GLY	6.0
1	I	119	TRP	6.0
4	P	8	GLU	6.0
2	N	160	ALA	6.0
1	B	112	ASP	5.9
1	B	237	THR	5.9
2	L	164	ALA	5.9
1	C	86	GLY	5.9
2	L	281	ARG	5.9
1	J	78	GLY	5.9
1	J	116	LYS	5.9
2	N	242	ALA	5.9
1	B	479	ALA	5.9

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Mol	Chain	Res	Type	RSRZ
2	F	121	PRO	5.9
2	N	456	LYS	5.9
1	C	356	ALA	5.9
2	M	118	PRO	5.9
1	B	478	ASP	5.8
1	I	559	PHE	5.8
1	A	251	VAL	5.8
1	B	267	VAL	5.8
2	M	77	GLU	5.8
1	A	349	GLY	5.8
2	L	411	TYR	5.8
2	M	26	ASP	5.8
1	A	117	TRP	5.8
2	F	363	ASN	5.8
1	C	175	LEU	5.8
1	C	46	THR	5.8
2	L	421	PHE	5.8
1	B	238	GLN	5.8
1	B	499	ALA	5.8
2	M	69	ALA	5.8
2	D	130	PHE	5.7
1	J	507	CYS	5.7
2	E	142	ASN	5.7
2	M	426	GLY	5.7
2	N	429	ASN	5.7
2	F	260	MET	5.7
1	C	375	GLU	5.7
2	L	401	GLU	5.7
1	K	220	MET	5.7
1	A	358	LEU	5.7
2	N	218	VAL	5.7
1	B	270	PRO	5.7
4	P	54	ASP	5.7
2	E	82	LEU	5.7
1	I	147	ILE	5.7
1	C	443	VAL	5.7
1	C	91	LEU	5.7
2	D	80	ALA	5.7
2	L	34	ASP	5.7
1	C	81	ASN	5.6
1	C	359	ALA	5.6
1	K	294	MET	5.6

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Mol	Chain	Res	Type	RSRZ
1	B	109	HIS	5.6
1	C	191	ARG	5.6
2	E	453	ARG	5.6
2	N	164	ALA	5.6
1	I	345	PRO	5.6
1	I	563	PHE	5.6
1	C	258	ARG	5.6
1	C	72	ALA	5.6
2	N	198	GLN	5.6
1	K	47	ALA	5.6
2	N	81	ARG	5.6
2	E	117	LEU	5.6
1	B	507	CYS	5.6
1	I	497	GLN	5.6
1	I	313	PHE	5.6
1	C	166	TYR	5.6
1	K	146	LYS	5.6
1	J	189	VAL	5.5
2	F	165	ALA	5.5
2	N	168	ALA	5.5
1	K	296	VAL	5.5
2	F	287	MET	5.5
2	E	135	ILE	5.5
1	K	314	ARG	5.5
2	N	63	THR	5.5
1	A	359	ALA	5.5
1	I	557	GLU	5.5
1	K	114	GLU	5.5
1	I	190	ARG	5.5
1	C	201	PRO	5.5
1	A	267	VAL	5.5
1	I	197	ARG	5.5
1	K	350	TYR	5.5
2	D	364	ASN	5.5
1	K	76	GLY	5.5
2	L	53	GLU	5.5
2	M	228	THR	5.5
1	J	559	PHE	5.5
2	D	310	GLN	5.5
2	N	402	ASP	5.4
1	C	70	PRO	5.4
1	A	143	PHE	5.4

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Mol	Chain	Res	Type	RSRZ
2	D	345	ARG	5.4
1	C	385	SER	5.4
1	J	472	GLY	5.4
2	D	28	ALA	5.4
4	P	71	LEU	5.4
1	A	77	PRO	5.4
2	N	219	LEU	5.4
2	E	40	GLY	5.4
1	I	127	ASP	5.4
2	F	315	SER	5.4
1	J	311	GLU	5.4
1	K	418	HIS	5.4
1	K	376	GLY	5.4
1	I	473	PRO	5.4
1	K	289	ALA	5.4
2	D	325	ILE	5.3
2	F	16	GLY	5.3
1	A	207	THR	5.3
1	I	144	THR	5.3
1	I	471	VAL	5.3
1	I	316	GLN	5.3
1	C	336	GLU	5.3
1	C	388	GLY	5.3
2	M	28	ALA	5.3
1	B	266	LEU	5.3
1	C	2	ILE	5.3
1	C	334	LEU	5.3
2	M	129	GLN	5.3
2	E	281	ARG	5.3
2	N	202	SER	5.3
4	H	75	ALA	5.3
2	N	82	LEU	5.3
1	J	22	ALA	5.3
2	F	273	ALA	5.3
1	K	519	ILE	5.3
1	I	289	ALA	5.3
2	L	123	ALA	5.3
1	I	165	GLU	5.3
1	K	492	GLU	5.3
1	C	4	GLY	5.2
2	E	315	SER	5.2
2	M	205	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
2	F	310	GLN	5.2
1	B	470	LEU	5.2
1	K	90	PRO	5.2
2	F	28	ALA	5.2
2	F	79	VAL	5.2
1	K	389	GLY	5.2
1	C	393	GLU	5.2
2	N	226	ASP	5.2
1	K	65	VAL	5.2
1	B	111	LEU	5.2
1	B	372	GLY	5.2
2	E	462	TYR	5.2
2	F	186	PRO	5.2
2	N	113	PRO	5.2
1	J	394	PRO	5.2
2	F	277	ILE	5.2
2	N	48	ILE	5.2
2	N	238	ALA	5.2
1	I	293	ASN	5.2
1	K	258	ARG	5.2
1	I	51	VAL	5.2
1	A	142	GLY	5.2
1	K	118	ALA	5.2
1	C	198	LYS	5.1
2	D	452	LYS	5.1
1	I	223	THR	5.1
2	L	160	ALA	5.1
2	F	20	PHE	5.1
2	F	205	ILE	5.1
1	I	194	PRO	5.1
2	D	354	PRO	5.1
1	K	181	LEU	5.1
2	E	28	ALA	5.1
1	A	156	ARG	5.1
1	K	553	TYR	5.1
2	M	146	ARG	5.1
1	A	320	VAL	5.1
1	K	79	MET	5.1
1	A	225	ALA	5.1
2	E	395	LEU	5.1
1	A	114	GLU	5.1
1	C	310	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	229	PRO	5.1
2	M	317	PRO	5.1
2	N	206	GLN	5.1
1	I	370	THR	5.1
1	A	551	ALA	5.0
1	I	38	GLU	5.0
1	I	186	THR	5.0
2	N	297	ARG	5.0
1	K	229	PRO	5.0
1	J	234	LYS	5.0
2	M	314	LEU	5.0
1	B	221	GLY	5.0
1	C	256	GLY	5.0
1	A	291	THR	5.0
1	C	179	THR	5.0
1	I	576	ALA	5.0
1	K	191	ARG	5.0
2	M	7	GLU	5.0
1	A	457	LEU	5.0
1	I	219	ALA	5.0
1	C	220	MET	5.0
3	O	162	ASN	5.0
2	F	63	THR	5.0
4	P	86	VAL	5.0
1	A	424	TRP	5.0
1	K	266	LEU	5.0
2	F	364	ASN	5.0
2	N	115	THR	5.0
1	J	346	ALA	5.0
1	C	29	LYS	5.0
1	C	261	GLU	4.9
1	I	32	GLU	4.9
1	C	475	ALA	4.9
1	I	256	GLY	4.9
1	A	1	MET	4.9
1	I	500	TYR	4.9
2	M	127	PRO	4.9
1	C	398	SER	4.9
1	I	198	LYS	4.9
2	M	143	THR	4.9
1	C	400	LEU	4.9
2	L	336	GLN	4.9

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Mol	Chain	Res	Type	RSRZ
2	N	27	LEU	4.9
1	A	130	ARG	4.9
1	I	474	ASP	4.9
1	K	417	ARG	4.9
2	M	439	ALA	4.9
1	B	464	LEU	4.9
1	J	303	ILE	4.9
2	E	339	LEU	4.9
1	K	469	GLN	4.9
2	E	137	THR	4.9
2	N	18	LEU	4.9
2	N	339	LEU	4.9
2	N	336	GLN	4.9
1	I	201	PRO	4.9
2	E	375	HIS	4.9
1	I	143	PHE	4.9
1	J	238	GLN	4.9
1	I	364	ARG	4.9
2	F	280	ARG	4.9
1	A	180	GLU	4.9
2	M	273	ALA	4.9
2	M	435	SER	4.9
2	E	121	PRO	4.9
1	K	75	LEU	4.9
2	D	88	MET	4.9
1	K	572	GLY	4.9
1	K	85	ASP	4.9
1	A	379	THR	4.9
2	D	222	ASN	4.9
1	B	407	TRP	4.8
1	I	185	HIS	4.8
2	D	240	THR	4.8
2	M	71	THR	4.8
2	F	11	ILE	4.8
2	N	277	ILE	4.8
1	K	261	GLU	4.8
2	F	259	ASP	4.8
2	F	346	LYS	4.8
2	F	89	LEU	4.8
1	I	566	ALA	4.8
1	I	368	VAL	4.8
4	P	11	GLN	4.8

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Mol	Chain	Res	Type	RSRZ
1	I	83	ILE	4.8
1	I	242	ALA	4.8
1	K	143	PHE	4.8
2	F	429	ASN	4.8
1	I	21	GLY	4.8
1	I	31	GLY	4.8
2	M	81	ARG	4.8
1	C	54	ASP	4.8
2	L	278	PRO	4.8
1	K	573	ALA	4.8
2	F	168	ALA	4.8
2	N	142	ASN	4.8
2	D	109	GLU	4.8
1	I	40	ILE	4.8
1	C	3	GLN	4.8
4	H	69	PRO	4.8
2	F	87	GLU	4.8
2	F	296	GLU	4.8
1	A	543	PRO	4.8
1	K	162	PRO	4.8
2	D	427	GLN	4.8
1	A	256	GLY	4.8
1	K	400	LEU	4.8
2	N	12	THR	4.8
1	I	134	VAL	4.8
2	E	421	PHE	4.7
2	F	242	ALA	4.7
1	A	26	ASP	4.7
1	I	183	MET	4.7
1	I	300	GLU	4.7
1	K	145	HIS	4.7
2	M	165	ALA	4.7
2	N	370	LYS	4.7
1	J	58	LEU	4.7
1	K	549	GLY	4.7
2	N	65	GLY	4.7
1	A	319	SER	4.7
2	D	259	ASP	4.7
1	I	379	THR	4.7
4	H	97	THR	4.7
2	N	421	PHE	4.7
1	C	289	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
2	M	15	SER	4.7
2	F	348	ILE	4.7
2	N	432	ILE	4.7
1	A	169	GLU	4.7
2	D	63	THR	4.7
2	F	142	ASN	4.7
2	F	235	PRO	4.7
2	E	310	GLN	4.7
2	E	374	ASP	4.7
1	I	41	ARG	4.7
2	M	453	ARG	4.7
2	M	310	GLN	4.7
1	K	187	TRP	4.7
1	K	385	SER	4.7
2	E	29	TYR	4.7
2	M	249	HIS	4.7
1	K	121	PRO	4.7
2	F	17	PRO	4.7
2	N	329	THR	4.7
2	M	37	ASP	4.7
1	K	442	ASN	4.6
1	I	58	LEU	4.6
2	L	385	ALA	4.6
1	A	187	TRP	4.6
1	A	447	TYR	4.6
1	I	562	TYR	4.6
1	C	68	GLY	4.6
4	H	37	VAL	4.6
1	K	45	ASP	4.6
4	P	9	THR	4.6
1	J	351	PRO	4.6
1	J	395	VAL	4.6
1	C	109	HIS	4.6
1	C	390	ASP	4.6
2	M	240	THR	4.6
1	C	290	ASN	4.6
2	F	222	ASN	4.6
1	A	72	ALA	4.6
2	E	396	VAL	4.6
1	A	546	GLU	4.6
1	A	88	GLN	4.6
1	K	202	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	J	305	VAL	4.6
1	K	183	MET	4.6
1	K	323	MET	4.6
2	E	357	SER	4.6
2	M	229	ILE	4.6
2	D	103	LEU	4.6
2	F	375	HIS	4.6
2	N	15	SER	4.6
2	N	340	SER	4.6
2	L	259	ASP	4.5
1	C	88	GLN	4.5
1	C	360	ALA	4.5
2	L	337	ILE	4.5
4	H	55	PRO	4.5
1	A	116	LYS	4.5
1	C	17	LYS	4.5
2	F	255	VAL	4.5
1	K	128	GLU	4.5
1	K	474	ASP	4.5
1	B	222	GLY	4.5
1	C	217	PRO	4.5
1	C	492	GLU	4.5
1	C	296	VAL	4.5
1	I	87	ILE	4.5
2	D	223	LYS	4.5
2	N	84	VAL	4.5
1	B	204	PRO	4.5
1	B	229	PRO	4.5
2	F	118	PRO	4.5
2	L	12	THR	4.5
1	I	299	ARG	4.5
1	B	195	VAL	4.5
1	J	558	GLU	4.5
4	P	1	MET	4.5
1	K	434	ALA	4.5
2	D	348	ILE	4.5
1	I	297	ALA	4.5
2	E	80	ALA	4.5
1	A	152	ASP	4.5
2	M	401	GLU	4.5
1	K	196	GLN	4.4
2	E	148	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
2	D	301	VAL	4.4
1	K	230	PHE	4.4
1	I	169	GLU	4.4
1	K	502	GLU	4.4
1	I	76	GLY	4.4
2	F	291	LEU	4.4
2	D	332	ILE	4.4
2	L	391	ASP	4.4
1	C	444	ALA	4.4
1	C	78	GLY	4.4
1	C	473	PRO	4.4
1	K	329	ARG	4.4
2	N	423	ILE	4.4
2	F	88	MET	4.4
1	B	199	LEU	4.4
1	J	261	GLU	4.4
1	A	57	GLY	4.4
1	A	165	GLU	4.4
1	I	86	GLY	4.4
1	I	492	GLU	4.4
1	B	473	PRO	4.4
1	A	562	TYR	4.4
1	A	190	ARG	4.4
1	K	109	HIS	4.4
4	P	84	HIS	4.4
1	C	530	ILE	4.4
2	L	32	ILE	4.4
2	M	390	VAL	4.4
3	G	142	ASN	4.4
1	I	91	LEU	4.4
1	C	74	GLU	4.4
1	K	73	VAL	4.4
1	K	311	GLU	4.4
1	K	110	ALA	4.3
2	D	288	TYR	4.3
2	F	83	GLY	4.3
2	L	152	ILE	4.3
1	C	509	MET	4.3
2	N	143	THR	4.3
1	K	325	ASP	4.3
2	F	302	GLU	4.3
2	N	220	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	16	ALA	4.3
1	I	73	VAL	4.3
1	I	82	GLY	4.3
1	B	114	GLU	4.3
1	K	43	ASP	4.3
2	F	336	GLN	4.3
2	D	229	ILE	4.3
1	A	174	VAL	4.3
2	N	136	SER	4.3
1	C	140	GLU	4.3
1	J	206	LEU	4.3
2	M	27	LEU	4.3
2	N	225	ASP	4.3
1	C	482	LEU	4.3
1	K	473	PRO	4.3
2	L	175	PRO	4.3
1	K	144	THR	4.3
2	D	350	PRO	4.3
2	E	252	HIS	4.3
2	D	342	GLU	4.3
2	E	207	GLU	4.3
2	D	64	THR	4.3
1	C	552	ARG	4.3
1	J	211	ILE	4.3
1	I	508	SER	4.3
2	E	356	PRO	4.3
2	F	325	ILE	4.3
1	C	267	VAL	4.3
2	F	366	VAL	4.3
1	I	139	PRO	4.2
1	K	351	PRO	4.2
1	K	173	VAL	4.2
2	N	224	ALA	4.2
1	A	91	LEU	4.2
1	A	494	PHE	4.2
1	C	71	LEU	4.2
1	J	349	GLY	4.2
1	C	394	PRO	4.2
1	I	339	SER	4.2
2	L	49	GLU	4.2
2	L	156	SER	4.2
1	C	510	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	K	291	THR	4.2
2	D	289	THR	4.2
2	F	261	THR	4.2
1	K	497	GLN	4.2
2	F	354	PRO	4.2
2	E	88	MET	4.2
4	H	5	ALA	4.2
1	C	277	THR	4.2
1	B	210	ARG	4.2
1	C	90	PRO	4.2
1	K	539	ILE	4.2
4	H	4	ILE	4.2
2	N	462	TYR	4.2
1	B	11	GLY	4.2
1	I	136	GLY	4.2
1	I	196	GLN	4.2
1	J	327	THR	4.2
2	D	228	THR	4.2
2	F	143	THR	4.2
1	C	448	PRO	4.2
1	C	16	ALA	4.2
2	E	83	GLY	4.2
2	F	299	GLY	4.2
1	B	9	ILE	4.2
1	K	213	ASP	4.2
2	N	165	ALA	4.2
2	L	142	ASN	4.2
1	A	375	GLU	4.2
2	D	38	GLY	4.2
2	M	128	GLU	4.2
2	F	359	SER	4.2
1	A	186	THR	4.2
2	E	12	THR	4.2
2	E	56	VAL	4.2
1	C	229	PRO	4.2
2	L	224	ALA	4.2
1	I	348	GLU	4.1
1	K	164	GLY	4.1
2	E	440	TRP	4.1
2	F	244	TYR	4.1
2	D	131	ILE	4.1
1	B	234	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
2	M	198	GLN	4.1
1	C	205	PHE	4.1
2	N	289	THR	4.1
2	N	324	PRO	4.1
1	K	348	GLU	4.1
2	L	339	LEU	4.1
2	N	422	PHE	4.1
2	F	175	PRO	4.1
1	C	13	ALA	4.1
2	D	446	LEU	4.1
2	N	68	LEU	4.1
1	B	108	VAL	4.1
2	N	366	VAL	4.1
1	I	19	MET	4.1
1	K	459	GLN	4.1
2	D	315	SER	4.1
1	I	321	ALA	4.1
1	A	327	THR	4.1
1	J	435	LEU	4.1
2	F	22	GLU	4.1
2	N	276	GLU	4.1
2	L	120	ASN	4.1
1	J	434	ALA	4.1
1	J	473	PRO	4.1
2	E	136	SER	4.1
1	J	400	LEU	4.1
1	I	536	ILE	4.1
3	G	44	ARG	4.1
1	C	493	ASP	4.1
2	E	362	MET	4.1
1	I	246	ASN	4.1
1	K	520	LEU	4.1
2	F	378	VAL	4.1
2	L	7	GLU	4.1
1	A	555	SER	4.1
2	M	409	ARG	4.1
1	C	320	VAL	4.1
4	P	97	THR	4.1
1	A	74	GLU	4.0
1	C	257	GLU	4.0
2	D	53	GLU	4.0
1	J	77	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	K	150	PRO	4.0
1	C	238	GLN	4.0
1	A	552	ARG	4.0
2	D	431	SER	4.0
1	J	207	THR	4.0
1	A	293	ASN	4.0
1	A	442	ASN	4.0
1	C	425	ASN	4.0
1	K	425	ASN	4.0
1	A	51	VAL	4.0
2	F	140	VAL	4.0
1	A	273	THR	4.0
1	C	188	PRO	4.0
2	F	226	ASP	4.0
1	I	376	GLY	4.0
1	K	68	GLY	4.0
1	A	20	LEU	4.0
2	L	27	LEU	4.0
2	L	371	THR	4.0
1	B	242	ALA	4.0
1	K	87	ILE	4.0
1	I	171	PRO	4.0
1	I	417	ARG	4.0
1	A	376	GLY	4.0
1	B	278	GLY	4.0
1	I	409	LEU	4.0
1	C	399	THR	4.0
1	C	300	GLU	4.0
1	J	451	ARG	4.0
1	J	134	VAL	4.0
1	C	183	MET	4.0
2	F	34	ASP	4.0
3	O	54	ASP	4.0
1	A	553	TYR	4.0
2	N	463	TYR	4.0
1	C	535	SER	4.0
2	N	435	SER	4.0
2	D	439	ALA	4.0
2	M	242	ALA	4.0
1	A	154	ARG	4.0
1	A	149	VAL	4.0
1	A	172	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	471	VAL	4.0
1	J	237	THR	4.0
1	K	471	VAL	4.0
2	D	445	MET	4.0
4	P	79	GLU	4.0
1	I	148	LEU	4.0
1	K	37	GLY	4.0
2	M	404	LEU	4.0
2	E	132	GLN	4.0
2	E	336	GLN	4.0
2	E	348	ILE	4.0
2	E	55	ALA	4.0
1	I	141	PHE	4.0
1	K	342	GLU	3.9
2	M	209	GLU	3.9
2	N	147	GLY	3.9
1	B	7	GLN	3.9
2	L	57	ILE	3.9
1	J	301	ALA	3.9
2	F	188	ALA	3.9
4	H	39	ARG	3.9
1	I	522	PHE	3.9
1	A	458	LEU	3.9
3	G	53	LEU	3.9
1	I	203	THR	3.9
1	K	271	GLU	3.9
2	L	400	GLY	3.9
2	N	28	ALA	3.9
1	I	172	VAL	3.9
1	I	443	VAL	3.9
1	K	172	VAL	3.9
3	G	162	ASN	3.9
1	A	577	LEU	3.9
1	I	150	PRO	3.9
1	K	457	LEU	3.9
2	D	447	PRO	3.9
2	L	104	PRO	3.9
2	E	22	GLU	3.9
1	K	72	ALA	3.9
1	K	242	ALA	3.9
2	L	124	ARG	3.9
2	L	19	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
2	L	412	LEU	3.9
2	N	412	LEU	3.9
2	D	175	PRO	3.9
1	K	367	LYS	3.9
2	E	86	LYS	3.9
2	M	25	LYS	3.9
2	F	10	GLY	3.9
2	F	347	GLY	3.9
1	C	268	GLU	3.9
1	A	515	ILE	3.9
2	D	48	ILE	3.9
2	N	383	TYR	3.9
1	A	214	VAL	3.9
2	D	385	ALA	3.9
2	N	204	PHE	3.9
1	I	39	ILE	3.9
1	A	235	THR	3.9
1	K	470	LEU	3.9
4	P	16	ALA	3.9
1	J	194	PRO	3.9
2	M	175	PRO	3.9
2	E	331	TYR	3.9
2	M	252	HIS	3.9
2	M	21	VAL	3.9
3	G	43	VAL	3.9
1	A	146	LYS	3.9
1	K	255	CYS	3.9
1	K	270	PRO	3.9
2	M	83	GLY	3.9
2	N	282	GLY	3.9
1	A	232	SER	3.9
1	C	58	LEU	3.9
1	K	430	LEU	3.9
2	L	280	ARG	3.9
2	L	382	LEU	3.9
2	N	76	VAL	3.9
2	E	329	THR	3.8
2	N	228	THR	3.8
2	D	448	GLN	3.8
1	A	151	PRO	3.8
1	A	306	GLY	3.8
1	K	241	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
2	F	117	LEU	3.8
3	O	19	ARG	3.8
1	A	486	VAL	3.8
1	C	251	VAL	3.8
1	K	267	VAL	3.8
1	B	311	GLU	3.8
1	I	538	GLU	3.8
2	D	23	ASN	3.8
2	N	315	SER	3.8
1	K	432	THR	3.8
2	F	197	THR	3.8
1	C	142	GLY	3.8
1	I	28	CYS	3.8
1	K	86	GLY	3.8
3	G	204	ARG	3.8
4	H	52	LEU	3.8
1	C	185	HIS	3.8
1	K	60	VAL	3.8
1	I	510	LYS	3.8
1	K	246	ASN	3.8
1	C	187	TRP	3.8
1	I	162	PRO	3.8
1	I	560	PRO	3.8
1	B	198	LYS	3.8
2	F	264	CYS	3.8
2	D	262	ASN	3.8
1	B	326	SER	3.8
1	C	291	THR	3.8
1	J	399	THR	3.8
1	C	222	GLY	3.8
2	E	204	PHE	3.8
2	F	172	THR	3.8
3	G	143	THR	3.8
2	D	51	SER	3.8
1	A	307	VAL	3.8
1	C	137	THR	3.8
1	I	403	VAL	3.8
2	D	204	PHE	3.8
2	F	204	PHE	3.8
2	M	346	LYS	3.8
1	A	356	ALA	3.8
1	C	45	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	K	228	GLY	3.7
1	I	66	SER	3.7
1	J	14	VAL	3.7
2	E	21	VAL	3.7
1	K	407	TRP	3.7
2	E	194	MET	3.7
2	F	331	TYR	3.7
2	D	30	GLY	3.7
2	L	194	MET	3.7
1	I	412	SER	3.7
2	E	309	THR	3.7
1	A	231	GLY	3.7
1	C	82	GLY	3.7
1	C	486	VAL	3.7
1	K	231	GLY	3.7
2	E	30	GLY	3.7
2	F	145	VAL	3.7
1	B	139	PRO	3.7
1	I	387	PRO	3.7
2	N	17	PRO	3.7
1	K	88	GLN	3.7
1	A	350	TYR	3.7
1	A	223	THR	3.7
2	L	223	LYS	3.7
2	E	378	VAL	3.7
2	M	56	VAL	3.7
2	E	243	GLU	3.7
2	M	60	PHE	3.7
1	B	295	PRO	3.7
1	I	446	ASP	3.7
1	J	446	ASP	3.7
2	N	186	PRO	3.7
1	A	290	ASN	3.7
2	F	436	LEU	3.7
2	F	74	SER	3.7
2	L	96	ILE	3.7
2	N	126	LYS	3.7
1	K	364	ARG	3.7
1	K	269	PHE	3.7
2	N	194	MET	3.7
2	D	22	GLU	3.7
2	E	127	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
2	N	151	PRO	3.7
1	I	135	LEU	3.7
1	K	493	ASP	3.7
2	E	416	ASP	3.7
2	L	416	ASP	3.7
1	I	187	TRP	3.7
2	L	48	ILE	3.7
2	D	188	ALA	3.7
2	M	164	ALA	3.7
1	I	182	LYS	3.7
1	A	144	THR	3.7
1	C	223	THR	3.7
1	C	108	VAL	3.7
1	C	546	GLU	3.7
1	A	112	ASP	3.7
1	I	312	TYR	3.7
4	H	11	GLN	3.7
1	B	230	PHE	3.7
2	M	366	VAL	3.7
2	M	12	THR	3.7
1	I	44	GLY	3.7
1	I	70	PRO	3.7
1	K	171	PRO	3.7
2	D	61	GLU	3.7
2	D	205	ILE	3.7
2	L	232	ILE	3.7
2	M	463	TYR	3.7
2	F	31	ALA	3.7
2	F	123	ALA	3.7
1	J	286	VAL	3.6
1	I	392	SER	3.6
1	I	137	THR	3.6
1	J	55	THR	3.6
1	A	185	HIS	3.6
1	C	87	ILE	3.6
1	B	140	GLU	3.6
1	I	336	GLU	3.6
1	K	33	GLU	3.6
2	F	276	GLU	3.6
1	I	333	ALA	3.6
2	N	411	TYR	3.6
1	I	129	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	391	MET	3.6
1	A	548	ILE	3.6
1	B	558	GLU	3.6
1	I	128	GLU	3.6
1	J	252	TYR	3.6
1	B	197	ARG	3.6
1	C	195	VAL	3.6
2	D	140	VAL	3.6
4	H	94	VAL	3.6
1	A	436	ASP	3.6
2	L	225	ASP	3.6
3	O	53	LEU	3.6
2	E	282	GLY	3.6
1	C	83	ILE	3.6
1	J	337	ILE	3.6
2	E	454	ILE	3.6
1	I	347	GLU	3.6
1	K	13	ALA	3.6
1	K	163	ALA	3.6
2	E	272	ALA	3.6
1	K	486	VAL	3.6
2	F	231	ARG	3.6
1	I	209	MET	3.6
1	K	26	ASP	3.6
2	N	452	LYS	3.6
2	F	312	PRO	3.6
2	M	218	VAL	3.6
1	A	148	LEU	3.6
1	C	380	ILE	3.6
2	E	330	GLY	3.6
2	D	120	ASN	3.6
2	N	288	TYR	3.6
1	I	74	GLU	3.6
4	P	87	GLU	3.6
1	I	373	GLY	3.6
1	J	63	PRO	3.6
2	D	24	ALA	3.6
2	D	68	LEU	3.6
2	D	361	LEU	3.6
2	F	462	TYR	3.6
2	L	252	HIS	3.6
1	K	441	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
2	L	450	GLU	3.6
1	A	196	GLN	3.6
1	C	539	ILE	3.6
1	I	88	GLN	3.6
1	I	422	ILE	3.6
2	D	428	GLN	3.6
2	L	132	GLN	3.6
4	P	74	ILE	3.6
1	K	254	GLY	3.6
1	C	49	VAL	3.5
1	J	108	VAL	3.5
1	K	214	VAL	3.5
1	B	500	TYR	3.5
1	C	52	TYR	3.5
2	F	80	ALA	3.5
2	N	286	TYR	3.5
3	G	141	ALA	3.5
1	A	425	ASN	3.5
2	D	136	SER	3.5
1	A	243	LYS	3.5
1	C	276	LYS	3.5
1	K	374	GLU	3.5
2	L	197	THR	3.5
2	L	381	GLN	3.5
1	K	205	PHE	3.5
2	D	235	PRO	3.5
2	L	220	PHE	3.5
2	L	231	ARG	3.5
2	M	358	LEU	3.5
1	J	200	ASP	3.5
1	J	475	ALA	3.5
2	L	251	TYR	3.5
1	C	555	SER	3.5
2	E	452	LYS	3.5
1	K	81	ASN	3.5
2	L	74	SER	3.5
3	G	201	ILE	3.5
1	J	57	GLY	3.5
1	C	395	VAL	3.5
2	E	130	PHE	3.5
2	N	190	VAL	3.5
1	J	528	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
2	E	398	ILE	3.5
2	F	57	ILE	3.5
2	L	131	ILE	3.5
1	I	498	ASN	3.5
1	K	180	GLU	3.5
2	E	85	SER	3.5
2	M	307	SER	3.5
1	B	57	GLY	3.5
2	N	382	LEU	3.5
3	O	55	GLN	3.5
1	A	204	PRO	3.5
2	L	461	LYS	3.5
2	M	131	ILE	3.5
2	L	95	GLY	3.5
4	P	24	SER	3.5
1	J	265	VAL	3.5
2	E	300	VAL	3.5
4	H	64	ARG	3.5
2	E	99	PRO	3.5
1	K	353	TYR	3.5
1	C	152	ASP	3.5
1	B	259	GLY	3.5
2	L	30	GLY	3.5
2	N	200	GLU	3.5
2	D	91	ARG	3.5
1	B	327	THR	3.5
1	C	370	THR	3.5
1	I	50	GLN	3.5
3	G	140	VAL	3.5
2	F	113	PRO	3.5
2	N	86	LYS	3.5
1	J	47	ALA	3.5
2	M	266	ALA	3.5
2	N	127	PRO	3.5
2	D	96	ILE	3.5
1	B	58	LEU	3.5
2	F	144	LEU	3.5
1	C	117	TRP	3.5
2	F	195	GLY	3.5
1	B	486	VAL	3.5
2	F	243	GLU	3.5
2	D	132	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
2	E	211	THR	3.5
1	A	360	ALA	3.5
2	L	17	PRO	3.5
4	H	26	ALA	3.5
2	L	321	ARG	3.4
1	A	162	PRO	3.4
1	A	490	ILE	3.4
1	B	50	GLN	3.4
1	K	398	SER	3.4
1	B	227	PRO	3.4
1	C	260	ASN	3.4
1	I	179	THR	3.4
1	J	229	PRO	3.4
1	J	383	ALA	3.4
2	L	159	PRO	3.4
2	E	73	VAL	3.4
4	P	22	GLY	3.4
2	N	87	GLU	3.4
1	I	192	ALA	3.4
1	C	75	LEU	3.4
1	K	281	LEU	3.4
2	D	142	ASN	3.4
2	F	240	THR	3.4
1	A	258	ARG	3.4
1	A	78	GLY	3.4
1	B	306	GLY	3.4
1	K	124	LYS	3.4
2	D	76	VAL	3.4
2	E	255	VAL	3.4
2	M	114	ILE	3.4
1	I	356	ALA	3.4
1	K	560	PRO	3.4
2	N	428	GLN	3.4
1	C	319	SER	3.4
1	K	290	ASN	3.4
2	N	64	THR	3.4
1	C	364	ARG	3.4
2	M	220	PHE	3.4
2	L	282	GLY	3.4
2	M	38	GLY	3.4
1	K	507	CYS	3.4
1	J	489	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	I	469	GLN	3.4
2	F	132	GLN	3.4
1	K	203	THR	3.4
1	C	483	VAL	3.4
2	N	146	ARG	3.4
3	G	188	ARG	3.4
1	J	233	GLY	3.4
1	A	70	PRO	3.4
1	C	146	LYS	3.4
1	C	433	SER	3.4
1	K	535	SER	3.4
1	B	246	ASN	3.4
1	J	79	MET	3.4
1	K	55	THR	3.4
1	J	11	GLY	3.4
2	D	432	ILE	3.4
2	M	232	ILE	3.4
1	I	495	LEU	3.4
2	D	328	LEU	3.4
1	C	405	ALA	3.4
1	J	118	ALA	3.4
3	G	144	GLU	3.4
1	J	562	TYR	3.4
2	E	149	LYS	3.4
2	M	288	TYR	3.4
2	F	41	ARG	3.4
1	A	385	SER	3.4
1	J	132	GLY	3.4
2	L	51	SER	3.4
2	D	172	THR	3.4
2	E	289	THR	3.4
2	L	94	ASN	3.4
2	L	261	THR	3.4
2	M	238	ALA	3.3
1	A	560	PRO	3.3
2	E	175	PRO	3.3
1	C	378	VAL	3.3
1	C	513	TYR	3.3
1	K	574	PHE	3.3
1	I	251	VAL	3.3
2	E	190	VAL	3.3
2	M	427	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	325	ASP	3.3
1	I	69	LEU	3.3
1	J	208	GLY	3.3
2	D	365	GLY	3.3
2	F	131	ILE	3.3
2	M	116	GLY	3.3
2	M	195	GLY	3.3
1	B	385	SER	3.3
1	C	240	SER	3.3
2	L	298	ALA	3.3
4	H	50	ALA	3.3
2	L	317	PRO	3.3
1	J	307	VAL	3.3
2	M	450	GLU	3.3
2	N	169	ARG	3.3
1	C	354	LEU	3.3
1	J	366	GLY	3.3
1	C	55	THR	3.3
2	L	39	THR	3.3
1	C	110	ALA	3.3
1	C	293	ASN	3.3
1	J	293	ASN	3.3
1	K	356	ALA	3.3
2	L	25	LYS	3.3
2	N	24	ALA	3.3
1	K	227	PRO	3.3
1	K	381	VAL	3.3
2	E	81	ARG	3.3
1	I	294	MET	3.3
2	E	49	GLU	3.3
1	C	196	GLN	3.3
2	N	256	ILE	3.3
1	C	474	ASP	3.3
1	K	517	LYS	3.3
2	L	307	SER	3.3
2	N	154	SER	3.3
1	B	77	PRO	3.3
1	C	501	HIS	3.3
2	F	288	TYR	3.3
2	M	138	ILE	3.3
1	J	316	GLN	3.3
1	I	575	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	J	264	ASP	3.3
1	A	563	PHE	3.3
1	B	508	SER	3.3
1	I	48	PHE	3.3
1	I	302	SER	3.3
1	K	411	ALA	3.3
2	D	31	ALA	3.3
1	K	399	THR	3.3
2	N	455	SER	3.3
1	B	49	VAL	3.3
1	C	286	VAL	3.3
1	C	305	VAL	3.3
2	L	81	ARG	3.3
2	M	173	VAL	3.3
1	J	323	MET	3.3
1	A	353	TYR	3.3
2	D	412	LEU	3.3
2	E	286	TYR	3.3
1	B	375	GLU	3.3
1	C	311	GLU	3.3
1	B	390	ASP	3.3
1	K	54	ASP	3.3
1	K	177	ASP	3.3
2	M	193	ALA	3.3
1	J	403	VAL	3.3
2	D	430	ARG	3.3
2	L	76	VAL	3.3
1	A	399	THR	3.3
2	F	384	SER	3.3
1	A	473	PRO	3.3
1	K	275	PRO	3.3
2	L	240	THR	3.3
2	L	322	THR	3.3
2	F	463	TYR	3.3
2	L	277	ILE	3.3
2	N	388	ASN	3.3
1	C	271	GLU	3.3
1	C	374	GLU	3.3
1	K	332	GLU	3.3
2	N	195	GLY	3.3
1	C	377	ALA	3.3
1	K	359	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
2	E	145	VAL	3.3
2	N	216	ARG	3.3
4	P	70	VAL	3.3
2	M	144	LEU	3.3
2	M	239	LEU	3.3
2	N	221	LEU	3.3
1	I	295	PRO	3.3
1	A	507	CYS	3.2
1	A	170	GLU	3.2
1	B	376	GLY	3.2
2	E	461	LYS	3.2
2	F	422	PHE	3.2
1	C	544	VAL	3.2
1	J	214	VAL	3.2
2	D	193	ALA	3.2
1	K	139	PRO	3.2
1	K	362	TYR	3.2
2	E	54	TYR	3.2
2	F	15	SER	3.2
2	F	252	HIS	3.2
2	M	115	THR	3.2
2	M	422	PHE	3.2
1	C	219	ALA	3.2
1	K	10	ALA	3.2
2	F	112	LEU	3.2
2	F	152	ILE	3.2
2	F	356	PRO	3.2
1	A	8	LYS	3.2
1	I	112	ASP	3.2
1	I	390	ASP	3.2
1	I	433	SER	3.2
2	F	12	THR	3.2
4	H	28	GLU	3.2
1	K	465	GLN	3.2
2	F	56	VAL	3.2
2	F	239	LEU	3.2
2	N	91	ARG	3.2
4	H	71	LEU	3.2
2	D	277	ILE	3.2
2	M	432	ILE	3.2
2	D	346	LYS	3.2
1	J	302	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	K	328	SER	3.2
2	E	299	GLY	3.2
1	A	299	ARG	3.2
1	B	193	ARG	3.2
1	I	311	GLU	3.2
2	L	276	GLU	3.2
1	K	239	GLN	3.2
2	M	123	ALA	3.2
1	C	536	ILE	3.2
2	F	313	ILE	3.2
2	F	13	TYR	3.2
1	A	21	GLY	3.2
2	M	119	LEU	3.2
1	I	120	THR	3.2
2	L	243	GLU	3.2
2	L	399	ILE	3.2
2	F	223	LYS	3.2
1	K	44	GLY	3.2
2	N	119	LEU	3.2
2	N	157	GLY	3.2
1	A	108	VAL	3.2
1	A	123	VAL	3.2
1	A	249	VAL	3.2
1	A	446	ASP	3.2
1	C	153	VAL	3.2
1	C	299	ARG	3.2
1	K	547	ARG	3.2
2	F	81	ARG	3.2
1	A	62	GLU	3.2
1	C	499	ALA	3.2
1	I	53	GLU	3.2
1	K	147	ILE	3.2
1	K	414	ALA	3.2
2	D	137	THR	3.2
2	D	168	ALA	3.2
2	F	138	ILE	3.2
2	F	156	SER	3.2
1	K	347	GLU	3.2
2	F	433	GLU	3.2
2	L	126	LYS	3.2
2	F	284	PRO	3.2
2	L	13	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
2	M	443	LEU	3.2
1	B	472	GLY	3.2
2	D	44	GLY	3.2
2	D	299	GLY	3.2
4	P	41	GLY	3.2
1	C	134	VAL	3.2
2	L	140	VAL	3.2
1	J	531	LYS	3.1
1	K	66	SER	3.1
2	M	23	ASN	3.1
2	M	388	ASN	3.1
1	C	470	LEU	3.1
1	I	322	LEU	3.1
4	H	33	LEU	3.1
1	J	563	PHE	3.1
1	A	487	GLY	3.1
1	C	323	MET	3.1
1	I	507	CYS	3.1
1	A	115	LYS	3.1
2	F	249	HIS	3.1
1	B	248	ASP	3.1
2	F	374	ASP	3.1
2	M	329	THR	3.1
2	E	161	ASN	3.1
1	I	380	ILE	3.1
1	A	55	THR	3.1
1	B	302	SER	3.1
1	K	35	LEU	3.1
2	F	185	GLU	3.1
2	M	221	LEU	3.1
2	L	310	GLN	3.1
2	M	289	THR	3.1
2	N	355	LEU	3.1
2	D	331	TYR	3.1
2	E	17	PRO	3.1
4	H	66	ARG	3.1
2	M	298	ALA	3.1
2	M	334	GLU	3.1
1	B	406	PHE	3.1
1	C	264	ASP	3.1
1	J	204	PRO	3.1
2	M	113	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
2	N	309	THR	3.1
2	D	231	ARG	3.1
2	D	241	VAL	3.1
1	B	233	GLY	3.1
1	C	454	ILE	3.1
1	K	262	MET	3.1
2	L	325	ILE	3.1
2	M	370	LYS	3.1
2	D	224	ALA	3.1
1	I	35	LEU	3.1
1	C	180	GLU	3.1
1	K	50	GLN	3.1
1	K	552	ARG	3.1
2	D	169	ARG	3.1
2	L	46	GLN	3.1
2	E	71	THR	3.1
2	E	154	SER	3.1
2	F	54	TYR	3.1
2	L	324	PRO	3.1
4	H	45	VAL	3.1
1	I	539	ILE	3.1
1	K	530	ILE	3.1
1	A	81	ASN	3.1
1	J	310	ALA	3.1
1	B	51	VAL	3.1
1	B	525	GLU	3.1
1	K	122	MET	3.1
1	A	179	THR	3.1
1	K	372	GLY	3.1
2	L	8	TYR	3.1
2	L	228	THR	3.1
2	L	318	ASP	3.1
2	N	391	ASP	3.1
1	A	163	ALA	3.1
1	A	49	VAL	3.1
1	K	169	GLU	3.1
1	K	300	GLU	3.1
2	D	128	GLU	3.1
2	E	265	GLU	3.1
2	L	16	GLY	3.0
1	K	458	LEU	3.0
2	E	221	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	292	ALA	3.0
2	F	191	PHE	3.0
1	A	197	ARG	3.0
1	C	145	HIS	3.0
1	K	123	VAL	3.0
1	C	402	ILE	3.0
1	I	509	MET	3.0
2	F	337	ILE	3.0
1	C	63	PRO	3.0
1	C	362	TYR	3.0
1	I	126	GLY	3.0
1	I	513	TYR	3.0
1	J	62	GLU	3.0
2	E	278	PRO	3.0
4	H	8	GLU	3.0
2	N	150	LEU	3.0
1	B	45	ASP	3.0
1	B	398	SER	3.0
1	C	118	ALA	3.0
1	C	232	SER	3.0
1	I	207	THR	3.0
1	K	200	ASP	3.0
1	K	264	ASP	3.0
2	E	258	THR	3.0
2	F	258	THR	3.0
2	N	384	SER	3.0
1	B	265	VAL	3.0
1	I	236	VAL	3.0
2	L	360	ARG	3.0
1	J	19	MET	3.0
2	N	252	HIS	3.0
1	A	135	LEU	3.0
1	B	400	LEU	3.0
1	I	227	PRO	3.0
1	J	20	LEU	3.0
1	K	233	GLY	3.0
1	K	506	TYR	3.0
4	P	53	PRO	3.0
1	C	355	ALA	3.0
1	I	152	ASP	3.0
1	J	315	ASP	3.0
1	J	398	SER	3.0

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Mol	Chain	Res	Type	RSRZ
2	L	71	THR	3.0
2	L	258	THR	3.0
1	I	250	VAL	3.0
1	K	548	ILE	3.0
2	L	68	LEU	3.0
2	L	254	LEU	3.0
2	M	339	LEU	3.0
2	N	239	LEU	3.0
1	C	184	TYR	3.0
1	J	352	PRO	3.0
1	J	543	PRO	3.0
2	L	463	TYR	3.0
1	C	348	GLU	3.0
1	I	33	GLU	3.0
2	F	342	GLU	3.0
2	N	129	GLN	3.0
1	A	153	VAL	3.0
1	I	123	VAL	3.0
1	J	488	ARG	3.0
1	K	286	VAL	3.0
2	L	136	SER	3.0
2	L	226	ASP	3.0
1	C	288	ILE	3.0
1	I	20	LEU	3.0
1	J	246	ASN	3.0
2	E	89	LEU	3.0
1	A	222	GLY	3.0
1	C	353	TYR	3.0
1	I	252	TYR	3.0
1	K	513	TYR	3.0
2	M	244	TYR	3.0
2	E	401	GLU	3.0
2	N	275	GLU	3.0
1	J	225	ALA	3.0
2	E	415	ALA	3.0
1	I	158	LYS	3.0
1	K	134	VAL	3.0
2	L	125	ARG	3.0
1	A	43	ASP	3.0
1	C	302	SER	3.0
2	L	408	ASP	3.0
2	M	14	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
4	P	48	ASP	3.0
1	I	181	LEU	3.0
4	H	51	LEU	3.0
2	N	295	TYR	3.0
1	A	485	GLU	3.0
1	B	551	ALA	3.0
1	I	116	LYS	3.0
1	I	477	GLN	3.0
1	B	211	ILE	3.0
1	C	407	TRP	3.0
2	N	280	ARG	3.0
2	N	254	LEU	3.0
1	A	398	SER	3.0
1	K	478	ASP	3.0
2	N	45	GLY	3.0
2	E	363	ASN	3.0
1	I	360	ALA	3.0
1	J	512	ALA	3.0
1	K	529	ALA	3.0
2	N	77	GLU	3.0
1	A	160	VAL	3.0
1	I	552	ARG	3.0
1	K	36	VAL	3.0
1	A	303	ILE	2.9
1	K	83	ILE	2.9
2	F	91	ARG	3.0
4	H	15	LEU	2.9
2	D	359	SER	2.9
1	I	243	LYS	2.9
1	A	73	VAL	2.9
1	J	251	VAL	2.9
1	J	492	GLU	2.9
2	F	109	GLU	2.9
1	A	400	LEU	2.9
2	N	381	GLN	2.9
1	C	43	ASP	2.9
1	C	478	ASP	2.9
1	K	120	THR	2.9
1	K	235	THR	2.9
2	L	234	THR	2.9
2	N	400	GLY	2.9
1	J	270	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	220	PHE	2.9
1	A	402	ILE	2.9
2	D	382	LEU	2.9
2	M	364	ASN	2.9
2	N	14	ILE	2.9
2	N	401	GLU	2.9
2	D	198	GLN	2.9
1	A	86	GLY	2.9
1	C	234	LYS	2.9
2	F	155	GLY	2.9
1	B	555	SER	2.9
1	I	351	PRO	2.9
1	K	207	THR	2.9
2	E	324	PRO	2.9
2	F	60	PHE	2.9
2	F	228	THR	2.9
2	M	204	PHE	2.9
2	M	371	THR	2.9
2	N	331	TYR	2.9
2	N	114	ILE	2.9
3	O	52	ALA	2.9
1	I	425	ASN	2.9
2	N	243	GLU	2.9
1	C	126	GLY	2.9
2	L	299	GLY	2.9
2	N	44	GLY	2.9
1	K	420	PRO	2.9
2	L	235	PRO	2.9
1	I	215	LEU	2.9
1	K	42	LEU	2.9
1	K	137	THR	2.9
2	D	357	SER	2.9
2	L	174	ARG	2.9
2	N	197	THR	2.9
3	O	146	ARG	2.9
4	H	62	LEU	2.9
1	A	145	HIS	2.9
1	B	294	MET	2.9
1	I	363	GLU	2.9
1	K	257	GLU	2.9
2	N	46	GLN	2.9
2	N	148	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
2	N	427	GLN	2.9
1	K	419	PHE	2.9
1	C	409	LEU	2.9
1	K	312	TYR	2.9
2	D	326	PRO	2.9
2	F	151	PRO	2.9
2	M	68	LEU	2.9
1	C	189	VAL	2.9
1	I	14	VAL	2.9
2	F	174	ARG	2.9
1	A	183	MET	2.9
1	C	209	MET	2.9
3	O	37	ALA	2.9
1	K	319	SER	2.9
2	D	143	THR	2.9
2	E	379	SER	2.9
1	A	502	GLU	2.9
1	I	59	LYS	2.9
1	I	564	GLU	2.9
1	K	375	GLU	2.9
2	L	183	LYS	2.9
2	L	230	GLU	2.9
1	A	246	ASN	2.9
2	M	247	PHE	2.9
2	E	361	LEU	2.9
2	F	257	LEU	2.9
1	A	211	ILE	2.9
1	B	190	ARG	2.9
1	K	89	ARG	2.9
1	C	508	SER	2.9
2	D	154	SER	2.9
1	C	367	LYS	2.9
1	I	200	ASP	2.9
2	L	26	ASP	2.9
1	B	348	GLU	2.9
1	C	574	PHE	2.9
1	K	415	PHE	2.9
1	K	424	TRP	2.9
2	F	254	LEU	2.9
2	E	11	ILE	2.8
1	A	323	MET	2.8
1	B	345	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	352	PRO	2.8
2	N	354	PRO	2.8
1	A	511	LYS	2.8
1	B	370	THR	2.8
1	I	8	LYS	2.8
2	E	72	SER	2.8
2	E	307	SER	2.8
1	C	213	ASP	2.8
2	N	290	ASP	2.8
1	C	343	GLU	2.8
1	I	415	PHE	2.8
1	A	238	GLN	2.8
1	A	317	GLY	2.8
2	E	146	ARG	2.8
2	L	341	ARG	2.8
2	L	141	MET	2.8
2	F	127	PRO	2.8
2	M	397	ALA	2.8
2	N	273	ALA	2.8
1	A	435	LEU	2.8
1	I	493	ASP	2.8
1	B	329	ARG	2.8
1	C	426	GLY	2.8
1	J	297	ALA	2.8
1	J	423	ASN	2.8
1	A	292	SER	2.8
1	I	292	SER	2.8
2	D	12	THR	2.8
1	A	164	GLY	2.8
1	K	82	GLY	2.8
1	K	244	TRP	2.8
1	K	248	ASP	2.8
2	E	200	GLU	2.8
2	N	152	ILE	2.8
2	N	302	GLU	2.8
2	N	325	ILE	2.8
3	G	55	GLN	2.8
1	J	255	CYS	2.8
2	F	238	ALA	2.8
2	N	31	ALA	2.8
2	L	262	ASN	2.8
1	J	540	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	302	SER	2.8
1	A	339	SER	2.8
1	C	79	MET	2.8
2	D	141	MET	2.8
2	E	455	SER	2.8
2	F	322	THR	2.8
2	F	449	GLY	2.8
2	L	22	GLU	2.8
2	L	413	GLN	2.8
2	M	184	GLU	2.8
2	N	296	GLU	2.8
2	E	319	ASP	2.8
1	A	22	ALA	2.8
1	A	188	PRO	2.8
2	M	150	LEU	2.8
1	C	313	PHE	2.8
1	K	313	PHE	2.8
1	A	60	VAL	2.8
2	F	300	VAL	2.8
2	L	297	ARG	2.8
1	A	221	GLY	2.8
1	C	349	GLY	2.8
1	I	11	GLY	2.8
2	L	195	GLY	2.8
1	C	424	TRP	2.8
1	I	115	LYS	2.8
1	I	375	GLU	2.8
1	A	355	ALA	2.8
1	B	312	TYR	2.8
1	K	316	GLN	2.8
2	D	230	GLU	2.8
2	L	431	SER	2.8
1	K	499	ALA	2.8
2	E	385	ALA	2.8
2	F	411	TYR	2.8
2	M	324	PRO	2.8
1	A	58	LEU	2.8
4	H	1	MET	2.8
1	B	568	LYS	2.8
2	N	25	LYS	2.8
1	C	50	GLN	2.8
1	I	235	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	377	ALA	2.8
2	F	419	GLU	2.8
2	M	387	ALA	2.8
4	H	27	GLU	2.8
2	F	27	LEU	2.8
2	F	357	SER	2.8
2	M	354	PRO	2.8
2	N	139	ASP	2.8
2	E	256	ILE	2.7
1	J	262	MET	2.7
1	J	382	GLY	2.7
1	K	132	GLY	2.7
4	P	17	GLY	2.7
1	A	331	ALA	2.7
1	I	244	TRP	2.7
1	J	52	TYR	2.7
2	M	46	GLN	2.7
2	N	19	LEU	2.7
2	M	72	SER	2.7
2	N	350	PRO	2.7
2	D	232	ILE	2.7
2	M	96	ILE	2.7
1	I	161	LYS	2.7
1	J	21	GLY	2.7
1	K	28	CYS	2.7
2	F	97	GLY	2.7
2	E	397	ALA	2.7
1	A	459	GLN	2.7
1	C	485	GLU	2.7
2	E	269	GLU	2.7
2	M	87	GLU	2.7
2	N	187	PHE	2.7
1	A	6	ILE	2.7
1	C	23	ARG	2.7
2	L	253	VAL	2.7
2	N	416	ASP	2.7
3	O	167	VAL	2.7
1	C	450	LEU	2.7
2	F	44	GLY	2.7
4	P	65	GLY	2.7
1	I	72	ALA	2.7
2	D	242	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	125	PRO	2.7
1	A	448	PRO	2.7
1	C	387	PRO	2.7
1	C	527	GLU	2.7
1	I	90	PRO	2.7
1	J	171	PRO	2.7
2	F	77	GLU	2.7
2	N	235	PRO	2.7
1	A	191	ARG	2.7
1	C	307	VAL	2.7
1	C	432	THR	2.7
1	K	288	ILE	2.7
2	D	14	ILE	2.7
1	I	60	VAL	2.7
1	I	195	VAL	2.7
2	D	79	VAL	2.7
2	D	300	VAL	2.7
2	L	63	THR	2.7
2	M	133	THR	2.7
2	M	379	SER	2.7
1	C	24	MET	2.7
1	K	158	LYS	2.7
1	C	315	ASP	2.7
1	C	76	GLY	2.7
1	C	246	ASN	2.7
2	M	161	ASN	2.7
2	F	55	ALA	2.7
3	G	163	ALA	2.7
1	I	480	GLU	2.7
1	K	477	GLN	2.7
1	A	286	VAL	2.7
1	K	209	MET	2.7
1	K	511	LYS	2.7
2	E	261	THR	2.7
2	F	133	THR	2.7
2	M	107	THR	2.7
1	C	328	SER	2.7
2	N	431	SER	2.7
2	L	395	LEU	2.7
1	A	404	GLY	2.7
1	I	132	GLY	2.7
1	A	141	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	E	273	ALA	2.7
1	A	252	TYR	2.7
1	C	84	TYR	2.7
2	E	422	PHE	2.7
1	A	309	ILE	2.7
1	B	386	PRO	2.7
1	A	340	ARG	2.7
1	K	32	GLU	2.7
1	K	265	VAL	2.7
1	I	34	GLY	2.7
1	A	54	ASP	2.7
1	C	504	ASP	2.7
1	K	315	ASP	2.7
1	A	16	ALA	2.7
1	J	551	ALA	2.7
2	E	191	PHE	2.7
2	L	462	TYR	2.7
1	C	422	ILE	2.7
2	L	135	ILE	2.7
1	A	124	LYS	2.7
1	C	64	VAL	2.7
1	I	124	LYS	2.7
2	M	253	VAL	2.7
1	I	441	GLU	2.7
1	K	571	GLN	2.7
2	D	434	GLU	2.7
2	E	143	THR	2.7
1	C	233	GLY	2.7
1	J	306	GLY	2.7
2	F	202	SER	2.7
1	I	324	ALA	2.6
1	K	152	ASP	2.6
2	D	139	ASP	2.6
2	E	37	ASP	2.6
2	M	403	ALA	2.6
1	C	548	ILE	2.6
1	J	523	TYR	2.6
2	L	100	ILE	2.6
2	M	13	TYR	2.6
2	D	47	VAL	2.6
2	F	241	VAL	2.6
2	M	79	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	M	304	LYS	2.6
2	M	341	ARG	2.6
1	C	111	LEU	2.6
1	I	540	LEU	2.6
1	K	165	GLU	2.6
2	L	115	THR	2.6
2	M	258	THR	2.6
1	A	429	SER	2.6
1	K	331	ALA	2.6
2	L	14	ILE	2.6
2	N	294	ILE	2.6
1	A	175	LEU	2.6
1	C	287	LEU	2.6
1	J	201	PRO	2.6
2	M	75	LEU	2.6
3	G	48	GLU	2.6
1	A	313	PHE	2.6
2	N	418	PHE	2.6
1	C	186	THR	2.6
1	C	526	ALA	2.6
2	N	71	THR	2.6
1	K	555	SER	2.6
2	F	154	SER	2.6
1	C	417	ARG	2.6
2	E	203	TYR	2.6
2	L	190	VAL	2.6
1	K	148	LEU	2.6
4	H	67	ASP	2.6
1	B	196	GLN	2.6
1	B	569	GLU	2.6
1	C	176	GLU	2.6
1	J	74	GLU	2.6
2	E	334	GLU	2.6
2	M	132	GLN	2.6
1	K	388	GLY	2.6
2	E	232	ILE	2.6
2	N	110	LYS	2.6
2	N	123	ALA	2.6
3	G	134	ALA	2.6
1	A	30	VAL	2.6
1	A	401	ARG	2.6
1	C	235	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	371	THR	2.6
1	K	111	LEU	2.6
2	N	217	SER	2.6
1	A	139	PRO	2.6
1	K	125	PRO	2.6
2	L	312	PRO	2.6
2	L	402	ASP	2.6
2	M	67	ASP	2.6
1	B	425	ASN	2.6
1	C	517	LYS	2.6
1	I	68	GLY	2.6
2	D	388	ASN	2.6
2	E	332	ILE	2.6
2	E	140	VAL	2.6
2	E	238	ALA	2.6
2	L	92	ARG	2.6
1	B	439	TYR	2.6
1	J	553	TYR	2.6
2	F	349	TYR	2.6
1	B	352	PRO	2.6
1	K	508	SER	2.6
4	H	7	PRO	2.6
4	H	6	ASP	2.6
2	M	130	PHE	2.6
1	C	363	GLU	2.6
1	I	259	GLY	2.6
4	P	12	GLY	2.6
1	B	299	ARG	2.6
1	C	324	ALA	2.6
1	J	321	ALA	2.6
2	E	266	ALA	2.6
1	B	308	THR	2.6
2	M	431	SER	2.6
1	J	424	TRP	2.6
1	I	43	ASP	2.6
1	I	216	PHE	2.6
2	L	93	PHE	2.6
1	C	373	GLY	2.6
1	I	466	GLU	2.6
1	J	445	GLU	2.6
2	F	206	GLN	2.6
1	J	499	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	192	ALA	2.6
2	N	255	VAL	2.6
1	A	46	THR	2.6
1	K	151	PRO	2.6
1	I	56	SER	2.5
2	E	202	SER	2.5
1	A	489	ILE	2.5
1	J	454	ILE	2.5
1	K	40	ILE	2.5
1	J	376	GLY	2.5
1	K	127	ASP	2.5
4	H	12	GLY	2.5
1	A	257	GLU	2.5
1	C	381	VAL	2.5
1	I	257	GLU	2.5
1	K	320	VAL	2.5
1	K	503	VAL	2.5
1	A	321	ALA	2.5
1	A	512	ALA	2.5
1	I	479	ALA	2.5
1	J	324	ALA	2.5
2	D	243	GLU	2.5
2	D	194	MET	2.5
2	F	439	ALA	2.5
2	L	91	ARG	2.5
2	N	264	CYS	2.5
1	K	184	TYR	2.5
2	M	349	TYR	2.5
1	I	420	PRO	2.5
1	I	524	LYS	2.5
1	K	431	PHE	2.5
2	E	418	PHE	2.5
2	N	60	PHE	2.5
4	H	9	THR	2.5
4	P	81	PHE	2.5
1	I	407	TRP	2.5
1	A	109	HIS	2.5
1	K	412	SER	2.5
2	F	219	LEU	2.5
2	N	454	ILE	2.5
1	A	68	GLY	2.5
1	K	368	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	378	VAL	2.5
1	J	72	ALA	2.5
1	J	163	ALA	2.5
2	E	188	ALA	2.5
2	N	420	ARG	2.5
2	N	58	GLN	2.5
4	H	54	ASP	2.5
2	L	222	ASN	2.5
1	A	9	ILE	2.5
1	I	430	LEU	2.5
1	J	235	THR	2.5
1	J	450	LEU	2.5
1	K	223	THR	2.5
2	E	438	ILE	2.5
1	B	443	VAL	2.5
2	D	85	SER	2.5
2	M	147	GLY	2.5
2	M	375	HIS	2.5
1	C	133	MET	2.5
1	K	479	ALA	2.5
2	F	362	MET	2.5
2	L	24	ALA	2.5
2	L	238	ALA	2.5
1	A	348	GLU	2.5
1	K	38	GLU	2.5
2	D	336	GLN	2.5
2	N	448	GLN	2.5
3	O	48	GLU	2.5
1	C	500	TYR	2.5
1	A	182	LYS	2.5
1	I	202	ASN	2.5
2	D	264	CYS	2.5
1	I	281	LEU	2.5
2	D	245	LEU	2.5
3	O	172	ILE	2.5
4	P	68	LEU	2.5
1	A	18	GLY	2.5
1	C	120	THR	2.5
2	F	134	GLY	2.5
2	N	306	GLY	2.5
1	B	331	ALA	2.5
2	L	154	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	N	188	ALA	2.5
2	N	307	SER	2.5
1	I	159	GLU	2.5
1	A	248	ASP	2.5
1	B	517	LYS	2.5
2	F	290	ASP	2.5
3	O	39	PHE	2.5
2	F	68	LEU	2.5
1	K	489	ILE	2.5
2	E	392	ILE	2.5
2	F	423	ILE	2.5
2	L	424	ASN	2.5
1	A	195	VAL	2.5
1	K	168	VAL	2.5
2	M	47	VAL	2.5
1	A	131	GLY	2.5
1	I	344	MET	2.5
1	I	391	MET	2.5
1	J	256	GLY	2.5
2	N	174	ARG	2.5
1	J	379	THR	2.5
1	K	521	ALA	2.5
1	K	456	GLU	2.5
2	M	58	GLN	2.5
2	M	126	LYS	2.5
2	M	419	GLU	2.5
2	M	452	LYS	2.5
1	A	215	LEU	2.5
1	B	446	ASP	2.5
1	B	559	PHE	2.5
1	C	252	TYR	2.5
1	C	281	LEU	2.5
2	E	26	ASP	2.5
2	E	225	ASP	2.5
2	E	314	LEU	2.5
2	F	408	ASP	2.5
2	L	113	PRO	2.5
2	M	423	ILE	2.5
1	C	168	VAL	2.5
1	K	236	VAL	2.5
1	A	119	TRP	2.5
1	C	231	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	349	GLY	2.5
1	K	344	MET	2.5
1	K	373	GLY	2.5
1	A	289	ALA	2.5
2	F	234	THR	2.5
2	N	333	THR	2.5
2	F	214	LEU	2.5
2	M	18	LEU	2.5
3	O	22	GLN	2.5
2	E	354	PRO	2.5
1	C	172	VAL	2.5
1	J	253	VAL	2.5
1	K	149	VAL	2.5
2	N	199	ARG	2.5
1	A	423	ASN	2.5
1	J	259	GLY	2.5
1	K	278	GLY	2.5
2	E	365	GLY	2.5
1	I	434	ALA	2.5
3	G	136	ALA	2.5
1	C	418	HIS	2.5
1	C	48	PHE	2.4
1	C	69	LEU	2.4
2	M	412	LEU	2.4
4	H	72	LEU	2.4
1	C	469	GLN	2.4
1	C	541	GLN	2.4
1	I	397	GLN	2.4
1	J	180	GLU	2.4
1	K	252	TYR	2.4
1	K	525	GLU	2.4
2	D	413	GLN	2.4
2	L	196	ILE	2.4
2	N	13	TYR	2.4
1	I	394	PRO	2.4
2	N	159	PRO	2.4
2	N	317	PRO	2.4
1	I	549	GLY	2.4
1	K	259	GLY	2.4
2	D	95	GLY	2.4
2	E	147	GLY	2.4
2	N	116	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	356	ALA	2.4
2	E	69	ALA	2.4
2	L	273	ALA	2.4
1	C	520	LEU	2.4
2	F	153	PHE	2.4
1	A	500	TYR	2.4
2	L	264	CYS	2.4
2	N	107	THR	2.4
1	I	502	GLU	2.4
1	J	300	GLU	2.4
1	K	238	GLN	2.4
2	E	156	SER	2.4
2	F	217	SER	2.4
2	F	379	SER	2.4
2	M	166	GLN	2.4
2	N	7	GLU	2.4
2	N	433	GLU	2.4
4	H	82	GLN	2.4
1	A	378	VAL	2.4
1	I	329	ARG	2.4
1	J	129	VAL	2.4
1	J	236	VAL	2.4
1	A	79	MET	2.4
1	J	401	ARG	2.4
1	K	386	PRO	2.4
2	D	324	PRO	2.4
2	N	396	VAL	2.4
1	K	446	ASP	2.4
2	L	330	GLY	2.4
1	C	318	PHE	2.4
2	D	459	ILE	2.4
2	E	270	ILE	2.4
2	D	244	TYR	2.4
1	K	67	THR	2.4
2	L	70	THR	2.4
1	C	449	GLU	2.4
1	J	227	PRO	2.4
1	J	412	SER	2.4
1	K	130	ARG	2.4
2	D	62	GLU	2.4
2	L	428	GLN	2.4
1	K	188	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	455	SER	2.4
4	H	73	PRO	2.4
2	F	126	LYS	2.4
1	A	177	ASP	2.4
1	A	479	ALA	2.4
1	B	264	ASP	2.4
1	C	528	ALA	2.4
1	I	199	LEU	2.4
1	J	42	LEU	2.4
1	J	112	ASP	2.4
2	F	389	GLY	2.4
2	N	30	GLY	2.4
2	N	158	LEU	2.4
3	O	142	ASN	2.4
1	A	506	TYR	2.4
1	I	350	TYR	2.4
1	K	185	HIS	2.4
1	I	486	VAL	2.4
1	K	23	ARG	2.4
2	N	59	VAL	2.4
4	H	47	VAL	2.4
1	A	347	GLU	2.4
1	A	363	GLU	2.4
1	B	342	GLU	2.4
1	J	569	GLU	2.4
1	K	170	GLU	2.4
2	M	287	MET	2.4
2	N	128	GLU	2.4
3	O	144	GLU	2.4
1	C	182	LYS	2.4
1	K	243	LYS	2.4
2	L	72	SER	2.4
1	A	208	GLY	2.4
2	L	157	GLY	2.4
1	K	310	ALA	2.4
2	D	298	ALA	2.4
2	F	171	ALA	2.4
2	F	397	ALA	2.4
1	B	315	ASP	2.4
2	F	318	ASP	2.4
1	C	51	VAL	2.4
2	L	255	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	N	268	ARG	2.4
1	K	268	GLU	2.4
1	K	327	THR	2.4
2	D	209	GLU	2.4
2	E	333	THR	2.4
2	N	166	GLN	2.4
3	G	158	THR	2.4
4	H	35	THR	2.4
1	J	215	LEU	2.4
1	K	58	LEU	2.4
2	N	436	LEU	2.4
1	B	13	ALA	2.4
2	E	31	ALA	2.4
2	N	69	ALA	2.4
1	J	490	ILE	2.4
1	J	45	ASP	2.4
2	L	374	ASP	2.4
1	A	41	ARG	2.4
1	K	64	VAL	2.4
1	K	218	VAL	2.4
2	N	281	ARG	2.4
2	D	429	ASN	2.4
1	A	394	PRO	2.4
1	J	188	PRO	2.4
1	B	180	GLU	2.4
1	K	175	LEU	2.4
2	L	151	PRO	2.4
2	D	248	GLU	2.4
2	M	170	GLN	2.4
1	C	306	GLY	2.4
1	K	404	GLY	2.4
1	K	533	GLY	2.4
2	N	271	GLY	2.4
1	A	377	ALA	2.4
1	I	9	ILE	2.4
1	C	200	ASP	2.4
2	E	84	VAL	2.4
2	M	391	ASP	2.4
1	J	304	TYR	2.4
1	K	276	LYS	2.4
2	D	436	LEU	2.4
1	I	188	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	280	PRO	2.3
1	A	38	GLU	2.3
1	C	53	GLU	2.3
1	C	571	GLN	2.3
1	I	238	GLN	2.3
3	G	205	GLU	2.3
2	N	211	THR	2.3
2	M	357	SER	2.3
4	H	31	SER	2.3
3	G	182	VAL	2.3
1	I	133	MET	2.3
1	A	493	ASP	2.3
1	J	390	ASP	2.3
1	K	537	ASP	2.3
2	F	29	TYR	2.3
2	M	290	ASP	2.3
4	H	48	ASP	2.3
1	I	423	ASN	2.3
1	A	53	GLU	2.3
1	A	132	GLY	2.3
1	C	309	ILE	2.3
2	F	266	ALA	2.3
2	N	403	ALA	2.3
1	I	285	THR	2.3
2	D	261	THR	2.3
1	I	65	VAL	2.3
2	E	384	SER	2.3
1	B	562	TYR	2.3
1	C	577	LEU	2.3
1	J	506	TYR	2.3
1	K	215	LEU	2.3
2	D	66	LEU	2.3
2	F	263	TYR	2.3
2	D	416	ASP	2.3
2	E	290	ASP	2.3
1	C	230	PHE	2.3
1	C	39	ILE	2.3
1	I	442	ASN	2.3
1	J	519	ILE	2.3
2	L	347	GLY	2.3
1	K	321	ALA	2.3
1	A	65	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	14	VAL	2.3
1	C	66	SER	2.3
1	J	69	LEU	2.3
1	J	240	SER	2.3
1	K	516	MET	2.3
2	E	355	LEU	2.3
2	E	442	LEU	2.3
2	N	257	LEU	2.3
2	N	29	TYR	2.3
2	E	247	PHE	2.3
2	E	350	PRO	2.3
2	N	327	ASP	2.3
1	C	132	GLY	2.3
1	I	454	ILE	2.3
1	K	454	ILE	2.3
2	E	303	GLY	2.3
2	L	285	GLY	2.3
2	M	97	GLY	2.3
1	A	316	GLN	2.3
1	I	414	ALA	2.3
1	C	441	GLU	2.3
1	I	81	ASN	2.3
2	F	338	GLN	2.3
2	F	425	GLN	2.3
1	I	189	VAL	2.3
1	K	554	VAL	2.3
2	N	73	VAL	2.3
1	A	220	MET	2.3
1	I	75	LEU	2.3
2	D	199	ARG	2.3
2	M	197	THR	2.3
1	A	184	TYR	2.3
2	D	104	PRO	2.3
2	E	313	ILE	2.3
2	D	45	GLY	2.3
2	E	323	HIS	2.3
2	M	294	ILE	2.3
1	I	382	GLY	2.3
4	H	85	ASP	2.3
2	L	55	ALA	2.3
1	A	497	GLN	2.3
1	B	218	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	250	VAL	2.3
1	K	159	GLU	2.3
2	D	43	ARG	2.3
2	F	275	GLU	2.3
1	A	133	MET	2.3
1	C	344	MET	2.3
1	C	119	TRP	2.3
1	A	362	TYR	2.3
2	E	13	TYR	2.3
1	C	204	PRO	2.3
2	L	10	GLY	2.3
1	A	29	LYS	2.3
1	B	325	ASP	2.3
1	K	247	ALA	2.3
2	F	69	ALA	2.3
1	B	371	LEU	2.3
1	I	378	VAL	2.3
1	I	381	VAL	2.3
2	D	218	VAL	2.3
1	A	122	MET	2.3
1	C	41	ARG	2.3
1	I	550	ARG	2.3
1	K	335	ARG	2.3
2	E	268	ARG	2.3
2	F	321	ARG	2.3
2	M	236	ARG	2.3
1	K	62	GLU	2.3
2	F	61	GLU	2.3
2	M	373	GLU	2.3
4	P	19	GLU	2.3
2	F	115	THR	2.3
1	A	288	ILE	2.3
1	J	226	ILE	2.3
2	M	154	SER	2.3
2	N	352	ILE	2.3
1	A	310	ALA	2.3
1	C	575	LYS	2.3
1	I	228	GLY	2.3
2	D	278	PRO	2.3
2	M	347	GLY	2.3
2	N	175	PRO	2.3
1	C	149	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	430	LEU	2.3
1	K	135	LEU	2.3
2	M	42	VAL	2.3
2	M	140	VAL	2.3
2	M	355	LEU	2.3
1	A	391	MET	2.3
1	I	220	MET	2.3
2	F	319	ASP	2.3
2	N	393	ARG	2.3
1	J	202	ASN	2.2
2	L	256	ILE	2.2
2	L	311	ILE	2.2
1	B	319	SER	2.2
1	C	352	PRO	2.2
1	I	245	SER	2.2
1	I	338	SER	2.2
2	D	15	SER	2.2
2	D	99	PRO	2.2
2	N	38	GLY	2.2
2	N	156	SER	2.2
1	C	333	ALA	2.2
2	D	267	LEU	2.2
2	F	82	LEU	2.2
2	L	18	LEU	2.2
1	B	258	ARG	2.2
1	C	325	ASP	2.2
2	F	170	GLN	2.2
2	F	353	ASP	2.2
2	N	408	ASP	2.2
1	A	343	GLU	2.2
1	I	558	GLU	2.2
1	J	447	TYR	2.2
2	N	23	ASN	2.2
2	N	120	ASN	2.2
1	A	432	THR	2.2
1	B	55	THR	2.2
1	K	273	THR	2.2
1	B	275	PRO	2.2
1	I	57	GLY	2.2
2	D	238	ALA	2.2
2	E	104	PRO	2.2
2	M	271	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	N	284	PRO	2.2
2	E	297	ARG	2.2
2	N	274	ARG	2.2
1	C	114	GLU	2.2
1	C	248	ASP	2.2
2	M	259	ASP	2.2
2	M	342	GLU	2.2
2	D	352	ILE	2.2
2	M	421	PHE	2.2
4	H	81	PHE	2.2
1	I	184	TYR	2.2
2	E	25	LYS	2.2
3	G	156	LYS	2.2
1	I	266	LEU	2.2
1	J	520	LEU	2.2
2	L	214	LEU	2.2
2	M	82	LEU	2.2
2	N	201	LEU	2.2
1	C	386	PRO	2.2
1	I	277	THR	2.2
1	I	323	MET	2.2
1	I	526	ALA	2.2
2	D	39	THR	2.2
2	D	460	GLY	2.2
2	E	113	PRO	2.2
2	F	324	PRO	2.2
2	L	116	GLY	2.2
2	N	231	ARG	2.2
1	A	525	GLU	2.2
1	A	428	TYR	2.2
1	I	476	LEU	2.2
1	I	523	TYR	2.2
2	F	139	ASP	2.2
2	M	318	ASP	2.2
1	A	178	GLY	2.2
1	A	202	ASN	2.2
1	B	554	VAL	2.2
1	A	333	ALA	2.2
1	A	366	GLY	2.2
1	I	178	GLY	2.2
1	I	468	VAL	2.2
1	K	51	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	173	VAL	2.2
1	A	420	PRO	2.2
1	B	10	ALA	2.2
1	B	201	PRO	2.2
1	C	89	ARG	2.2
2	E	271	GLY	2.2
2	L	403	ALA	2.2
2	M	45	GLY	2.2
2	N	171	ALA	2.2
1	A	396	THR	2.2
1	B	66	SER	2.2
1	C	40	ILE	2.2
1	C	519	ILE	2.2
1	I	80	LEU	2.2
1	K	480	GLU	2.2
2	E	404	LEU	2.2
2	D	226	ASP	2.2
2	F	67	ASP	2.2
2	F	283	TYR	2.2
2	D	396	VAL	2.2
1	A	259	GLY	2.2
1	B	567	MET	2.2
1	C	224	ALA	2.2
1	C	228	GLY	2.2
1	I	113	ARG	2.2
2	F	281	ARG	2.2
1	C	297	ALA	2.2
1	C	346	ALA	2.2
2	D	123	ALA	2.2
2	M	17	PRO	2.2
2	M	159	PRO	2.2
2	N	262	ASN	2.2
1	C	392	SER	2.2
1	I	555	SER	2.2
2	F	48	ILE	2.2
3	O	201	ILE	2.2
1	C	507	CYS	2.2
2	M	203	TYR	2.2
2	D	50	VAL	2.2
1	A	44	GLY	2.2
1	J	567	MET	2.2
2	N	34	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	47	ALA	2.2
2	F	90	GLY	2.2
1	I	275	PRO	2.2
2	N	326	PRO	2.2
2	F	94	ASN	2.2
1	A	575	LYS	2.2
2	M	348	ILE	2.2
2	E	68	LEU	2.2
3	G	28	LEU	2.2
1	A	250	VAL	2.2
1	B	469	GLN	2.2
1	I	320	VAL	2.2
2	M	29	TYR	2.2
2	M	295	TYR	2.2
2	M	88	MET	2.2
2	M	297	ARG	2.2
2	N	287	MET	2.2
1	I	315	ASP	2.1
1	I	475	ALA	2.1
1	J	85	ASP	2.1
2	D	213	ALA	2.1
2	M	186	PRO	2.1
4	P	101	ASP	2.1
1	K	48	PHE	2.1
1	I	111	LEU	2.1
1	I	458	LEU	2.1
2	L	158	LEU	2.1
2	M	19	LEU	2.1
2	M	219	LEU	2.1
2	N	328	LEU	2.1
1	C	167	THR	2.1
1	J	308	THR	2.1
1	K	396	THR	2.1
1	B	236	VAL	2.1
1	C	218	VAL	2.1
1	C	265	VAL	2.1
3	G	2	SER	2.1
2	D	260	MET	2.1
2	F	58	GLN	2.1
2	N	265	GLU	2.1
1	B	453	ALA	2.1
1	J	221	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	219	ALA	2.1
1	B	15	ILE	2.1
2	N	149	LYS	2.1
2	N	94	ASN	2.1
1	J	67	THR	2.1
2	E	115	THR	2.1
1	A	488	ARG	2.1
1	K	302	SER	2.1
2	E	349	TYR	2.1
2	N	453	ARG	2.1
2	E	166	GLN	2.1
1	C	57	GLY	2.1
1	I	110	ALA	2.1
1	I	155	GLY	2.1
1	K	514	GLY	2.1
2	D	49	GLU	2.1
1	K	361	PHE	2.1
2	D	451	LEU	2.1
2	M	135	ILE	2.1
2	N	311	ILE	2.1
2	N	380	ASP	2.1
2	E	218	VAL	2.1
2	M	120	ASN	2.1
1	I	516	MET	2.1
2	D	462	TYR	2.1
2	E	92	ARG	2.1
1	C	414	ALA	2.1
1	C	505	ALA	2.1
1	C	565	GLU	2.1
1	I	208	GLY	2.1
2	E	97	GLY	2.1
2	E	419	GLU	2.1
2	L	90	GLY	2.1
2	N	357	SER	2.1
2	E	205	ILE	2.1
2	F	66	LEU	2.1
2	L	440	TRP	2.1
2	M	20	PHE	2.1
1	J	353	TYR	2.1
2	L	172	THR	2.1
2	M	234	THR	2.1
1	A	354	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	464	LEU	2.1
1	K	131	GLY	2.1
1	K	409	LEU	2.1
2	F	116	GLY	2.1
2	L	134	GLY	2.1
2	N	132	GLN	2.1
4	H	80	ALA	2.1
4	P	40	GLY	2.1
1	A	87	ILE	2.1
1	B	125	PRO	2.1
1	B	330	TRP	2.1
1	I	121	PRO	2.1
1	J	87	ILE	2.1
2	F	51	SER	2.1
2	L	435	SER	2.1
2	N	215	SER	2.1
1	K	160	VAL	2.1
1	J	299	ARG	2.1
1	K	274	ASP	2.1
2	D	297	ARG	2.1
2	E	320	ASP	2.1
4	H	3	VAL	2.1
2	M	237	MET	2.1
2	M	393	ARG	2.1
3	O	196	ARG	2.1
4	P	67	ASP	2.1
1	I	353	TYR	2.1
1	K	52	TYR	2.1
1	A	576	ALA	2.1
1	B	366	GLY	2.1
1	C	18	GLY	2.1
1	B	570	ILE	2.1
1	C	269	PHE	2.1
1	C	576	ALA	2.1
1	I	67	THR	2.1
1	I	205	PHE	2.1
1	I	572	GLY	2.1
1	K	136	GLY	2.1
1	K	505	ALA	2.1
2	M	333	THR	2.1
2	M	369	GLY	2.1
1	K	536	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	N	348	ILE	2.1
1	K	455	SER	2.1
1	K	546	GLU	2.1
1	A	236	VAL	2.1
2	N	241	VAL	2.1
1	C	401	ARG	2.1
2	F	453	ARG	2.1
2	D	78	ASP	2.1
1	J	312	TYR	2.1
2	D	19	LEU	2.1
2	D	221	LEU	2.1
4	H	18	LEU	2.1
1	B	40	ILE	2.1
1	B	303	ILE	2.1
1	C	242	ALA	2.1
1	C	453	ALA	2.1
1	I	231	GLY	2.1
1	I	269	PHE	2.1
2	D	363	ASN	2.1
2	F	213	ALA	2.1
4	P	20	GLY	2.1
1	C	396	THR	2.1
2	F	309	THR	2.1
2	M	64	THR	2.1
2	M	309	THR	2.1
2	L	340	SER	2.1
1	A	253	VAL	2.1
1	K	391	MET	2.0
2	D	92	ARG	2.0
1	A	161	LYS	2.0
1	K	234	LYS	2.0
1	I	410	ASP	2.0
4	P	36	LEU	2.0
1	I	553	TYR	2.0
1	J	439	TYR	2.0
1	C	479	ALA	2.0
1	J	61	GLY	2.0
1	J	242	ALA	2.0
1	J	254	GLY	2.0
1	K	487	GLY	2.0
2	D	100	ILE	2.0
2	N	11	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	461	GLU	2.0
1	C	128	GLU	2.0
1	J	140	GLU	2.0
1	B	433	SER	2.0
1	K	544	VAL	2.0
2	L	396	VAL	2.0
1	K	322	LEU	2.0
2	M	436	LEU	2.0
2	N	314	LEU	2.0
1	B	431	PHE	2.0
1	J	536	ILE	2.0
2	D	392	ILE	2.0
2	F	130	PHE	2.0
2	L	205	ILE	2.0
1	A	213	ASP	2.0
1	B	389	GLY	2.0
1	C	382	GLY	2.0
1	I	512	ALA	2.0
1	A	121	PRO	2.0
1	B	70	PRO	2.0
1	B	437	PRO	2.0
1	C	227	PRO	2.0
2	E	351	PRO	2.0
1	J	179	THR	2.0
1	K	189	VAL	2.0
2	L	329	THR	2.0
2	N	293	THR	2.0
1	A	113	ARG	2.0
1	A	364	ARG	2.0
2	L	430	ARG	2.0
1	I	29	LYS	2.0
2	D	219	LEU	2.0
2	L	315	SER	2.0
2	M	136	SER	2.0
1	I	519	ILE	2.0
3	O	176	ILE	2.0
1	A	110	ALA	2.0
1	C	487	GLY	2.0
1	A	397	GLN	2.0
1	I	130	ARG	2.0
1	J	239	GLN	2.0
2	F	190	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	111	ARG	2.0
2	F	440	TRP	2.0
1	I	42	LEU	2.0
1	K	577	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.