



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:16 AM UTC

PDB ID : 8GPU / pdb_00008gpu
Title : YFV_E_YD6Fab_prefusion
Authors : Li, Y.; Wu, L.; Qi, J.; Yan, J.; Gao, G.F.
Deposited on : 2022-08-27
Resolution : 2.79 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:

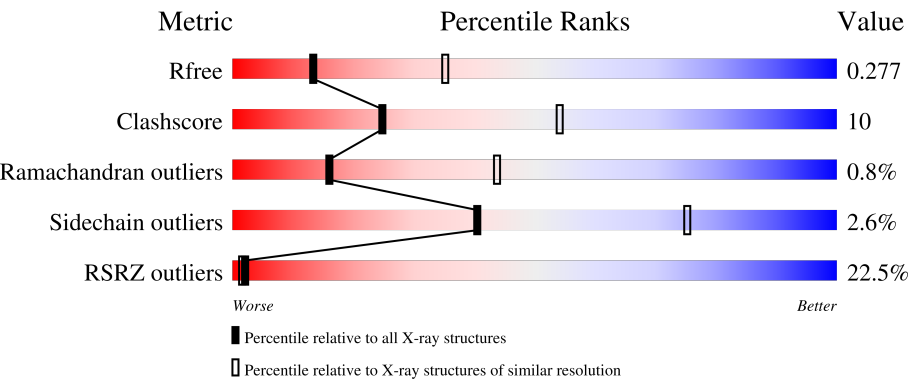
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	398	<div><div>11%</div><div>78%</div><div>20%</div><div>..</div></div>
1	B	398	<div><div>11%</div><div>71%</div><div>24%</div><div>..</div></div>
1	E	398	<div><div>17%</div><div>72%</div><div>24%</div><div>..</div></div>
1	I	398	<div><div>14%</div><div>79%</div><div>16%</div><div>...</div></div>
1	M	398	<div><div>28%</div><div>75%</div><div>21%</div><div>...</div></div>

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Mol	Chain	Length	Quality of chain
1	P	398	
2	C	217	
2	F	217	
2	H	217	
2	J	217	
2	N	217	
2	Q	217	
3	D	217	
3	G	217	
3	K	217	
3	L	217	
3	O	217	
3	R	217	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 37132 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 Envelope protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	1	0
			2997	1877	518	582	20			
1	E	392	Total	C	N	O	S	0	0	0
			2985	1868	515	582	20			
1	B	388	Total	C	N	O	S	0	1	0
			2965	1861	512	572	20			
1	I	388	Total	C	N	O	S	0	0	0
			2952	1853	508	571	20			
1	M	388	Total	C	N	O	S	0	0	0
			2950	1851	508	571	20			
1	P	388	Total	C	N	O	S	0	0	0
			2950	1851	508	571	20			

- Molecule 2 is a protein called YD6Fab_H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1623	1028	270	318	7			
2	F	216	Total	C	N	O	S	0	0	0
			1623	1028	270	318	7			
2	C	216	Total	C	N	O	S	0	0	0
			1623	1028	270	318	7			
2	J	211	Total	C	N	O	S	0	0	0
			1591	1010	264	310	7			
2	N	216	Total	C	N	O	S	0	0	0
			1623	1028	270	318	7			
2	Q	216	Total	C	N	O	S	0	0	0
			1623	1028	270	318	7			

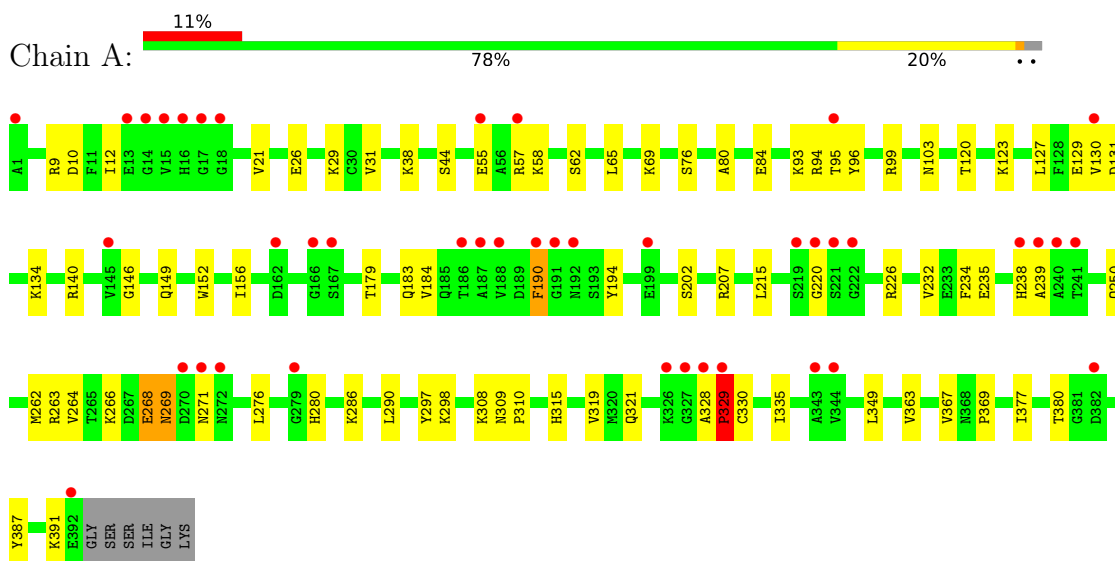
- Molecule 3 is a protein called YD6Fab_L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1601	1004	267	325	5			
3	G	216	Total	C	N	O	S	0	0	0
			1614	1010	268	330	6			
3	D	213	Total	C	N	O	S	0	0	0
			1594	1000	266	323	5			
3	K	214	Total	C	N	O	S	0	0	0
			1601	1004	267	325	5			
3	O	217	Total	C	N	O	S	0	0	0
			1623	1015	270	332	6			
3	R	213	Total	C	N	O	S	0	0	0
			1594	1000	266	323	5			

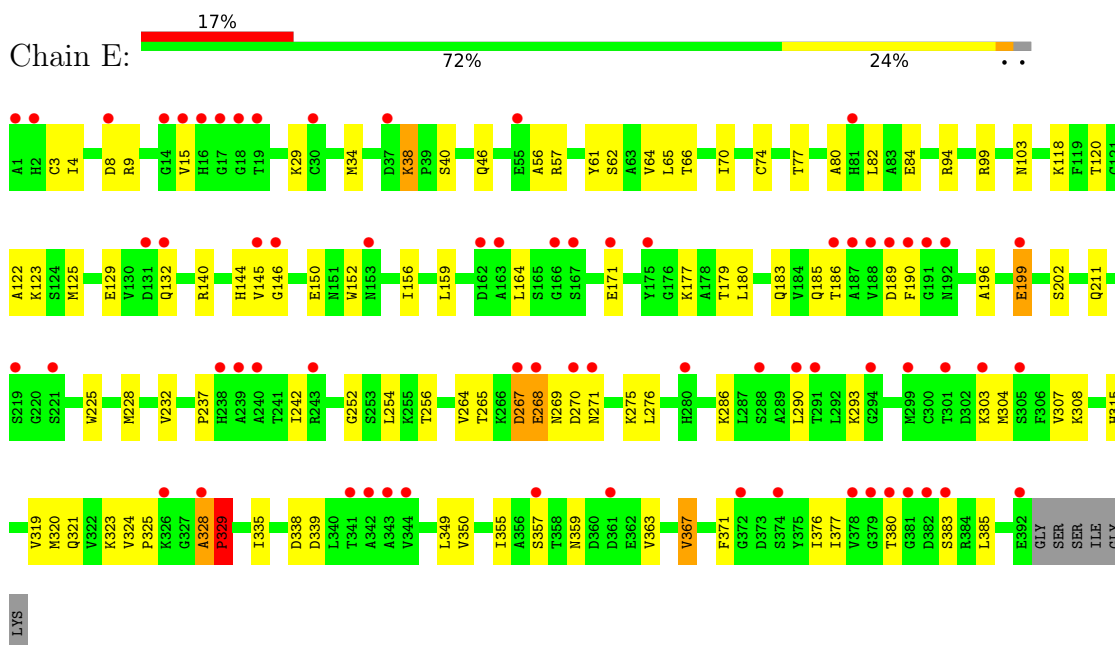
3 Residue-property plots [i](#)

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.

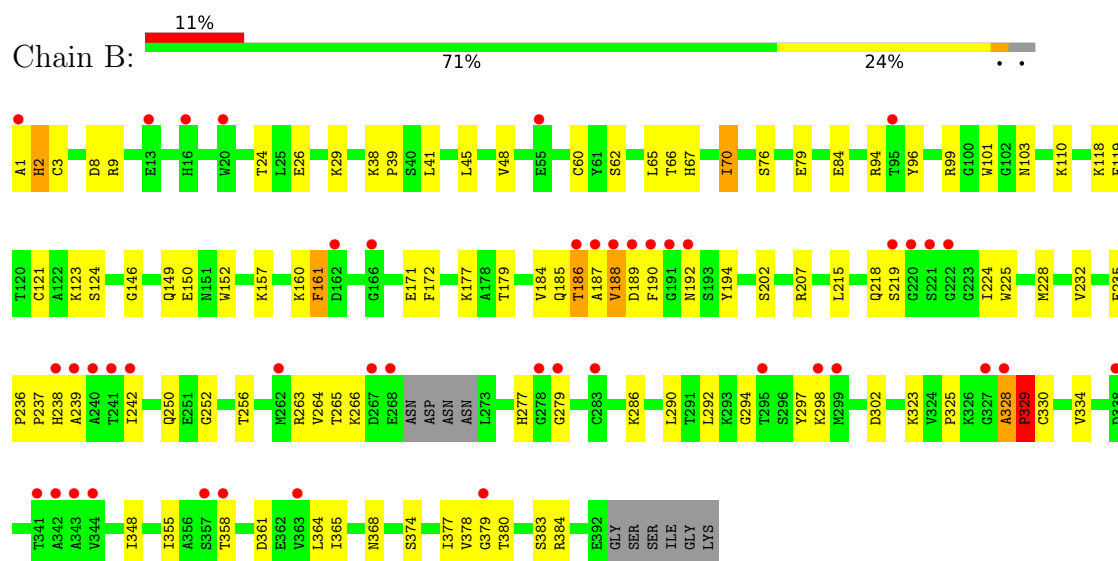
• Molecule 1: Envelope protein



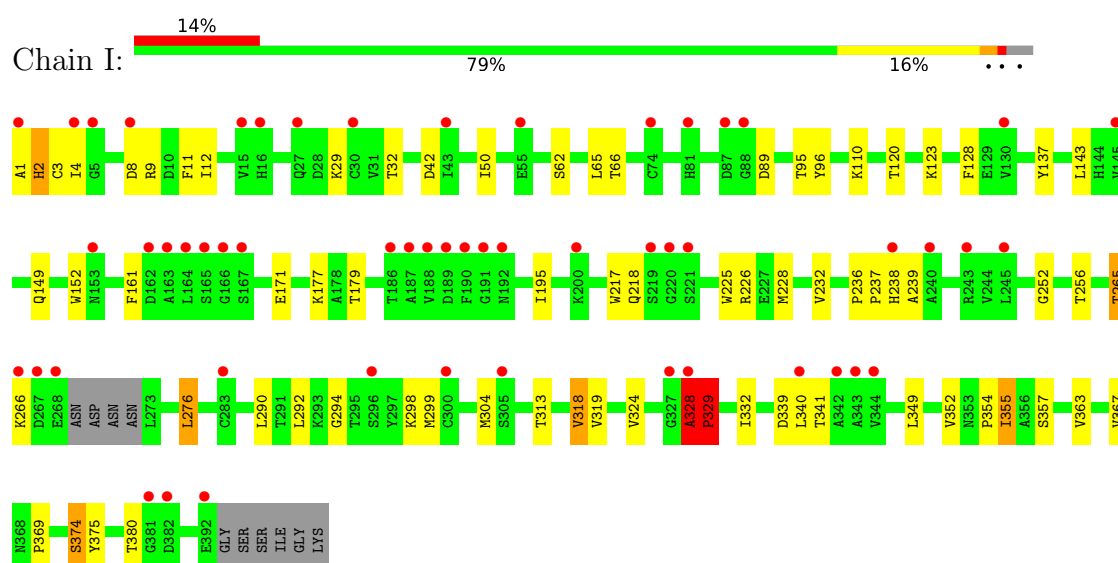
• Molecule 1: Envelope protein



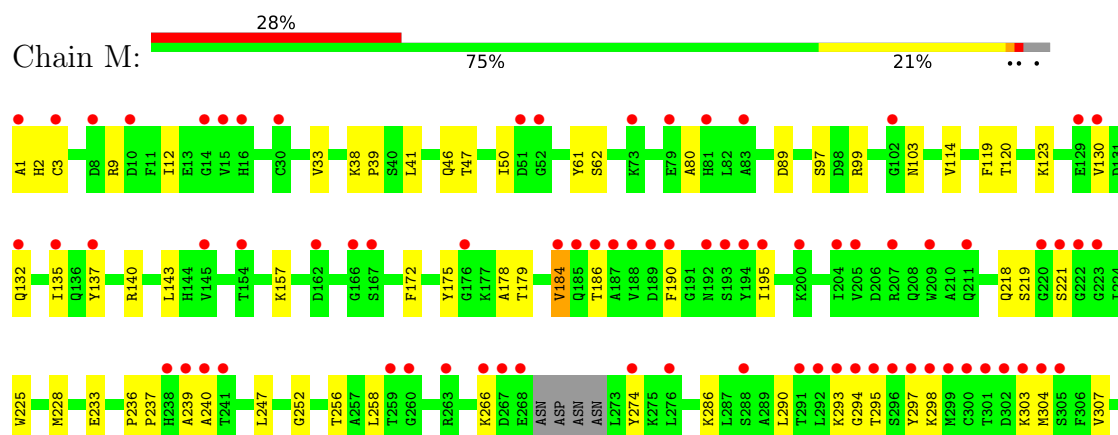
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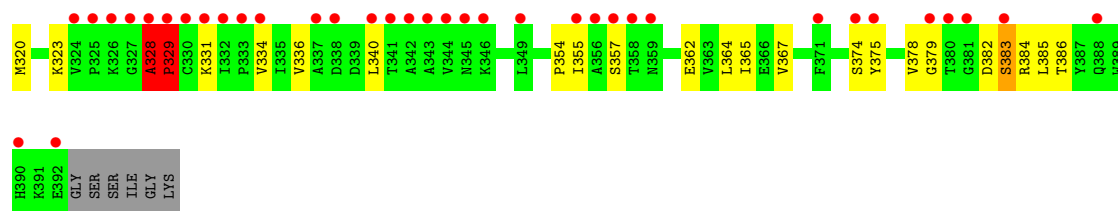


• Molecule 1: Envelope protein

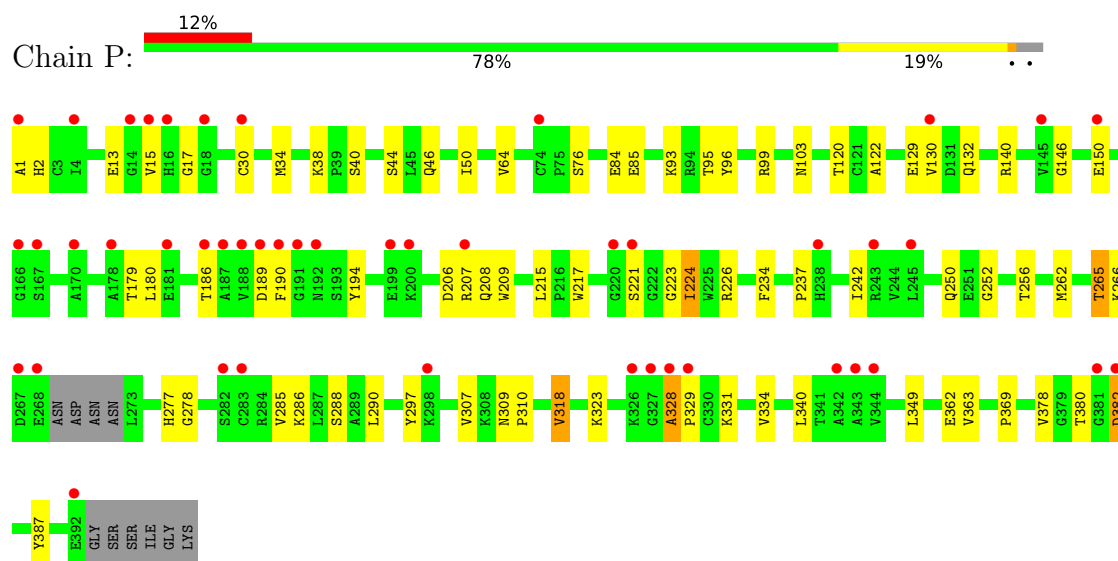


• Molecule 1: Envelope protein

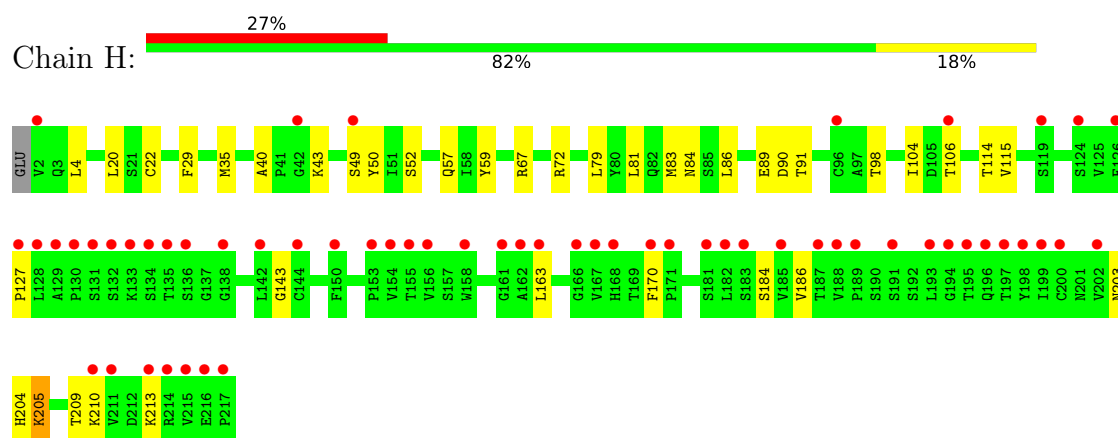




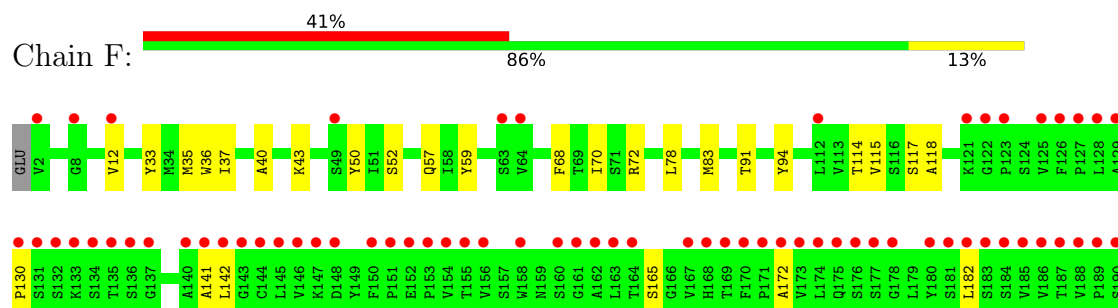
• Molecule 1: Envelope protein

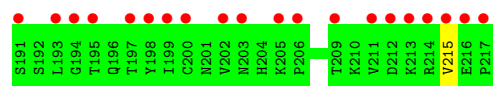


• Molecule 2: YD6Fab_H

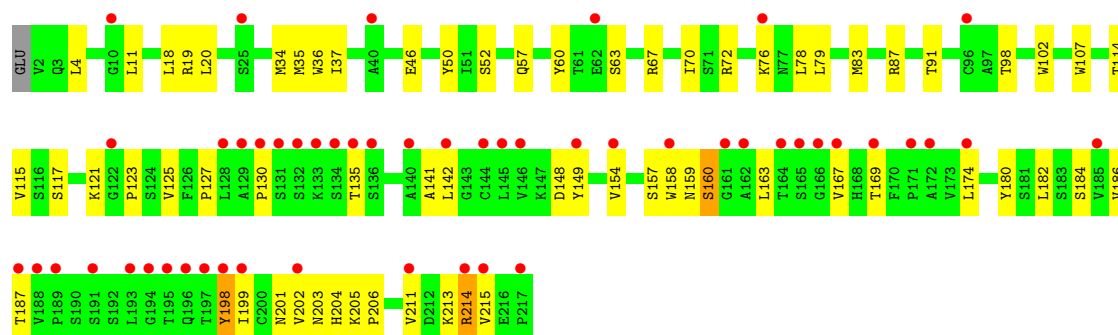


• Molecule 2: YD6Fab_H

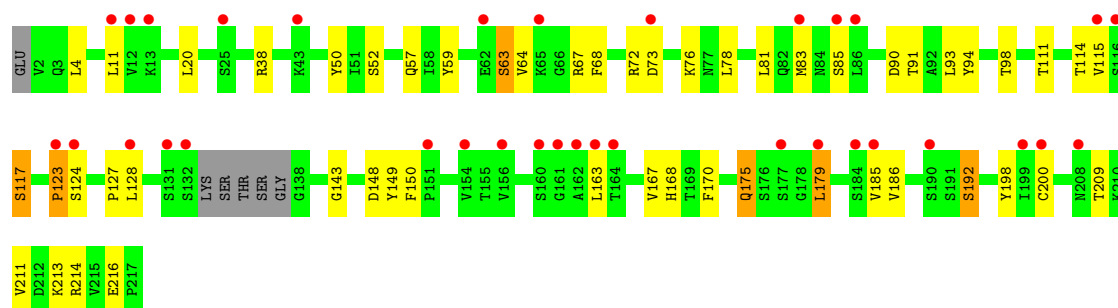
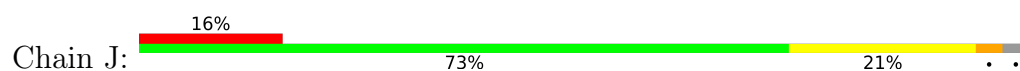




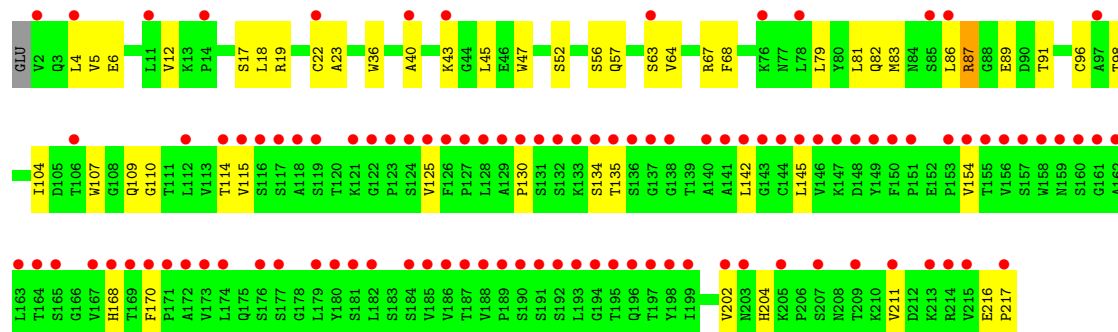
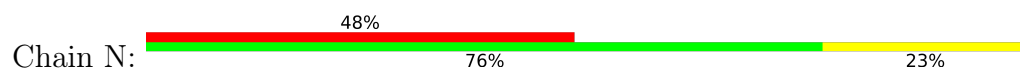
• Molecule 2: YD6Fab_H



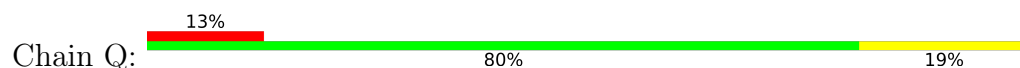
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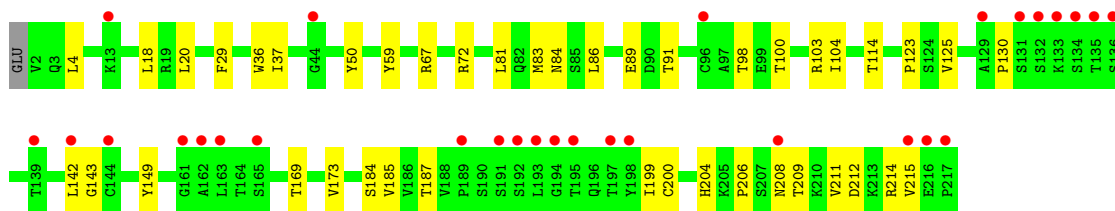


• Molecule 2: YD6Fab_H

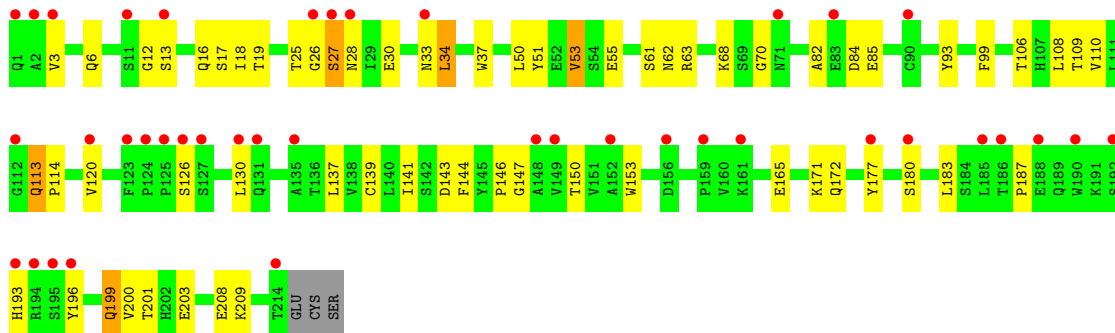


• Molecule 2: YD6Fab_H

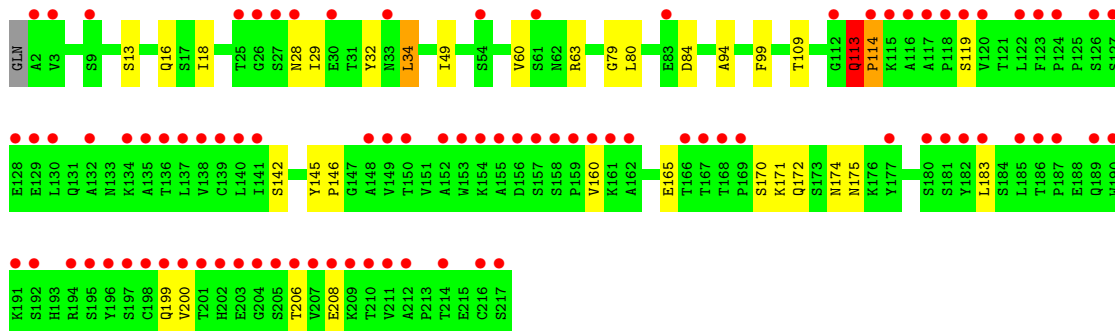
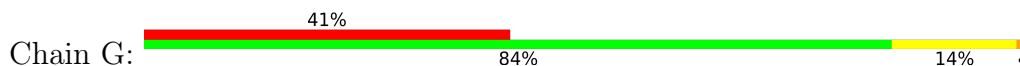




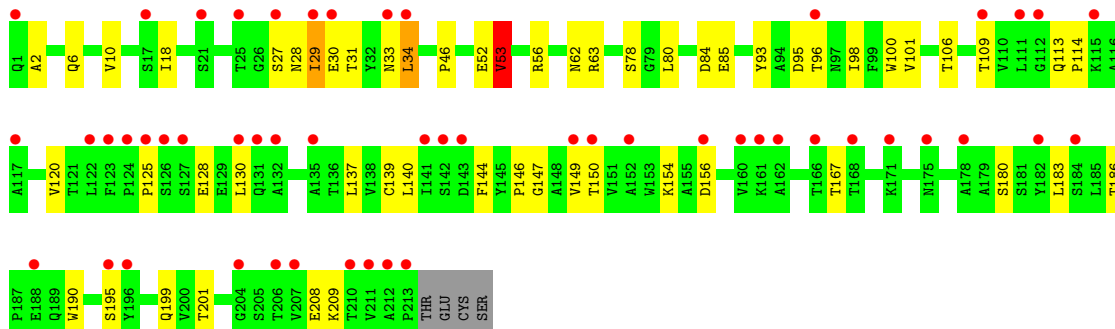
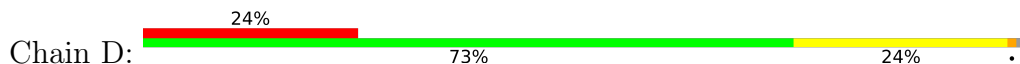
• Molecule 3: YD6Fab_L



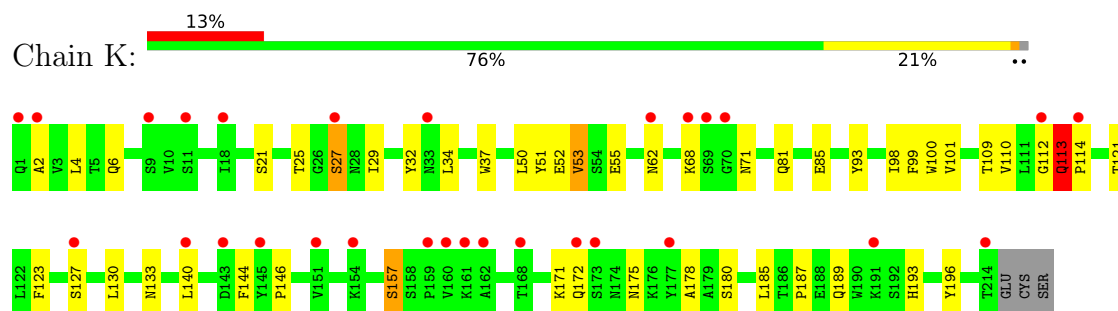
• Molecule 3: YD6Fab_L



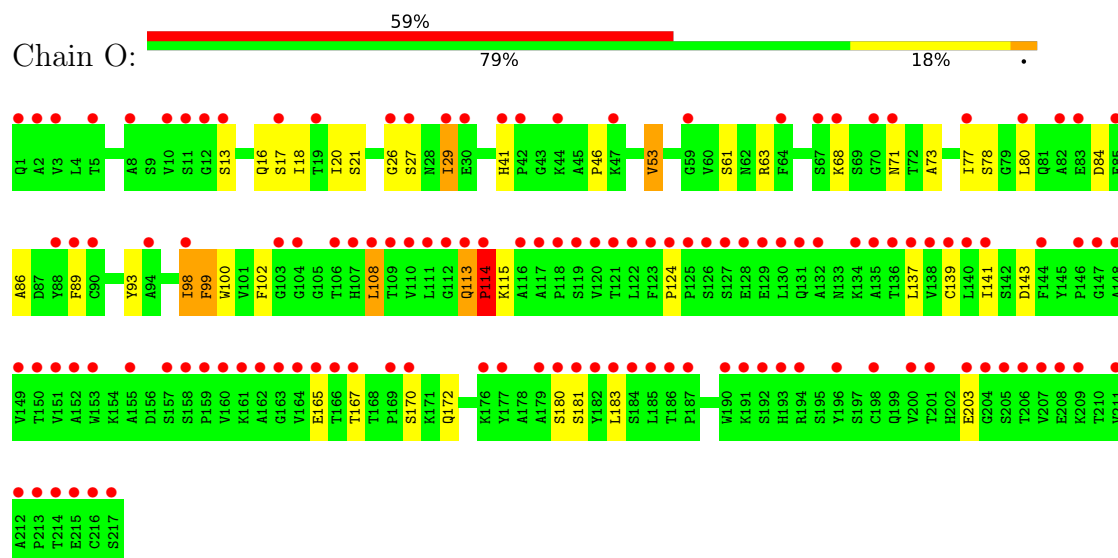
• Molecule 3: YD6Fab_L



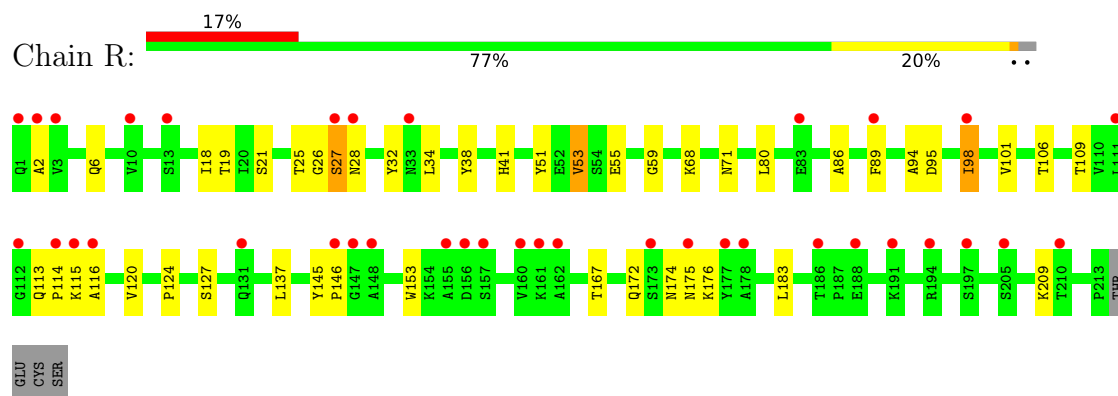
- Molecule 3: YD6Fab_L



- Molecule 3: YD6Fab_L



- Molecule 3: YD6Fab_L



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	157.26Å 278.00Å 354.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.57 – 2.79 42.57 – 2.79	Depositor EDS
% Data completeness (in resolution range)	85.4 (42.57-2.79) 85.3 (42.57-2.79)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.244 , 0.279 0.243 , 0.277	Depositor DCC
R_{free} test set	8337 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.006 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	37132	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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	0.17	0/3061	0.38	0/4153
1	B	0.18	0/3025	0.40	0/4102
1	E	0.20	0/3045	0.46	4/4132 (0.1%)
1	I	0.16	0/3011	0.37	3/4084 (0.1%)
1	M	0.21	0/3009	0.48	5/4081 (0.1%)
1	P	0.18	0/3009	0.43	1/4081 (0.0%)
2	C	0.24	0/1662	0.50	2/2262 (0.1%)
2	F	0.20	0/1662	0.44	2/2262 (0.1%)
2	H	0.18	0/1662	0.40	0/2262
2	J	0.20	0/1629	0.46	1/2217 (0.0%)
2	N	0.19	0/1662	0.40	0/2262
2	Q	0.19	0/1662	0.35	0/2262
3	D	0.28	0/1634	0.56	0/2232
3	G	0.27	0/1654	0.54	3/2258 (0.1%)
3	K	0.28	0/1641	0.55	2/2242 (0.1%)
3	L	0.32	0/1641	0.58	0/2242
3	O	0.32	0/1663	0.61	1/2270 (0.0%)
3	R	0.31	0/1634	0.52	0/2232
All	All	0.22	0/37966	0.46	24/51636 (0.0%)

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	B	0	1
1	I	0	1
3	K	0	1
All	All	0	3

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	382	ASP	N-CA-C	-12.33	98.24	113.28
1	M	383	SER	N-CA-C	-8.24	102.78	112.92
3	O	114	PRO	N-CA-CB	-8.14	94.70	103.25
2	F	118	ALA	CA-C-N	6.82	134.23	122.64
2	F	118	ALA	C-N-CA	6.82	134.23	122.64
1	E	329	PRO	CA-N-CD	-6.43	102.99	112.00
1	I	328	ALA	CA-C-N	6.39	127.82	119.84
1	I	328	ALA	C-N-CA	6.39	127.82	119.84
1	M	328	ALA	CA-C-N	6.35	127.78	119.84
1	M	328	ALA	C-N-CA	6.35	127.78	119.84
3	G	29	ILE	N-CA-C	-6.18	107.84	113.71
1	M	382	ASP	CB-CA-C	6.11	121.02	110.94
1	E	329	PRO	N-CA-CB	-6.08	96.87	103.25
1	I	329	PRO	CA-N-CD	-5.88	103.77	112.00
3	K	113	GLN	CA-C-N	5.85	127.16	119.84
3	K	113	GLN	C-N-CA	5.85	127.16	119.84
1	E	328	ALA	CA-C-N	5.78	127.06	119.84
1	E	328	ALA	C-N-CA	5.78	127.06	119.84
2	C	117	SER	CA-C-N	5.78	129.31	120.82
2	C	117	SER	C-N-CA	5.78	129.31	120.82
2	J	117	SER	CA-C-O	-5.65	114.53	120.58
1	M	329	PRO	CA-N-CD	-5.28	104.60	112.00
3	G	113	GLN	CA-C-N	5.01	126.10	119.84
3	G	113	GLN	C-N-CA	5.01	126.10	119.84

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	328	ALA	Mainchain
1	I	328	ALA	Mainchain
3	K	112	GLY	Mainchain

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	2997	0	2934	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2965	0	2908	81	0
1	E	2985	0	2911	58	0
1	I	2952	0	2893	40	0
1	M	2950	0	2886	53	0
1	P	2950	0	2886	57	0
2	C	1623	0	1595	48	0
2	F	1623	0	1595	17	0
2	H	1623	0	1595	26	0
2	J	1591	0	1561	38	0
2	N	1623	0	1595	39	0
2	Q	1623	0	1595	26	0
3	D	1594	0	1541	38	0
3	G	1614	0	1553	20	0
3	K	1601	0	1548	41	0
3	L	1601	0	1548	39	0
3	O	1623	0	1564	45	0
3	R	1594	0	1541	32	0
All	All	37132	0	36249	716	0

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 10.

All (716) 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)
1:P:328:ALA:CB	1:P:329:PRO:HD2	1.72	1.19
2:C:76:LYS:O	2:C:78:LEU:HD23	1.43	1.18
3:O:113:GLN:CG	3:O:114:PRO:HD3	1.76	1.14
1:P:328:ALA:HB1	1:P:329:PRO:CD	1.79	1.13
3:O:113:GLN:CB	3:O:114:PRO:HD3	1.78	1.12
1:P:328:ALA:CB	1:P:329:PRO:CD	2.25	1.12
1:A:328:ALA:HB1	1:A:329:PRO:HD2	1.16	1.10
1:P:328:ALA:HB3	1:P:329:PRO:HD2	1.30	1.06
1:B:328:ALA:HB1	1:B:329:PRO:CD	1.87	1.05
1:B:328:ALA:HB1	1:B:329:PRO:HD2	1.40	1.04
3:O:113:GLN:HG3	3:O:114:PRO:CD	1.88	1.04
3:O:113:GLN:HB2	3:O:114:PRO:HD3	1.38	1.03
3:O:20:ILE:HD11	3:O:108:LEU:CD1	1.91	0.99
3:K:113:GLN:HB2	3:K:114:PRO:HD3	1.44	0.98
1:A:328:ALA:HB1	1:A:329:PRO:CD	1.95	0.96
1:B:187:ALA:HB2	1:B:279:GLY:HA3	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:113:GLN:HG3	3:O:114:PRO:HD3	1.49	0.90
1:P:328:ALA:HB1	1:P:329:PRO:HD3	1.51	0.90
1:E:329:PRO:HD3	1:E:357:SER:O	1.72	0.89
1:A:328:ALA:CB	1:A:329:PRO:HD2	2.01	0.89
3:D:109:THR:HG21	3:D:146:PRO:HB3	1.55	0.87
1:P:179:THR:HB	1:P:286:LYS:HB3	1.56	0.86
1:M:303:LYS:HA	1:M:383:SER:OG	1.76	0.85
2:J:123:PRO:HB3	2:J:149:TYR:HB3	1.58	0.85
2:C:76:LYS:O	2:C:78:LEU:CD2	2.24	0.84
3:O:113:GLN:CB	3:O:114:PRO:CD	2.57	0.82
3:G:113:GLN:CG	3:G:114:PRO:HD3	2.09	0.82
3:O:113:GLN:CG	3:O:114:PRO:CD	2.50	0.82
2:H:163:LEU:HD21	2:H:186:VAL:HG21	1.61	0.81
3:K:29:ILE:HG22	3:K:68:LYS:HE3	1.62	0.80
1:B:265:THR:HG1	1:B:277:HIS:HE2	1.30	0.80
3:G:113:GLN:HG2	3:G:114:PRO:CD	2.12	0.79
1:B:328:ALA:CB	1:B:329:PRO:HD2	2.11	0.79
3:O:20:ILE:HD11	3:O:108:LEU:HD11	1.63	0.78
3:O:113:GLN:HB2	3:O:114:PRO:CD	2.15	0.77
2:N:170:PHE:HD2	3:O:180:SER:HB3	1.49	0.77
3:G:113:GLN:HG3	3:G:114:PRO:HD3	1.66	0.77
2:C:142:LEU:HD11	2:C:198:TYR:HE2	1.51	0.76
3:O:113:GLN:HG3	3:O:114:PRO:HD2	1.64	0.76
3:L:113:GLN:HB2	3:L:114:PRO:CD	2.16	0.76
2:C:167:VAL:HG22	2:C:186:VAL:HG12	1.69	0.76
1:M:323:LYS:HG3	1:M:362:GLU:HG2	1.68	0.75
3:G:113:GLN:CG	3:G:114:PRO:CD	2.64	0.75
3:G:113:GLN:HG2	3:G:114:PRO:HD2	1.69	0.74
3:L:113:GLN:HB2	3:L:114:PRO:HD3	1.71	0.73
1:E:303:LYS:HA	1:E:383:SER:HB3	1.70	0.72
1:P:95:THR:HG22	1:P:96:TYR:H	1.55	0.72
3:K:113:GLN:HB2	3:K:114:PRO:CD	2.19	0.71
2:C:127:PRO:HG3	2:C:213:LYS:HG3	1.73	0.71
3:D:113:GLN:HG2	3:D:114:PRO:HD2	1.72	0.71
3:D:113:GLN:HG2	3:D:114:PRO:CD	2.21	0.71
2:F:130:PRO:HB3	2:F:142:LEU:HD11	1.73	0.70
1:M:99:ARG:HA	1:M:103:ASN:HD21	1.58	0.69
3:K:29:ILE:O	3:K:68:LYS:NZ	2.22	0.69
3:R:172:GLN:N	3:R:176:LYS:O	2.21	0.69
1:E:304:MET:HG2	1:E:324:VAL:HG22	1.74	0.68
2:N:91:THR:HG23	2:N:114:THR:HA	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:32:TYR:HB3	3:G:34:LEU:HD23	1.76	0.68
2:Q:199:ILE:HG12	2:Q:214:ARG:HG2	1.74	0.68
2:C:142:LEU:HD13	2:C:215:VAL:HG11	1.75	0.67
1:P:146:GLY:HA3	1:P:363:VAL:HG23	1.77	0.67
3:D:29:ILE:O	3:D:31:THR:N	2.27	0.67
1:A:235:GLU:OE2	1:B:263:ARG:NH1	2.27	0.67
3:K:85:GLU:HG3	3:K:109:THR:HA	1.77	0.66
2:J:170:PHE:HE2	3:K:180:SER:HB3	1.59	0.66
3:R:53:VAL:HG11	3:R:68:LYS:HB2	1.77	0.66
2:J:175:GLN:H	2:J:175:GLN:HE21	1.42	0.65
1:M:50:ILE:HD11	1:M:190:PHE:HE2	1.62	0.65
3:O:18:ILE:HG21	3:O:108:LEU:HD21	1.78	0.65
1:P:323:LYS:HG3	1:P:362:GLU:HG2	1.77	0.65
1:B:84:GLU:OE1	1:B:84:GLU:N	2.30	0.65
1:B:328:ALA:HB1	1:B:329:PRO:HD3	1.78	0.65
1:E:171:GLU:HB3	1:E:177:LYS:HB3	1.79	0.65
1:P:130:VAL:HG11	1:P:190:PHE:CZ	2.32	0.65
3:R:32:TYR:HB3	3:R:34:LEU:HD23	1.79	0.65
1:E:267:ASP:OD2	1:E:275:LYS:NZ	2.21	0.64
1:A:179:THR:HB	1:A:286:LYS:HB3	1.77	0.64
3:O:20:ILE:CD1	3:O:108:LEU:CD1	2.70	0.64
3:G:63:ARG:NH1	3:G:79:GLY:O	2.30	0.64
3:O:139:CYS:HB3	3:O:181:SER:OG	1.98	0.64
3:G:171:LYS:HE3	3:G:175:ASN:HA	1.80	0.64
1:I:332:ILE:HB	1:I:354:PRO:HB2	1.80	0.63
3:D:34:LEU:HA	3:D:52:GLU:HA	1.79	0.63
3:D:63:ARG:NH2	3:D:84:ASP:OD2	2.30	0.63
1:M:328:ALA:HB1	1:M:329:PRO:HD2	1.80	0.63
2:N:18:LEU:HD12	2:N:19:ARG:H	1.63	0.63
2:J:64:VAL:HB	2:J:68:PHE:HD2	1.64	0.63
3:O:77:ILE:HD13	3:O:80:LEU:HD13	1.80	0.63
2:H:91:THR:HG23	2:H:114:THR:HA	1.79	0.63
2:F:91:THR:HG23	2:F:114:THR:HA	1.78	0.63
1:I:62:SER:HB3	1:I:123:LYS:HB2	1.80	0.63
1:I:329:PRO:HD3	1:I:357:SER:O	1.99	0.62
1:E:179:THR:HB	1:E:286:LYS:HB3	1.81	0.62
2:C:160:SER:HA	2:C:201:ASN:OD1	1.99	0.62
1:E:40:SER:HB2	1:E:144:HIS:HB2	1.80	0.62
3:R:113:GLN:HB3	3:R:114:PRO:CD	2.30	0.62
2:Q:143:GLY:HA3	2:Q:185:VAL:HG12	1.80	0.62
1:A:310:PRO:HD2	1:A:387:TYR:HD2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:154:VAL:HG12	2:N:204:HIS:HD2	1.64	0.62
2:C:35:MET:HB3	2:C:50:TYR:HD1	1.65	0.62
2:Q:91:THR:HG23	2:Q:114:THR:HA	1.81	0.62
2:C:11:LEU:HD12	2:C:11:LEU:O	2.00	0.61
2:H:50:TYR:HB3	2:H:59:TYR:HB2	1.80	0.61
2:F:36:TRP:HD1	2:F:70:ILE:HD12	1.65	0.61
2:J:148:ASP:HA	2:J:179:LEU:HD13	1.81	0.61
3:K:185:LEU:HD22	3:K:189:GLN:HB3	1.83	0.61
1:A:84:GLU:N	1:A:84:GLU:OE1	2.31	0.61
3:L:85:GLU:HB2	3:L:110:VAL:HG22	1.83	0.61
3:L:113:GLN:CB	3:L:114:PRO:CD	2.76	0.61
1:P:206:ASP:OD1	1:P:208:GLN:N	2.34	0.61
1:E:152:TRP:O	1:E:156:ILE:HG13	2.00	0.61
3:R:174:ASN:ND2	3:R:176:LYS:HD2	2.16	0.61
3:K:109:THR:HG21	3:K:146:PRO:HB3	1.83	0.60
1:E:62:SER:HB3	1:E:123:LYS:HB2	1.83	0.60
1:E:99:ARG:HA	1:E:103:ASN:HD21	1.66	0.60
1:A:99:ARG:HA	1:A:103:ASN:HD21	1.65	0.60
3:L:33:ASN:OD1	3:L:68:LYS:NZ	2.34	0.60
1:I:328:ALA:HB1	1:I:329:PRO:HD2	1.82	0.60
3:L:137:LEU:HD13	3:L:183:LEU:HD23	1.83	0.60
3:G:28:ASN:HA	3:G:94:ALA:HA	1.84	0.60
2:J:163:LEU:HD21	2:J:186:VAL:HG21	1.83	0.60
3:L:62:ASN:ND2	3:R:59:GLY:HA3	2.16	0.60
1:I:294:GLY:HA3	1:I:355:ILE:HD11	1.83	0.60
3:R:26:GLY:O	3:R:71:ASN:ND2	2.33	0.60
1:A:130:VAL:HG21	1:A:190:PHE:CE1	2.36	0.59
1:B:38:LYS:NZ	1:B:290:LEU:O	2.32	0.59
2:C:130:PRO:HB3	2:C:142:LEU:HB3	1.84	0.59
1:P:130:VAL:HG11	1:P:190:PHE:CE1	2.37	0.59
3:R:174:ASN:HD21	3:R:176:LYS:HD2	1.66	0.59
2:J:123:PRO:CB	2:J:149:TYR:HB3	2.32	0.59
2:N:19:ARG:NH1	2:N:82:GLN:OE1	2.35	0.59
3:D:113:GLN:CG	3:D:114:PRO:CD	2.81	0.59
3:R:95:ASP:OD1	3:R:98:ILE:HB	2.02	0.59
1:M:46:GLN:HG2	1:M:47:THR:HG23	1.82	0.59
3:O:53:VAL:HG11	3:O:68:LYS:HG3	1.85	0.59
1:A:131:ASP:HB3	1:A:134:LYS:HG3	1.83	0.59
2:N:22:CYS:HB3	2:N:79:LEU:HB3	1.85	0.59
3:L:13:SER:H	3:L:16:GLN:HE22	1.50	0.59
3:G:113:GLN:HB3	3:G:145:TYR:CE2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:125:PRO:HD2	3:D:190:TRP:CZ2	2.38	0.59
3:D:156:ASP:OD1	3:D:195:SER:N	2.26	0.59
3:K:113:GLN:CB	3:K:114:PRO:CD	2.81	0.59
1:M:62:SER:HB3	1:M:123:LYS:HB2	1.84	0.59
2:C:11:LEU:HD12	2:C:11:LEU:C	2.28	0.58
1:E:268:GLU:O	1:E:270:ASP:N	2.29	0.58
1:B:3:CYS:HB3	1:B:9:ARG:HG3	1.85	0.58
3:O:63:ARG:NH2	3:O:84:ASP:OD2	2.35	0.58
2:C:157:SER:O	2:C:201:ASN:N	2.37	0.58
1:P:297:TYR:O	1:P:331:LYS:NZ	2.37	0.58
1:A:58:LYS:HG3	1:A:220:GLY:HA2	1.84	0.58
1:B:265:THR:OG1	1:B:277:HIS:NE2	2.23	0.58
1:M:137:TYR:CE1	1:M:184:VAL:HG22	2.39	0.58
1:B:187:ALA:HB2	1:B:279:GLY:CA	2.29	0.58
2:C:52:SER:O	2:C:72:ARG:NH1	2.37	0.58
1:A:93:LYS:HD2	1:A:234:PHE:HB2	1.85	0.58
3:G:13:SER:H	3:G:16:GLN:NE2	2.02	0.58
3:O:63:ARG:NH1	3:O:78:SER:O	2.37	0.58
2:N:87:ARG:HD3	2:N:89:GLU:OE1	2.04	0.57
1:A:369:PRO:HG2	1:A:391:LYS:HE3	1.86	0.57
1:B:294:GLY:HA3	1:B:297:TYR:CE2	2.39	0.57
2:J:73:ASP:HB3	2:J:78:LEU:HB2	1.86	0.57
1:M:225:TRP:HB2	1:M:228:MET:HE3	1.85	0.57
3:L:120:VAL:O	3:L:209:LYS:NZ	2.30	0.57
2:C:20:LEU:HD13	2:C:83:MET:HE2	1.86	0.57
3:K:37:TRP:HB2	3:K:50:LEU:HB2	1.87	0.57
1:A:297:TYR:HB3	1:A:330:CYS:HA	1.87	0.57
3:K:113:GLN:CB	3:K:114:PRO:HD3	2.23	0.57
1:A:238[A]:HIS:CG	1:A:239:ALA:N	2.73	0.57
2:F:35:MET:HB3	2:F:50:TYR:HD1	1.70	0.57
2:J:91:THR:HG23	2:J:114:THR:HA	1.86	0.57
3:L:143:ASP:OD1	3:L:172:GLN:NE2	2.31	0.57
1:B:334:VAL:HG22	1:B:378:VAL:HG22	1.87	0.57
2:N:5:VAL:HG22	2:N:23:ALA:HB3	1.86	0.56
1:A:69:LYS:NZ	1:A:84:GLU:OE2	2.36	0.56
1:B:358:THR:OG1	1:B:361:ASP:OD1	2.23	0.56
3:G:63:ARG:HH22	3:G:84:ASP:CG	2.14	0.56
2:J:52:SER:O	2:J:72:ARG:NH1	2.38	0.56
2:Q:142:LEU:HD13	2:Q:215:VAL:HG11	1.88	0.56
1:A:298:LYS:O	1:A:330:CYS:HB2	2.06	0.56
3:L:199:GLN:HB3	3:L:208:GLU:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:GLY:O	1:E:256:THR:HG23	2.06	0.56
1:B:265:THR:HG22	1:B:266:LYS:H	1.70	0.56
2:C:36:TRP:HD1	2:C:70:ILE:HD12	1.70	0.56
1:E:202:SER:HB2	1:E:264:VAL:HB	1.88	0.56
1:B:39:PRO:HD2	1:B:290:LEU:HB3	1.87	0.56
1:B:328:ALA:CB	1:B:329:PRO:CD	2.65	0.56
1:I:95:THR:HG22	1:I:96:TYR:H	1.70	0.56
3:R:18:ILE:HD12	3:R:19:THR:H	1.71	0.56
1:E:125:MET:HE2	1:E:254:LEU:HD13	1.88	0.55
3:G:49:ILE:HA	3:G:60:VAL:HG21	1.87	0.55
1:P:132:GLN:HE21	1:P:190:PHE:HB3	1.70	0.55
1:A:183:GLN:HG2	1:A:184:VAL:O	2.06	0.55
2:C:76:LYS:C	2:C:78:LEU:HD23	2.29	0.55
2:J:128:LEU:HB3	3:K:123:PHE:CE2	2.41	0.55
2:J:192:SER:OG	2:J:198:TYR:OH	2.22	0.55
2:Q:18:LEU:HB3	2:Q:83:MET:HE3	1.88	0.55
1:I:265:THR:HG22	1:I:266:LYS:H	1.71	0.55
3:L:150:THR:HB	3:L:201:THR:HB	1.89	0.55
2:J:73:ASP:N	2:J:78:LEU:O	2.36	0.55
2:J:185:VAL:HG11	3:K:140:LEU:HD13	1.87	0.55
1:E:125:MET:SD	1:E:196:ALA:HB1	2.47	0.55
3:D:120:VAL:O	3:D:209:LYS:NZ	2.40	0.55
1:B:192:ASN:C	1:B:207:ARG:HG3	2.32	0.55
3:D:154:LYS:HE2	3:D:199:GLN:HE22	1.72	0.55
1:I:339:ASP:OD1	1:I:341:THR:N	2.36	0.55
1:B:238[A]:HIS:CG	1:B:239:ALA:N	2.73	0.54
2:C:63:SER:O	2:C:67:ARG:NH1	2.40	0.54
3:K:6:GLN:HB2	3:K:21:SER:O	2.08	0.54
3:O:18:ILE:HG22	3:O:77:ILE:CG1	2.37	0.54
1:P:215:LEU:HD21	1:P:250:GLN:HG3	1.89	0.54
1:E:61:TYR:CZ	1:E:123:LYS:HB3	2.42	0.54
2:J:52:SER:HB3	2:J:57:GLN:HB2	1.89	0.54
1:B:62:SER:HB3	1:B:123:LYS:HB2	1.88	0.54
1:B:99:ARG:NH1	1:B:103:ASN:O	2.36	0.54
3:D:56:ARG:HH11	3:D:62:ASN:HA	1.71	0.54
1:I:4:ILE:HD13	1:I:319:VAL:HG11	1.88	0.54
1:M:307:VAL:HG23	1:M:323:LYS:HB2	1.89	0.54
3:R:2:ALA:HB3	3:R:101:VAL:HG11	1.89	0.54
1:P:189:ASP:HB2	1:P:262:MET:HE1	1.89	0.54
3:K:2:ALA:HB1	3:K:101:VAL:HG11	1.89	0.54
1:P:132:GLN:NE2	1:P:190:PHE:HB3	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:219:SER:O	1:M:221:SER:N	2.37	0.54
2:J:175:GLN:NE2	2:J:179:LEU:O	2.41	0.54
1:M:329:PRO:HD3	1:M:357:SER:O	2.08	0.54
2:N:52:SER:HB2	2:N:57:GLN:HB2	1.90	0.54
1:P:310:PRO:HD2	1:P:387:TYR:CD2	2.43	0.54
3:R:41:HIS:CD2	3:R:86:ALA:HB2	2.43	0.54
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.90	0.54
1:P:309:ASN:HB3	1:P:387:TYR:HE2	1.73	0.54
2:F:172:ALA:HB2	2:F:182:LEU:HD23	1.90	0.53
3:L:33:ASN:HA	3:L:68:LYS:NZ	2.24	0.53
1:A:80:ALA:O	1:A:94:ARG:NH2	2.36	0.53
3:L:30:GLU:OE2	3:D:28:ASN:ND2	2.42	0.53
1:M:175:TYR:CZ	1:M:293:LYS:HB3	2.43	0.53
2:H:86:LEU:HB3	2:H:115:VAL:HG21	1.90	0.53
3:K:81:GLN:O	3:K:110:VAL:HG21	2.09	0.53
1:M:379:GLY:HA3	1:M:384:ARG:HA	1.89	0.53
2:N:68:PHE:HD1	2:N:83:MET:HA	1.74	0.53
3:O:53:VAL:HG11	3:O:68:LYS:CG	2.38	0.53
2:Q:4:LEU:HD11	2:Q:98:THR:HG23	1.89	0.53
3:R:2:ALA:CB	3:R:101:VAL:HG11	2.38	0.53
3:R:27:SER:O	3:R:28:ASN:HB2	2.07	0.53
1:A:215:LEU:HD21	1:A:250:GLN:HG3	1.91	0.53
3:G:199:GLN:HB3	3:G:208:GLU:HG2	1.91	0.53
2:C:203:ASN:HD21	2:C:205:LYS:NZ	2.06	0.53
2:J:11:LEU:HD21	2:J:150:PHE:HZ	1.74	0.53
2:N:64:VAL:HB	2:N:68:PHE:CD2	2.43	0.53
1:A:202:SER:HB2	1:A:264:VAL:O	2.09	0.53
2:Q:200:CYS:O	2:Q:212:ASP:HA	2.09	0.53
1:A:308:LYS:HB2	1:A:321:GLN:HB2	1.92	0.52
2:J:170:PHE:CE2	3:K:180:SER:HB3	2.40	0.52
2:N:36:TRP:CE2	2:N:81:LEU:HB2	2.43	0.52
3:O:20:ILE:HD11	3:O:108:LEU:HD13	1.84	0.52
1:P:15:VAL:HG22	1:P:17:GLY:H	1.75	0.52
1:I:3:CYS:HB3	1:I:9:ARG:NE	2.24	0.52
2:Q:169:THR:HG23	2:Q:184:SER:HB2	1.91	0.52
2:C:123:PRO:HB3	2:C:149:TYR:HB3	1.91	0.52
1:A:65:LEU:HD11	1:A:232:VAL:HG22	1.90	0.52
2:H:170:PHE:HD2	3:L:180:SER:HB3	1.74	0.52
2:F:130:PRO:HB3	2:F:142:LEU:CD1	2.39	0.52
1:E:8:ASP:HB3	1:E:29:LYS:HG2	1.91	0.52
2:C:11:LEU:HA	2:C:114:THR:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:298:LYS:NZ	1:I:328:ALA:O	2.42	0.52
1:M:354:PRO:O	1:M:355:ILE:HD13	2.10	0.52
3:D:167:THR:HG23	3:D:180:SER:O	2.10	0.52
1:B:70:ILE:HD11	1:B:242:ILE:HB	1.92	0.51
1:A:309:ASN:HB3	1:A:387:TYR:HE2	1.75	0.51
2:H:4:LEU:HD11	2:H:98:THR:HG23	1.92	0.51
2:N:47:TRP:HZ2	3:O:98:ILE:O	1.93	0.51
1:I:238:HIS:CG	1:I:239:ALA:N	2.77	0.51
2:J:143:GLY:HA3	2:J:185:VAL:HG12	1.91	0.51
2:C:125:VAL:HG21	2:C:202:VAL:HG21	1.92	0.51
1:M:1:ALA:HB3	1:M:140:ARG:HB3	1.92	0.51
1:P:64:VAL:HG23	1:P:122:ALA:HB2	1.92	0.51
1:B:171:GLU:HA	1:B:177:LYS:HA	1.92	0.51
2:C:121:LYS:HD2	2:C:148:ASP:O	2.09	0.51
1:I:349:LEU:HD12	1:I:367:VAL:HG13	1.91	0.51
2:J:127:PRO:HD3	2:J:213:LYS:HE3	1.92	0.51
1:P:99:ARG:HA	1:P:103:ASN:HD21	1.75	0.51
3:K:4:LEU:HD22	3:K:29:ILE:HD11	1.92	0.51
2:N:4:LEU:HD11	2:N:98:THR:HG23	1.93	0.51
1:A:55:GLU:OE2	1:A:220:GLY:HA3	2.10	0.51
2:H:52:SER:HB3	2:H:57:GLN:HB2	1.93	0.51
1:B:294:GLY:HA3	1:B:297:TYR:CD2	2.45	0.51
3:L:34:LEU:HD11	3:L:93:TYR:HB3	1.93	0.51
3:D:2:ALA:HB3	3:D:101:VAL:HG21	1.93	0.51
1:P:132:GLN:HE21	1:P:186:THR:HB	1.75	0.51
1:E:64:VAL:HG13	1:E:122:ALA:HB2	1.92	0.50
1:E:80:ALA:O	1:E:94:ARG:NH2	2.45	0.50
3:K:127:SER:HA	3:K:130:LEU:HD12	1.91	0.50
2:F:50:TYR:HB3	2:F:59:TYR:HB2	1.92	0.50
1:B:26:GLU:HB2	1:B:29:LYS:HD2	1.93	0.50
1:B:237:PRO:HG3	1:B:242:ILE:HD11	1.93	0.50
2:N:45:LEU:HD12	3:O:89:PHE:CD2	2.47	0.50
1:I:89:ASP:HA	1:I:228:MET:HE1	1.93	0.50
2:J:214:ARG:HD3	2:J:216:GLU:HG3	1.94	0.50
1:M:12:ILE:O	1:M:33:VAL:HA	2.11	0.50
1:M:252:GLY:O	1:M:256:THR:HG23	2.12	0.50
1:A:310:PRO:HD2	1:A:387:TYR:CD2	2.46	0.50
3:L:146:PRO:HD2	3:L:203:GLU:OE2	2.12	0.50
2:J:68:PHE:CD1	2:J:83:MET:HA	2.47	0.50
2:J:73:ASP:OD2	2:J:76:LYS:HB2	2.12	0.50
2:Q:130:PRO:HG3	2:Q:142:LEU:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:THR:HG22	1:A:96:TYR:H	1.77	0.50
1:B:179:THR:HB	1:B:286:LYS:HB3	1.94	0.50
2:C:130:PRO:HB3	2:C:142:LEU:HD23	1.94	0.50
3:D:130:LEU:H	3:D:130:LEU:HD12	1.77	0.50
1:A:152:TRP:O	1:A:156:ILE:HG13	2.12	0.49
1:I:292:LEU:HD21	1:I:352:VAL:HG12	1.94	0.49
1:P:93:LYS:HD2	1:P:234:PHE:HB2	1.94	0.49
1:B:185:GLN:O	1:B:187:ALA:N	2.44	0.49
1:B:225:TRP:HB2	1:B:228:MET:HE3	1.94	0.49
3:L:37:TRP:HB2	3:L:50:LEU:HB2	1.94	0.49
1:E:150:GLU:H	1:E:150:GLU:CD	2.20	0.49
3:G:109:THR:HG21	3:G:146:PRO:HB3	1.94	0.49
1:I:304:MET:HG2	1:I:324:VAL:HG22	1.93	0.49
3:K:193:HIS:HB2	3:K:196:TYR:HE1	1.76	0.49
1:P:265:THR:OG1	1:P:277:HIS:NE2	2.34	0.49
1:A:335:ILE:HG13	1:A:377:ILE:HB	1.95	0.49
2:H:20:LEU:HD12	2:H:81:LEU:HD23	1.93	0.49
1:I:149:GLN:HG2	1:I:152:TRP:CE3	2.47	0.49
3:K:51:TYR:O	3:K:55:GLU:HB2	2.11	0.49
2:N:40:ALA:HB3	2:N:43:LYS:HB2	1.95	0.49
3:K:29:ILE:HG22	3:K:68:LYS:CE	2.40	0.49
2:N:202:VAL:HB	2:N:211:VAL:HG22	1.93	0.49
1:E:338:ASP:OD1	1:E:338:ASP:N	2.46	0.49
2:C:87:ARG:O	2:C:115:VAL:HG21	2.13	0.49
3:D:150:THR:HB	3:D:201:THR:HB	1.94	0.49
1:M:178:ALA:HB2	1:M:290:LEU:HD13	1.95	0.49
3:R:113:GLN:HB3	3:R:114:PRO:HD3	1.95	0.49
3:D:85:GLU:OE1	3:D:109:THR:HA	2.13	0.49
1:I:252:GLY:O	1:I:256:THR:HG23	2.12	0.49
1:P:328:ALA:HB1	1:P:329:PRO:HD2	1.53	0.49
1:E:66:THR:HG22	1:E:118:LYS:H	1.76	0.49
2:F:35:MET:SD	2:F:37:ILE:HD11	2.53	0.49
2:C:91:THR:HG23	2:C:114:THR:HA	1.94	0.49
2:N:36:TRP:NE1	2:N:81:LEU:HB2	2.28	0.49
1:A:12:ILE:HD12	1:A:31:VAL:HG11	1.95	0.48
1:B:45:LEU:HD11	1:B:48:VAL:HG23	1.94	0.48
1:B:149:GLN:HE21	1:B:150:GLU:HG3	1.78	0.48
3:K:27:SER:O	3:K:29:ILE:N	2.33	0.48
1:M:132:GLN:CD	1:M:132:GLN:H	2.20	0.48
3:O:18:ILE:HG22	3:O:77:ILE:HG13	1.94	0.48
1:P:334:VAL:O	1:P:349:LEU:HD11	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ARG:HA	1:B:103:ASN:HD21	1.78	0.48
1:I:137:TYR:CZ	1:I:161:PHE:HB2	2.48	0.48
2:N:89:GLU:OE1	2:N:89:GLU:N	2.36	0.48
3:O:165:GLU:OE1	3:O:165:GLU:HA	2.13	0.48
2:Q:83:MET:HB3	2:Q:86:LEU:HD21	1.94	0.48
1:B:119:PHE:CD1	1:B:228:MET:HE2	2.48	0.48
2:Q:50:TYR:HB3	2:Q:59:TYR:HB2	1.95	0.48
1:E:34:MET:CE	1:E:350:VAL:HA	2.44	0.48
1:E:46:GLN:HG3	1:E:140:ARG:NH2	2.28	0.48
2:C:199:ILE:HG22	2:C:213:LYS:C	2.39	0.48
1:P:217:TRP:CZ2	1:P:226:ARG:HD3	2.47	0.48
1:A:26:GLU:HB2	1:A:29:LYS:HD2	1.95	0.48
1:A:194:TYR:CE2	1:A:207:ARG:HG3	2.49	0.48
3:D:63:ARG:HH22	3:D:84:ASP:CG	2.22	0.48
3:D:128:GLU:N	3:D:128:GLU:OE1	2.46	0.48
2:Q:204:HIS:CD2	2:Q:206:PRO:HD2	2.47	0.48
3:D:95:ASP:OD1	3:D:98:ILE:HG12	2.13	0.48
1:M:97:SER:OG	1:M:239:ALA:HA	2.13	0.48
1:M:218:GLN:HB2	1:M:225:TRP:CZ3	2.48	0.48
3:G:172:GLN:HG3	3:G:174:ASN:OD1	2.14	0.48
1:B:188:VAL:HG12	1:B:188:VAL:O	2.12	0.48
2:C:18:LEU:HD12	2:C:19:ARG:H	1.79	0.48
2:C:159:ASN:OD1	2:C:198:TYR:HA	2.13	0.48
1:I:374:SER:OG	1:I:375:TYR:N	2.46	0.48
3:O:124:PRO:HA	3:O:137:LEU:HD23	1.94	0.48
1:A:76:SER:HB3	1:P:130:VAL:O	2.13	0.48
2:H:83:MET:HE2	2:H:86:LEU:HD21	1.94	0.48
1:E:38:LYS:NZ	1:E:290:LEU:O	2.28	0.48
1:B:185:GLN:C	1:B:187:ALA:H	2.21	0.48
2:C:141:ALA:HB2	2:C:187:THR:HG22	1.96	0.48
2:C:107:TRP:CE3	3:D:46:PRO:HG2	2.49	0.48
2:J:185:VAL:HG11	3:K:140:LEU:CD1	2.43	0.48
3:L:82:ALA:HA	3:L:110:VAL:HG21	1.96	0.47
1:M:266:LYS:NZ	1:M:266:LYS:HB3	2.29	0.47
3:D:139:CYS:C	3:D:140:LEU:HD23	2.39	0.47
2:J:4:LEU:HD11	2:J:98:THR:HG23	1.96	0.47
1:B:38:LYS:HD2	1:B:290:LEU:HB2	1.96	0.47
1:M:157:LYS:HE2	1:M:172:PHE:CD1	2.49	0.47
2:Q:20:LEU:HG	2:Q:83:MET:HE2	1.96	0.47
1:E:320:MET:HE1	1:E:376:ILE:HG21	1.96	0.47
2:Q:89:GLU:N	2:Q:89:GLU:OE1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:GLU:OE1	1:E:150:GLU:N	2.41	0.47
3:D:56:ARG:NH1	3:D:62:ASN:HA	2.30	0.47
3:K:157:SER:O	3:K:157:SER:OG	2.22	0.47
1:A:190:PHE:HE2	1:A:276:LEU:HD13	1.79	0.47
1:E:129:GLU:HG2	1:B:76:SER:HA	1.96	0.47
1:E:225:TRP:HB2	1:E:228:MET:HE3	1.96	0.47
1:E:335:ILE:HG13	1:E:377:ILE:HB	1.97	0.47
2:F:68:PHE:CZ	2:F:83:MET:HE2	2.50	0.47
1:M:293:LYS:HG2	1:M:294:GLY:N	2.29	0.47
1:A:266:LYS:NZ	1:A:271:ASN:O	2.35	0.47
3:L:139:CYS:HB2	3:L:153:TRP:CH2	2.49	0.47
1:B:96:TYR:HB3	1:B:110:LYS:HB3	1.97	0.47
1:B:218:GLN:HG2	1:B:219:SER:H	1.80	0.47
2:C:142:LEU:HD11	2:C:198:TYR:CE2	2.38	0.47
1:M:240:ALA:HB1	2:N:56:SER:HB2	1.96	0.47
1:I:339:ASP:OD1	1:I:340:LEU:N	2.48	0.47
3:O:143:ASP:OD1	3:O:172:GLN:NE2	2.37	0.47
1:A:38:LYS:NZ	1:A:290:LEU:O	2.41	0.47
1:A:238[A]:HIS:CG	1:A:239:ALA:H	2.33	0.47
1:A:328:ALA:CB	1:A:329:PRO:CD	2.70	0.47
2:H:22:CYS:HB3	2:H:79:LEU:HB3	1.97	0.47
3:L:34:LEU:CD1	3:L:93:TYR:HB3	2.44	0.47
3:L:85:GLU:HG3	3:L:108:LEU:O	2.15	0.47
1:B:94:ARG:HG3	1:B:94:ARG:HH11	1.80	0.47
1:B:190:PHE:C	1:B:192:ASN:H	2.23	0.47
3:K:121:THR:HG22	3:K:123:PHE:CE1	2.49	0.47
1:E:145:VAL:HG12	1:E:146:GLY:H	1.80	0.47
1:B:66:THR:HG22	1:B:118:LYS:H	1.78	0.47
1:B:161:PHE:N	1:B:161:PHE:HD1	2.13	0.47
1:I:96:TYR:HB3	1:I:110:LYS:HB3	1.96	0.47
3:K:185:LEU:HD11	3:K:196:TYR:CE2	2.50	0.47
1:M:61:TYR:CZ	1:M:123:LYS:HB3	2.50	0.47
2:Q:125:VAL:HB	2:Q:211:VAL:HG11	1.96	0.47
1:I:65:LEU:HD11	1:I:232:VAL:HG22	1.97	0.46
1:I:313:THR:HG22	1:I:319:VAL:HG22	1.96	0.46
3:O:99:PHE:HD1	3:O:99:PHE:HA	1.62	0.46
1:P:180:LEU:HD23	1:P:180:LEU:HA	1.78	0.46
3:R:98:ILE:HD12	3:R:98:ILE:HA	1.71	0.46
3:G:18:ILE:HG23	3:G:80:LEU:HD21	1.98	0.46
2:C:125:VAL:CG2	2:C:202:VAL:HG21	2.46	0.46
2:J:68:PHE:CE1	2:J:83:MET:HG2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:50:ILE:CD1	1:P:130:VAL:HG13	2.44	0.46
3:L:51:TYR:O	3:L:55:GLU:HB2	2.16	0.46
1:I:128:PHE:HB2	1:I:195:ILE:HB	1.97	0.46
2:J:20:LEU:HD22	2:J:111:THR:HG21	1.98	0.46
1:P:129:GLU:HG3	1:P:194:TYR:HE1	1.80	0.46
1:P:307:VAL:CG2	1:P:323:LYS:HB2	2.46	0.46
2:J:67:ARG:NH1	2:J:90:ASP:OD2	2.35	0.46
3:O:71:ASN:OD1	3:R:25:THR:HG23	2.16	0.46
1:P:252:GLY:O	1:P:256:THR:HG23	2.15	0.46
3:R:109:THR:HG21	3:R:146:PRO:HB3	1.96	0.46
1:A:44:SER:OG	1:A:140:ARG:HB2	2.16	0.46
2:H:170:PHE:CD2	3:L:180:SER:HB3	2.50	0.46
2:H:204:HIS:HB3	2:H:209:THR:HB	1.98	0.46
2:C:37:ILE:HD12	2:C:107:TRP:CH2	2.50	0.46
1:P:129:GLU:HG3	1:P:194:TYR:CE1	2.50	0.46
1:B:60:CYS:HB2	1:B:225:TRP:CZ3	2.51	0.46
2:C:60:TYR:CE1	2:C:70:ILE:HG22	2.51	0.46
2:J:93:LEU:HD12	2:J:111:THR:C	2.40	0.46
2:H:203:ASN:OD1	2:H:205:LYS:NZ	2.49	0.46
1:E:82:LEU:HB3	1:E:84:GLU:HG2	1.97	0.46
1:B:67:HIS:HB3	3:D:96:THR:HG23	1.97	0.46
3:O:137:LEU:HD12	3:O:183:LEU:HD23	1.98	0.46
3:R:32:TYR:HB3	3:R:34:LEU:CD2	2.45	0.46
1:E:3:CYS:HB3	1:E:9:ARG:HG3	1.97	0.46
2:J:67:ARG:HD2	2:J:85:SER:O	2.16	0.46
1:M:3:CYS:HB3	1:M:9:ARG:NE	2.30	0.46
3:R:116:ALA:HB3	3:R:145:TYR:N	2.30	0.46
1:A:226:ARG:HH22	1:P:85:GLU:HG2	1.81	0.46
3:L:63:ARG:NH1	3:L:84:ASP:OD2	2.49	0.46
1:E:132:GLN:NE2	1:E:190:PHE:O	2.49	0.46
1:B:161:PHE:N	1:B:161:PHE:CD1	2.84	0.46
3:L:171:LYS:HD3	3:L:177:TYR:CE1	2.51	0.46
2:F:40:ALA:HB3	2:F:43:LYS:HB2	1.98	0.46
1:B:65:LEU:HD21	1:B:232:VAL:HG21	1.98	0.46
1:B:265:THR:HG1	1:B:277:HIS:CD2	2.33	0.46
2:C:91:THR:OG1	2:C:115:VAL:HG22	2.16	0.46
3:K:25:THR:O	3:K:71:ASN:ND2	2.49	0.46
3:K:133:ASN:HA	3:K:187:PRO:HG3	1.98	0.46
1:P:206:ASP:OD1	1:P:207:ARG:N	2.49	0.46
3:O:13:SER:HB2	3:O:16:GLN:NE2	2.30	0.45
3:R:28:ASN:HA	3:R:94:ALA:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:38:TYR:HB2	3:R:89:PHE:HB2	1.98	0.45
2:F:52:SER:HB3	2:F:57:GLN:HB2	1.97	0.45
1:B:146:GLY:HA2	1:B:364:LEU:O	2.16	0.45
1:A:129:GLU:HG3	1:A:194:TYR:CE1	2.51	0.45
1:B:379:GLY:HA3	1:B:384:ARG:HA	1.98	0.45
1:I:177:LYS:NZ	1:I:179:THR:OG1	2.49	0.45
3:K:144:PHE:CE1	3:K:178:ALA:HA	2.51	0.45
1:P:46:GLN:HG3	1:P:140:ARG:HE	1.81	0.45
2:Q:100:THR:O	2:Q:103:ARG:HG2	2.16	0.45
3:L:25:THR:O	3:L:27:SER:N	2.48	0.45
3:D:34:LEU:H	3:D:34:LEU:HG	1.64	0.45
2:J:209:THR:HG22	2:J:211:VAL:HG23	1.97	0.45
3:K:32:TYR:HB3	3:K:34:LEU:HD23	1.97	0.45
1:M:320:MET:HG2	1:M:365:ILE:HB	1.96	0.45
1:M:374:SER:OG	1:M:375:TYR:N	2.49	0.45
2:N:109:GLN:NE2	2:N:110:GLY:O	2.49	0.45
1:P:329:PRO:O	1:P:329:PRO:HG2	2.17	0.45
2:C:204:HIS:CE1	2:C:206:PRO:HG2	2.51	0.45
1:M:297:TYR:O	1:M:331:LYS:NZ	2.41	0.45
1:P:334:VAL:HG22	1:P:378:VAL:HG22	1.97	0.45
3:R:53:VAL:CG1	3:R:68:LYS:HB2	2.46	0.45
1:B:202:SER:HB2	1:B:264:VAL:O	2.17	0.45
2:C:154:VAL:HG12	2:C:182:LEU:HD21	1.99	0.45
1:M:334:VAL:HG22	1:M:378:VAL:HG13	1.98	0.45
3:O:115:LYS:HD2	3:O:203:GLU:HG3	1.99	0.45
2:H:143:GLY:HA3	2:H:184:SER:O	2.17	0.45
3:K:113:GLN:OE1	3:K:114:PRO:HD2	2.16	0.45
1:M:233:GLU:HG3	1:M:247:LEU:HD21	1.98	0.45
2:N:47:TRP:CZ2	3:O:99:PHE:HB2	2.51	0.45
2:N:130:PRO:HB3	2:N:142:LEU:HB3	1.98	0.45
3:O:29:ILE:HD13	3:O:73:ALA:HB2	1.98	0.45
2:H:98:THR:OG1	2:H:106:THR:OG1	2.22	0.45
1:E:4:ILE:HD13	1:E:319:VAL:HG11	1.98	0.45
1:E:304:MET:HE3	1:E:304:MET:HB2	1.90	0.45
1:I:50:ILE:HD11	1:I:276:LEU:HD21	1.99	0.45
2:J:50:TYR:HB3	2:J:59:TYR:HB2	1.98	0.45
1:M:179:THR:HB	1:M:286:LYS:HB3	1.97	0.45
1:E:304:MET:O	1:E:385:LEU:HD21	2.17	0.45
2:N:6:GLU:HG2	2:N:96:CYS:SG	2.57	0.45
2:Q:29:PHE:O	2:Q:72:ARG:NH2	2.49	0.45
2:C:202:VAL:HG22	2:C:211:VAL:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:95:ASP:OD1	3:D:95:ASP:N	2.49	0.45
1:E:349:LEU:HD12	1:E:367:VAL:HG12	2.00	0.44
1:B:297:TYR:HE1	1:B:329:PRO:HB3	1.81	0.44
2:N:154:VAL:HG12	2:N:204:HIS:CD2	2.49	0.44
1:A:26:GLU:HG2	1:A:280:HIS:HB3	2.00	0.44
1:E:308:LYS:HG3	1:E:321:GLN:HB2	2.00	0.44
1:M:50:ILE:HD11	1:M:190:PHE:CE2	2.49	0.44
2:H:203:ASN:OD1	2:H:210:LYS:HG2	2.17	0.44
3:L:130:LEU:HD22	3:L:187:PRO:HB3	1.99	0.44
1:I:318:VAL:HG12	1:I:369:PRO:HD3	1.98	0.44
1:P:237:PRO:HB3	1:P:242:ILE:HG12	1.99	0.44
1:B:302:ASP:N	1:B:302:ASP:OD1	2.50	0.44
3:D:63:ARG:HB3	3:D:78:SER:O	2.17	0.44
1:M:1:ALA:HA	1:M:2:HIS:HA	1.62	0.44
1:B:160:LYS:C	1:B:161:PHE:HD1	2.26	0.44
1:P:206:ASP:HB3	1:P:209:TRP:HB3	1.99	0.44
1:E:307:VAL:CG2	1:E:323:LYS:HB2	2.48	0.44
1:E:371:PHE:CD1	1:E:371:PHE:N	2.86	0.44
2:F:12:VAL:O	2:F:115:VAL:HA	2.18	0.44
2:J:38:ARG:HD3	2:J:94:TYR:CE2	2.53	0.44
2:N:168:HIS:HB3	2:N:170:PHE:HE1	1.83	0.44
3:O:113:GLN:CD	3:O:114:PRO:HD3	2.38	0.44
1:B:157:LYS:HG2	1:B:172:PHE:CE1	2.53	0.44
3:R:115:LYS:HG2	3:R:116:ALA:N	2.32	0.44
3:O:17:SER:HA	3:O:77:ILE:O	2.18	0.43
3:O:93:TYR:HA	3:O:100:TRP:HA	2.00	0.43
1:E:9:ARG:HB3	1:E:315:HIS:CD2	2.52	0.43
1:E:186:THR:HA	1:E:189:ASP:OD2	2.19	0.43
1:B:121:CYS:SG	1:B:124:SER:HB3	2.58	0.43
1:I:299:MET:HE3	1:I:299:MET:HB3	1.74	0.43
1:M:135:ILE:HD13	1:M:186:THR:HG21	1.99	0.43
2:H:20:LEU:HB2	2:H:81:LEU:HB3	2.00	0.43
2:H:205:LYS:HA	2:H:205:LYS:HD3	1.71	0.43
2:C:135:THR:HG22	2:C:135:THR:O	2.16	0.43
3:K:171:LYS:HD2	3:K:175:ASN:HA	2.00	0.43
1:P:34:MET:HG2	1:P:40:SER:OG	2.18	0.43
3:R:6:GLN:HG3	3:R:106:THR:OG1	2.18	0.43
1:A:130:VAL:O	1:P:76:SER:HB3	2.18	0.43
3:L:6:GLN:HG3	3:L:106:THR:OG1	2.18	0.43
2:N:47:TRP:CE2	3:O:99:PHE:HB2	2.54	0.43
2:Q:208:ASN:O	2:Q:208:ASN:CG	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LYS:HB3	1:A:266:LYS:HE2	1.69	0.43
2:H:35:MET:SD	2:H:104:ILE:HG12	2.58	0.43
1:E:56:ALA:O	1:B:79:GLU:HG3	2.19	0.43
1:B:377:ILE:HG23	1:B:384:ARG:HD3	1.99	0.43
2:C:169:THR:HG22	2:C:184:SER:HB2	2.01	0.43
1:I:171:GLU:HA	1:I:177:LYS:HA	2.00	0.43
2:J:168:HIS:CD2	3:K:178:ALA:HB3	2.54	0.43
1:M:364:LEU:C	1:M:365:ILE:HD13	2.43	0.43
1:A:349:LEU:HD12	1:A:367:VAL:HG22	2.01	0.43
2:H:29:PHE:O	2:H:72:ARG:NH2	2.52	0.43
1:B:252:GLY:O	1:B:256:THR:HG23	2.18	0.43
1:I:218:GLN:HB2	1:I:225:TRP:CZ3	2.54	0.43
3:K:34:LEU:HA	3:K:52:GLU:HA	2.01	0.43
2:N:45:LEU:HD12	3:O:89:PHE:CE2	2.54	0.43
2:N:68:PHE:CE1	2:N:83:MET:HE3	2.54	0.43
1:P:221:SER:O	1:P:223:GLY:N	2.43	0.43
3:L:53:VAL:CG1	3:L:68:LYS:HB2	2.48	0.43
1:E:65:LEU:HD21	1:E:232:VAL:HG13	2.01	0.43
1:E:74:CYS:O	1:E:77:THR:HB	2.19	0.43
3:G:160:VAL:HG11	3:G:183:LEU:HD11	1.99	0.43
1:B:103:ASN:HD22	1:B:239:ALA:HB1	1.84	0.43
3:D:6:GLN:HG3	3:D:106:THR:OG1	2.19	0.43
1:I:217:TRP:CZ2	1:I:226:ARG:HD3	2.53	0.43
1:M:130:VAL:HG22	1:M:195:ILE:HG13	2.01	0.43
3:L:33:ASN:CG	3:L:68:LYS:HZ1	2.23	0.43
1:E:267:ASP:O	1:E:269:ASN:N	2.52	0.43
3:D:33:ASN:O	3:D:53:VAL:HG12	2.19	0.43
1:M:38:LYS:HG3	1:M:290:LEU:O	2.19	0.43
3:L:141:ILE:HG12	3:L:200:VAL:HG21	2.00	0.43
1:E:237:PRO:HB3	1:E:242:ILE:HG12	2.01	0.43
1:M:340:LEU:HD21	1:M:386:THR:HG21	2.01	0.43
3:L:18:ILE:HG12	3:L:19:THR:N	2.34	0.42
2:H:127:PRO:O	3:L:126:SER:OG	2.36	0.42
3:L:33:ASN:HA	3:L:68:LYS:HZ1	1.84	0.42
1:B:215:LEU:HD21	1:B:250:GLN:HG3	2.01	0.42
3:K:99:PHE:O	3:K:100:TRP:CG	2.72	0.42
1:M:336:VAL:HG21	1:M:367:VAL:HG11	2.01	0.42
1:P:30:CYS:HB2	1:P:44:SER:HB3	2.01	0.42
1:P:84:GLU:OE1	1:P:84:GLU:N	2.48	0.42
1:P:265:THR:HG22	1:P:266:LYS:H	1.84	0.42
1:P:340:LEU:HD23	1:P:340:LEU:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:GLU:O	1:E:199:GLU:HG2	2.19	0.42
2:C:142:LEU:HD21	2:C:198:TYR:OH	2.18	0.42
3:D:137:LEU:HB2	3:D:183:LEU:HB3	2.01	0.42
3:R:124:PRO:HA	3:R:137:LEU:HD13	2.02	0.42
1:B:323:LYS:HE3	1:B:325:PRO:HD3	2.02	0.42
1:M:304:MET:O	1:M:385:LEU:HD21	2.18	0.42
2:N:36:TRP:CZ2	2:N:79:LEU:HD23	2.55	0.42
2:Q:123:PRO:HD2	2:Q:209:THR:HG21	2.00	0.42
3:L:193:HIS:HB2	3:L:196:TYR:HE1	1.84	0.42
2:F:52:SER:O	2:F:72:ARG:NH1	2.53	0.42
1:M:218:GLN:HB2	1:M:225:TRP:CE3	2.54	0.42
1:P:38:LYS:NZ	1:P:290:LEU:O	2.35	0.42
2:Q:36:TRP:CG	2:Q:81:LEU:HD22	2.55	0.42
1:I:11:PHE:C	1:I:12:ILE:HD13	2.44	0.42
2:Q:89:GLU:CD	2:Q:89:GLU:H	2.27	0.42
2:C:52:SER:HB3	2:C:57:GLN:HB2	2.00	0.42
3:D:10:VAL:HG23	3:D:18:ILE:HD11	2.00	0.42
1:I:238:HIS:CG	1:I:239:ALA:H	2.38	0.42
1:M:195:ILE:HG21	1:M:274:TYR:CD2	2.54	0.42
2:N:87:ARG:O	2:N:115:VAL:HG21	2.20	0.42
2:N:134:SER:O	2:N:135:THR:OG1	2.31	0.42
1:B:149:GLN:HA	1:B:152:TRP:CG	2.55	0.42
1:B:334:VAL:HG21	1:B:365:ILE:HD13	2.02	0.42
1:I:1:ALA:HA	1:I:2:HIS:HA	1.64	0.42
2:J:68:PHE:HB3	2:J:81:LEU:HD11	2.02	0.42
2:Q:123:PRO:HB3	2:Q:149:TYR:HB3	2.01	0.42
1:A:310:PRO:HA	1:A:319:VAL:O	2.19	0.42
1:E:183:GLN:NE2	1:E:185:GLN:OE1	2.53	0.42
1:B:149:GLN:HA	1:B:152:TRP:CD2	2.54	0.42
3:D:28:ASN:HD22	3:D:28:ASN:HA	1.69	0.42
1:M:33:VAL:CG2	1:M:41:LEU:HB3	2.50	0.42
1:M:236:PRO:HA	1:M:237:PRO:HD3	1.90	0.42
1:P:95:THR:HG22	1:P:96:TYR:N	2.30	0.42
1:E:159:LEU:HD12	1:E:180:LEU:HD12	2.01	0.42
2:F:142:LEU:HD23	2:F:215:VAL:CG1	2.50	0.42
2:J:128:LEU:HB3	3:K:123:PHE:CD2	2.55	0.42
3:R:51:TYR:O	3:R:55:GLU:HB2	2.19	0.42
1:A:268:GLU:O	1:A:269:ASN:C	2.63	0.41
2:H:67:ARG:NH1	2:H:90:ASP:OD2	2.48	0.41
1:E:329:PRO:CD	1:E:357:SER:O	2.56	0.41
1:M:39:PRO:HB2	1:M:143:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:37:ILE:HD11	2:Q:104:ILE:HD13	2.02	0.41
1:A:146:GLY:HA3	1:A:363:VAL:HG13	2.00	0.41
2:C:4:LEU:HD11	2:C:98:THR:HG23	2.01	0.41
1:B:194:TYR:CD2	1:B:207:ARG:HG2	2.55	0.41
2:J:167:VAL:HG22	2:J:186:VAL:HB	2.02	0.41
3:K:62:ASN:OD1	3:K:62:ASN:N	2.51	0.41
3:K:171:LYS:HG3	3:K:172:GLN:N	2.36	0.41
1:E:57:ARG:NH2	1:E:211:GLN:HG2	2.35	0.41
1:E:264:VAL:HG22	1:E:276:LEU:HD13	2.03	0.41
3:D:199:GLN:HB3	3:D:208:GLU:HG3	2.02	0.41
1:M:320:MET:HE2	1:M:320:MET:HB3	1.96	0.41
1:P:318:VAL:HG12	1:P:369:PRO:HD3	2.01	0.41
2:Q:143:GLY:HA2	2:Q:185:VAL:HA	2.01	0.41
2:H:35:MET:HB3	2:H:50:TYR:HD1	1.86	0.41
3:G:200:VAL:O	3:G:206:THR:HA	2.20	0.41
1:B:186:THR:C	1:B:188:VAL:N	2.77	0.41
1:B:236:PRO:HA	1:B:237:PRO:HD3	1.88	0.41
1:M:119:PHE:CD1	1:M:228:MET:HE2	2.56	0.41
2:F:83:MET:HE1	2:F:94:TYR:CZ	2.56	0.41
2:C:214:ARG:HH11	2:C:214:ARG:CG	2.33	0.41
2:N:63:SER:O	2:N:67:ARG:NH2	2.54	0.41
2:N:125:VAL:HA	2:N:145:LEU:O	2.20	0.41
1:P:224:ILE:HD12	1:P:226:ARG:HG3	2.01	0.41
1:E:293:LYS:O	1:E:355:ILE:HD11	2.20	0.41
1:B:348:ILE:HB	1:B:368:ASN:HB3	2.03	0.41
3:O:41:HIS:CD2	3:O:86:ALA:HB2	2.56	0.41
3:O:167:THR:HG21	3:O:180:SER:H	1.85	0.41
1:P:150:GLU:H	1:P:150:GLU:HG3	1.57	0.41
1:A:9:ARG:HD2	1:A:315:HIS:ND1	2.35	0.41
1:A:190:PHE:CE2	1:A:276:LEU:HD13	2.56	0.41
1:B:1:ALA:HA	1:B:2:HIS:HA	1.67	0.41
3:O:61:SER:OG	3:O:63:ARG:HG3	2.20	0.41
1:P:262:MET:SD	1:P:278:GLY:HA3	2.61	0.41
1:A:262:MET:HE3	1:A:262:MET:HB2	1.79	0.41
1:A:263:ARG:NH1	1:B:235:GLU:OE2	2.54	0.41
3:L:12:GLY:O	3:L:110:VAL:HA	2.21	0.41
1:E:34:MET:HE3	1:E:350:VAL:HA	2.03	0.41
1:B:99:ARG:HD3	1:B:239:ALA:O	2.21	0.41
3:D:80:LEU:HD12	3:D:80:LEU:HA	1.82	0.41
1:I:66:THR:HG23	3:K:93:TYR:CZ	2.56	0.41
1:M:298:LYS:NZ	1:M:328:ALA:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:67:ARG:HB3	2:Q:84:ASN:O	2.21	0.41
3:R:120:VAL:O	3:R:209:LYS:HE3	2.20	0.41
2:H:67:ARG:HB3	2:H:84:ASN:O	2.21	0.41
1:I:143:LEU:HD21	1:I:290:LEU:HD21	2.02	0.41
1:I:236:PRO:HA	1:I:237:PRO:HD3	1.92	0.41
3:K:99:PHE:HB3	3:K:100:TRP:CE3	2.55	0.41
1:M:80:ALA:HB3	1:M:114:VAL:HG23	2.02	0.41
2:F:141:ALA:C	2:F:142:LEU:HD12	2.46	0.40
1:B:298:LYS:O	1:B:330:CYS:HB2	2.22	0.40
1:P:1:ALA:HA	1:P:2:HIS:HA	1.73	0.40
3:R:175:ASN:OD1	3:R:175:ASN:N	2.53	0.40
1:A:57:ARG:HB2	1:A:127:LEU:HD12	2.04	0.40
1:E:325:PRO:O	1:E:359:ASN:HB3	2.21	0.40
1:B:39:PRO:HD3	1:B:292:LEU:HD13	2.03	0.40
1:B:194:TYR:CE2	1:B:207:ARG:HG2	2.56	0.40
2:C:158:TRP:HA	2:C:199:ILE:O	2.21	0.40
2:C:174:LEU:HD13	2:C:180:TYR:CE1	2.55	0.40
3:D:144:PHE:CE1	3:D:147:GLY:HA2	2.56	0.40
2:J:63:SER:OG	2:J:64:VAL:HG13	2.21	0.40
1:M:258:LEU:HD23	1:M:258:LEU:HA	1.87	0.40
2:N:86:LEU:HD23	2:N:86:LEU:HA	1.84	0.40
2:N:107:TRP:CE3	3:O:46:PRO:HG2	2.56	0.40
3:R:153:TRP:CE3	3:R:183:LEU:HD12	2.56	0.40
2:H:205:LYS:N	2:H:205:LYS:HE2	2.37	0.40
3:L:144:PHE:CE2	3:L:147:GLY:HA2	2.57	0.40
3:D:93:TYR:HA	3:D:100:TRP:HA	2.03	0.40
2:N:104:ILE:HD12	3:O:102:PHE:HZ	1.86	0.40
1:A:62:SER:HB3	1:A:123:LYS:HB2	2.03	0.40
3:L:70:GLY:HA3	3:D:27:SER:HA	2.03	0.40
1:E:70:ILE:H	2:F:33:TYR:HH	1.66	0.40
3:G:172:GLN:H	3:G:172:GLN:HG2	1.66	0.40
1:B:8:ASP:OD2	1:B:29:LYS:HE2	2.22	0.40
2:C:34:MET:HB3	2:C:79:LEU:HD22	2.03	0.40
1:I:8:ASP:HB3	1:I:29:LYS:HG2	2.04	0.40
1:I:32:THR:OG1	1:I:42:ASP:OD1	2.35	0.40
2:N:12:VAL:O	2:N:115:VAL:HA	2.22	0.40
2:N:216:GLU:HG2	2:N:217:PRO:HD2	2.04	0.40
2:Q:173:VAL:HB	3:R:167:THR:HG22	2.02	0.40
1:A:149:GLN:NE2	1:B:101:TRP:O	2.55	0.40
1:A:226:ARG:NH2	1:P:85:GLU:HG2	2.37	0.40
1:B:67:HIS:CE1	2:C:102:TRP:CD1	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:6:GLN:HB2	3:R:21:SER:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	391/398 (98%)	369 (94%)	19 (5%)	3 (1%)	16	44
1	B	385/398 (97%)	363 (94%)	19 (5%)	3 (1%)	16	44
1	E	390/398 (98%)	367 (94%)	19 (5%)	4 (1%)	12	38
1	I	384/398 (96%)	363 (94%)	19 (5%)	2 (0%)	24	55
1	M	384/398 (96%)	365 (95%)	17 (4%)	2 (0%)	24	55
1	P	384/398 (96%)	364 (95%)	19 (5%)	1 (0%)	36	66
2	C	214/217 (99%)	203 (95%)	10 (5%)	1 (0%)	24	55
2	F	214/217 (99%)	208 (97%)	6 (3%)	0	100	100
2	H	214/217 (99%)	205 (96%)	9 (4%)	0	100	100
2	J	207/217 (95%)	197 (95%)	8 (4%)	2 (1%)	12	38
2	N	214/217 (99%)	202 (94%)	12 (6%)	0	100	100
2	Q	214/217 (99%)	205 (96%)	9 (4%)	0	100	100
3	D	211/217 (97%)	199 (94%)	9 (4%)	3 (1%)	9	30
3	G	214/217 (99%)	197 (92%)	15 (7%)	2 (1%)	14	41
3	K	212/217 (98%)	194 (92%)	16 (8%)	2 (1%)	14	41
3	L	212/217 (98%)	198 (93%)	10 (5%)	4 (2%)	6	22
3	O	215/217 (99%)	201 (94%)	8 (4%)	6 (3%)	4	14
3	R	211/217 (97%)	196 (93%)	13 (6%)	2 (1%)	14	41
All	All	4870/4992 (98%)	4596 (94%)	237 (5%)	37 (1%)	16	44

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	PRO
3	L	26	GLY
1	E	267	ASP
1	E	268	GLU
1	E	329	PRO
1	B	329	PRO
2	C	160	SER
3	D	30	GLU
1	I	329	PRO
2	J	123	PRO
1	M	329	PRO
3	O	26	GLY
3	O	99	PHE
3	O	113	GLN
3	O	114	PRO
1	P	328	ALA
1	A	268	GLU
3	L	27	SER
3	G	99	PHE
3	D	53	VAL
2	J	124	SER
3	R	27	SER
3	L	99	PHE
1	A	269	ASN
3	G	114	PRO
1	B	186	THR
3	K	113	GLN
1	M	328	ALA
1	I	328	ALA
3	L	53	VAL
3	O	53	VAL
1	E	328	ALA
3	D	29	ILE
3	O	98	ILE
3	K	53	VAL
1	B	188	VAL
3	R	53	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain 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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	327/330 (99%)	321 (98%)	6 (2%)	51	82
1	B	322/330 (98%)	309 (96%)	13 (4%)	28	63
1	E	324/330 (98%)	312 (96%)	12 (4%)	30	65
1	I	320/330 (97%)	311 (97%)	9 (3%)	38	73
1	M	319/330 (97%)	315 (99%)	4 (1%)	61	86
1	P	319/330 (97%)	310 (97%)	9 (3%)	38	73
2	C	182/183 (100%)	178 (98%)	4 (2%)	45	78
2	F	182/183 (100%)	179 (98%)	3 (2%)	55	83
2	H	182/183 (100%)	178 (98%)	4 (2%)	45	78
2	J	178/183 (97%)	171 (96%)	7 (4%)	28	64
2	N	182/183 (100%)	180 (99%)	2 (1%)	65	87
2	Q	182/183 (100%)	181 (100%)	1 (0%)	81	93
3	D	179/183 (98%)	175 (98%)	4 (2%)	45	78
3	G	182/183 (100%)	176 (97%)	6 (3%)	33	69
3	K	180/183 (98%)	176 (98%)	4 (2%)	45	78
3	L	180/183 (98%)	171 (95%)	9 (5%)	22	54
3	O	183/183 (100%)	176 (96%)	7 (4%)	29	64
3	R	179/183 (98%)	176 (98%)	3 (2%)	53	83
All	All	4102/4176 (98%)	3995 (97%)	107 (3%)	40	75

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASP
1	A	21	VAL
1	A	120	THR
1	A	190	PHE
1	A	329	PRO
1	A	380	THR

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Mol	Chain	Res	Type
2	H	49	SER
2	H	89	GLU
2	H	205	LYS
2	H	213	LYS
3	L	3	VAL
3	L	17	SER
3	L	28	ASN
3	L	34	LEU
3	L	61	SER
3	L	109	THR
3	L	113	GLN
3	L	165	GLU
3	L	199	GLN
1	E	15	VAL
1	E	38	LYS
1	E	120	THR
1	E	164	LEU
1	E	199	GLU
1	E	265	THR
1	E	271	ASN
1	E	329	PRO
1	E	339	ASP
1	E	363	VAL
1	E	367	VAL
1	E	380	THR
2	F	78	LEU
2	F	117	SER
2	F	165	SER
3	G	34	LEU
3	G	113	GLN
3	G	119	SER
3	G	142	SER
3	G	165	GLU
3	G	170	SER
1	B	2	HIS
1	B	24	THR
1	B	41	LEU
1	B	70	ILE
1	B	161	PHE
1	B	184	VAL
1	B	189	ASP
1	B	224	ILE

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Mol	Chain	Res	Type
1	B	329	PRO
1	B	355	ILE
1	B	374	SER
1	B	380	THR
1	B	383	SER
2	C	46	GLU
2	C	163	LEU
2	C	198	TYR
2	C	214	ARG
3	D	34	LEU
3	D	53	VAL
3	D	149	VAL
3	D	186	THR
1	I	2	HIS
1	I	120	THR
1	I	265	THR
1	I	276	LEU
1	I	318	VAL
1	I	355	ILE
1	I	363	VAL
1	I	374	SER
1	I	380	THR
2	J	63	SER
2	J	115	VAL
2	J	117	SER
2	J	175	GLN
2	J	179	LEU
2	J	192	SER
2	J	200	CYS
3	K	27	SER
3	K	53	VAL
3	K	98	ILE
3	K	157	SER
1	M	89	ASP
1	M	120	THR
1	M	184	VAL
1	M	295	THR
2	N	17	SER
2	N	87	ARG
3	O	21	SER
3	O	27	SER
3	O	29	ILE

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Mol	Chain	Res	Type
3	O	108	LEU
3	O	114	PRO
3	O	141	ILE
3	O	170	SER
1	P	13	GLU
1	P	120	THR
1	P	224	ILE
1	P	265	THR
1	P	285	VAL
1	P	288	SER
1	P	318	VAL
1	P	380	THR
1	P	382	ASP
2	Q	187	THR
3	R	80	LEU
3	R	98	ILE
3	R	127	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	229	HIS
2	H	57	GLN
2	H	201	ASN
3	L	28	ASN
3	L	62	ASN
3	L	199	GLN
1	E	211	GLN
3	G	16	GLN
3	G	113	GLN
3	G	133	ASN
1	B	144	HIS
1	B	149	GLN
1	B	280	HIS
2	C	82	GLN
2	C	203	ASN
3	D	28	ASN
3	D	62	ASN
1	I	16	HIS
1	I	185	GLN
1	I	321	GLN

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Mol	Chain	Res	Type
2	J	82	GLN
2	J	84	ASN
2	J	203	ASN
3	K	1	GLN
1	M	238	HIS
1	M	359	ASN
2	N	77	ASN
2	N	84	ASN
2	N	175	GLN
1	P	132	GLN
1	P	144	HIS
1	P	230	HIS
1	P	359	ASN
2	Q	109	GLN
3	R	41	HIS
3	R	107	HIS

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	392/398 (98%)	0.74	42 (10%) 11 8	19, 42, 93, 181	1 (0%)
1	B	388/398 (97%)	0.83	44 (11%) 10 7	21, 47, 99, 144	1 (0%)
1	E	392/398 (98%)	1.00	68 (17%) 4 3	24, 51, 118, 163	0
1	I	388/398 (97%)	0.85	54 (13%) 6 5	21, 46, 95, 186	0
1	M	388/398 (97%)	1.49	111 (28%) 1 1	32, 60, 131, 235	0
1	P	388/398 (97%)	0.85	46 (11%) 9 7	18, 47, 98, 175	0
2	C	216/217 (99%)	1.27	51 (23%) 2 1	21, 67, 159, 238	0
2	F	216/217 (99%)	1.90	88 (40%) 0 0	26, 96, 210, 253	0
2	H	216/217 (99%)	1.32	59 (27%) 1 1	20, 74, 168, 234	0
2	J	211/217 (97%)	1.06	34 (16%) 4 4	17, 66, 100, 162	0
2	N	216/217 (99%)	2.21	104 (48%) 0 0	38, 113, 227, 268	0
2	Q	216/217 (99%)	0.65	29 (13%) 7 5	9, 44, 137, 215	0
3	D	213/217 (98%)	1.31	52 (24%) 2 1	22, 73, 124, 173	0
3	G	216/217 (99%)	1.72	89 (41%) 0 0	30, 87, 177, 237	0
3	K	214/217 (98%)	1.05	29 (13%) 7 5	21, 66, 114, 153	0
3	L	214/217 (98%)	1.16	40 (18%) 3 2	22, 72, 126, 186	0
3	O	217/217 (100%)	2.68	128 (58%) 0 0	46, 140, 231, 292	0
3	R	213/217 (98%)	1.10	37 (17%) 4 3	21, 67, 115, 146	0
All	All	4914/4992 (98%)	1.22	1105 (22%) 2 1	9, 60, 164, 292	2 (0%)

All (1105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	238[A]	HIS	8.9
3	O	123	PHE	8.3
2	F	127	PRO	8.2

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Mol	Chain	Res	Type	RSRZ
3	D	123	PHE	7.6
1	P	187	ALA	7.5
1	I	187	ALA	7.2
1	E	190	PHE	7.1
1	M	190	PHE	7.1
3	L	2	ALA	7.1
3	R	1	GLN	7.1
1	M	294	GLY	7.1
3	O	180	SER	7.1
1	I	268	GLU	7.1
3	O	207	VAL	7.0
3	D	29	ILE	6.9
3	O	148	ALA	6.8
1	M	268	GLU	6.8
1	M	188	VAL	6.8
1	A	188	VAL	6.6
2	N	142	LEU	6.6
2	H	131	SER	6.6
1	P	268	GLU	6.5
3	G	199	GLN	6.5
1	A	187	ALA	6.5
2	F	163	LEU	6.5
2	C	193	LEU	6.4
2	N	177	SER	6.3
1	A	328	ALA	6.3
3	O	112	GLY	6.3
1	M	344	VAL	6.3
1	M	293	LYS	6.3
2	N	135	THR	6.3
2	C	198	TYR	6.3
1	M	274	TYR	6.2
3	O	108	LEU	6.2
2	F	187	THR	6.2
3	O	153	TRP	6.1
1	P	130	VAL	6.1
3	O	110	VAL	6.1
2	C	135	THR	6.0
2	F	145	LEU	6.0
1	M	327	GLY	5.9
1	M	240	ALA	5.9
3	O	125	PRO	5.9
1	B	268	GLU	5.8

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Mol	Chain	Res	Type	RSRZ
1	E	187	ALA	5.8
1	P	190	PHE	5.8
3	O	10	VAL	5.8
1	M	220	GLY	5.7
1	A	382	ASP	5.7
1	I	164	LEU	5.7
2	Q	133	LYS	5.7
1	I	188	VAL	5.7
3	D	166	THR	5.7
2	J	132	SER	5.6
2	Q	131	SER	5.6
1	I	328	ALA	5.6
2	F	176	SER	5.6
1	A	166	GLY	5.6
1	M	295	THR	5.6
2	H	193	LEU	5.5
2	N	124	SER	5.5
2	F	144	CYS	5.5
3	O	71	ASN	5.5
2	N	133	LYS	5.5
3	G	196	TYR	5.5
2	F	141	ALA	5.5
1	M	192	ASN	5.4
2	H	133	LYS	5.4
3	O	200	VAL	5.4
1	A	240	ALA	5.4
3	R	162	ALA	5.4
3	O	206	THR	5.4
3	O	124	PRO	5.3
3	D	34	LEU	5.3
3	O	160	VAL	5.3
3	O	121	THR	5.3
1	M	16	HIS	5.3
1	M	187	ALA	5.3
2	N	145	LEU	5.3
2	N	125	VAL	5.3
3	G	127	SER	5.2
3	O	204	GLY	5.2
2	C	133	LYS	5.2
2	Q	163	LEU	5.2
2	J	73	ASP	5.2
3	O	111	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	I	145	VAL	5.2
3	K	112	GLY	5.2
3	O	183	LEU	5.2
1	B	328	ALA	5.1
2	J	162	ALA	5.1
3	R	2	ALA	5.1
1	B	189	ASP	5.1
3	K	33	ASN	5.1
1	M	1	ALA	5.1
3	O	140	LEU	5.1
2	H	132	SER	5.1
1	E	344	VAL	5.1
2	N	169	THR	5.1
2	N	128	LEU	5.1
2	N	179	LEU	5.1
1	M	298	LYS	5.1
2	F	198	TYR	5.1
3	G	157	SER	5.1
3	O	190	TRP	5.0
1	A	130	VAL	5.0
2	F	202	VAL	5.0
2	N	131	SER	5.0
2	N	136	SER	5.0
2	N	163	LEU	5.0
2	J	116	SER	5.0
1	B	186	THR	5.0
3	O	159	PRO	4.9
2	F	199	ILE	4.9
2	F	146	VAL	4.9
1	E	186	THR	4.9
1	I	166	GLY	4.9
3	G	161	LYS	4.9
1	M	299	MET	4.9
1	E	145	VAL	4.9
3	G	33	ASN	4.8
1	A	238[A]	HIS	4.8
3	O	3	VAL	4.8
2	N	141	ALA	4.8
1	P	188	VAL	4.8
2	N	154	VAL	4.8
3	L	124	PRO	4.8
1	A	17	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	343	ALA	4.8
2	H	129	ALA	4.8
2	F	184	SER	4.8
1	A	221	SER	4.7
1	I	190	PHE	4.7
3	O	201	THR	4.7
2	N	156	VAL	4.7
3	G	2	ALA	4.7
2	F	133	LYS	4.7
1	I	238	HIS	4.7
3	R	3	VAL	4.7
1	I	382	ASP	4.6
3	O	209	LYS	4.6
1	P	15	VAL	4.6
1	E	328	ALA	4.6
2	Q	162	ALA	4.6
2	F	135	THR	4.6
1	M	297	TYR	4.6
1	B	191	GLY	4.6
2	N	127	PRO	4.6
1	P	186	THR	4.6
2	N	123	PRO	4.6
1	M	328	ALA	4.5
1	E	238	HIS	4.5
1	P	14	GLY	4.5
2	F	131	SER	4.5
3	R	188	GLU	4.5
1	A	1	ALA	4.5
3	O	122	LEU	4.5
2	N	198	TYR	4.5
3	O	196	TYR	4.5
1	I	220	GLY	4.5
3	O	166	THR	4.5
1	B	267	ASP	4.5
3	O	151	VAL	4.5
1	B	1	ALA	4.5
1	A	16	HIS	4.4
1	M	337	ALA	4.4
3	O	179	ALA	4.4
3	G	26	GLY	4.4
1	M	358	THR	4.4
1	I	167	SER	4.4

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Mol	Chain	Res	Type	RSRZ
2	Q	191	SER	4.4
2	N	193	LEU	4.4
3	G	198	CYS	4.4
2	F	142	LEU	4.4
3	L	214	THR	4.4
3	G	206	THR	4.4
1	E	16	HIS	4.4
3	L	13	SER	4.4
3	O	127	SER	4.4
3	G	159	PRO	4.4
1	E	15	VAL	4.4
3	G	3	VAL	4.4
2	C	131	SER	4.3
3	D	1	GLN	4.3
2	N	202	VAL	4.3
2	F	174	LEU	4.3
3	O	214	THR	4.3
2	N	129	ALA	4.3
2	N	187	THR	4.3
2	N	211	VAL	4.3
3	G	154	LYS	4.3
1	P	1	ALA	4.3
1	P	167	SER	4.3
2	N	116	SER	4.3
3	O	205	SER	4.3
1	P	191	GLY	4.3
2	H	215	VAL	4.3
2	F	215	VAL	4.3
2	N	168	HIS	4.2
2	N	160	SER	4.2
2	Q	135	THR	4.2
1	A	145	VAL	4.2
3	G	200	VAL	4.2
3	D	122	LEU	4.2
1	I	343	ALA	4.2
2	C	129	ALA	4.2
3	O	117	ALA	4.2
2	N	126	PHE	4.2
3	O	135	ALA	4.2
1	B	327	GLY	4.2
2	F	128	LEU	4.2
3	O	82	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
3	D	213	PRO	4.1
1	M	355	ILE	4.1
2	N	85	SER	4.1
3	D	141	ILE	4.1
1	A	186	THR	4.1
1	B	188	VAL	4.1
2	F	162	ALA	4.1
1	M	267	ASP	4.1
1	P	267	ASP	4.1
1	A	190	PHE	4.1
1	M	357	SER	4.1
3	K	140	LEU	4.1
3	O	41	HIS	4.1
3	G	150	THR	4.1
2	N	130	PRO	4.1
2	N	199	ILE	4.1
1	M	296	SER	4.1
2	F	217	PRO	4.1
3	O	42	PRO	4.1
1	E	14	GLY	4.1
1	E	146	GLY	4.1
1	B	220	GLY	4.1
3	O	64	PHE	4.1
1	M	193	SER	4.1
2	F	154	VAL	4.1
3	O	198	CYS	4.0
2	F	130	PRO	4.0
2	F	188	VAL	4.0
3	D	152	ALA	4.0
3	O	2	ALA	4.0
2	N	158	TRP	4.0
3	G	214	THR	4.0
1	M	15	VAL	4.0
2	N	146	VAL	4.0
2	N	167	VAL	4.0
2	N	191	SER	4.0
2	N	189	PRO	4.0
1	B	222	GLY	4.0
1	M	52	GLY	4.0
1	I	267	ASP	4.0
3	G	207	VAL	4.0
2	N	155	THR	3.9

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Mol	Chain	Res	Type	RSRZ
2	H	217	PRO	3.9
3	K	1	GLN	3.9
2	C	214	ARG	3.9
3	L	188	GLU	3.9
3	G	135	ALA	3.9
3	G	152	ALA	3.9
1	M	81	HIS	3.9
3	O	104	GLY	3.9
1	M	145	VAL	3.9
2	N	217	PRO	3.9
3	D	127	SER	3.9
1	M	239	ALA	3.9
2	H	166	GLY	3.9
2	F	125	VAL	3.9
2	F	186	VAL	3.9
3	L	149	VAL	3.9
2	F	123	PRO	3.9
2	N	63	SER	3.9
3	G	180	SER	3.9
1	E	342	ALA	3.9
1	I	163	ALA	3.9
1	M	300	CYS	3.9
2	F	206	PRO	3.8
1	I	165	SER	3.8
3	O	27	SER	3.8
3	O	8	ALA	3.8
2	N	171	PRO	3.8
1	M	132	GLN	3.8
1	M	301	THR	3.8
2	F	155	THR	3.8
3	O	217	SER	3.8
3	O	162	ALA	3.8
3	O	138	VAL	3.8
1	M	266	LYS	3.8
3	O	182	TYR	3.8
3	G	185	LEU	3.8
2	F	177	SER	3.8
3	O	17	SER	3.8
2	F	129	ALA	3.8
3	G	148	ALA	3.8
3	G	212	ALA	3.8
2	N	170	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
2	F	147	LYS	3.8
3	G	186	THR	3.7
2	Q	132	SER	3.7
2	N	137	GLY	3.7
3	G	209	LYS	3.7
1	E	192	ASN	3.7
1	M	221	SER	3.7
3	R	115	LYS	3.7
2	J	163	LEU	3.7
3	D	25	THR	3.7
2	N	190	SER	3.7
2	H	167	VAL	3.7
2	F	185	VAL	3.7
2	C	188	VAL	3.7
1	I	186	THR	3.7
1	I	4	ILE	3.7
1	P	189	ASP	3.7
2	H	187	THR	3.7
1	E	1	ALA	3.7
2	N	40	ALA	3.7
1	M	184	VAL	3.7
3	G	122	LEU	3.6
3	O	98	ILE	3.6
1	M	331	LYS	3.6
3	O	139	CYS	3.6
1	M	211	GLN	3.6
3	G	130	LEU	3.6
3	O	109	THR	3.6
2	H	198	TYR	3.6
2	Q	194	GLY	3.6
2	C	132	SER	3.6
2	F	211	VAL	3.6
2	C	196	GLN	3.6
3	O	30	GLU	3.6
3	G	136	THR	3.6
2	N	118	ALA	3.6
3	R	89	PHE	3.6
3	O	150	THR	3.6
3	D	156	ASP	3.6
3	L	125	PRO	3.6
1	B	190	PHE	3.6
1	E	383	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	361	ASP	3.5
1	B	240	ALA	3.5
1	A	15	VAL	3.5
1	M	324	VAL	3.5
1	P	145	VAL	3.5
2	F	156	VAL	3.5
2	F	181	SER	3.5
2	J	160	SER	3.5
1	A	220	GLY	3.5
3	K	172	GLN	3.5
3	G	182	TYR	3.5
3	R	13	SER	3.5
1	P	4	ILE	3.5
2	H	144	CYS	3.5
1	M	186	THR	3.5
3	L	135	ALA	3.5
3	R	116	ALA	3.5
3	O	146	PRO	3.5
2	N	188	VAL	3.5
3	O	137	LEU	3.5
3	O	77	ILE	3.5
3	O	126	SER	3.5
2	C	195	THR	3.5
2	N	147	LYS	3.5
3	R	28	ASN	3.5
1	B	279	GLY	3.5
1	I	1	ALA	3.5
3	K	2	ALA	3.5
2	F	189	PRO	3.5
2	N	153	PRO	3.5
2	F	182	LEU	3.5
2	H	214	ARG	3.5
1	M	383	SER	3.4
2	F	136	SER	3.4
1	M	326	LYS	3.4
3	O	132	ALA	3.4
3	R	155	ALA	3.4
2	F	193	LEU	3.4
3	O	130	LEU	3.4
2	C	145	LEU	3.4
2	F	214	ARG	3.4
1	E	188	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	167	SER	3.4
3	R	177	TYR	3.4
2	F	209	THR	3.4
1	A	13	GLU	3.4
3	L	148	ALA	3.4
2	F	126	PHE	3.4
2	N	184	SER	3.4
3	G	197	SER	3.4
1	M	291	THR	3.4
3	K	214	THR	3.4
1	B	379	GLY	3.4
3	G	216	CYS	3.4
3	O	185	LEU	3.4
1	B	16	HIS	3.4
3	G	120	VAL	3.4
2	H	213	LYS	3.3
1	A	219	SER	3.3
2	C	165	SER	3.3
3	L	27	SER	3.3
1	P	16	HIS	3.3
2	F	122	GLY	3.3
2	F	178	GLY	3.3
3	R	112	GLY	3.3
3	R	131	GLN	3.3
2	N	173	VAL	3.3
3	L	3	VAL	3.3
3	O	191	LYS	3.3
2	C	134	SER	3.3
3	O	11	SER	3.3
2	C	189	PRO	3.3
2	Q	193	LEU	3.3
1	E	132	GLN	3.3
1	M	238	HIS	3.3
1	M	260	GLY	3.3
1	M	390	HIS	3.3
1	A	192	ASN	3.3
3	L	71	ASN	3.3
2	C	158	TRP	3.3
3	K	9	SER	3.3
2	J	128	LEU	3.3
1	E	294	GLY	3.3
3	L	1	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	192	ASN	3.3
1	P	192	ASN	3.3
3	O	120	VAL	3.3
1	A	329	PRO	3.3
2	F	151	PRO	3.3
2	C	197	THR	3.3
1	B	262	MET	3.3
1	M	166	GLY	3.3
1	P	326	LYS	3.3
3	O	26	GLY	3.3
3	O	163	GLY	3.3
1	P	342	ALA	3.3
2	Q	129	ALA	3.3
3	G	117	ALA	3.3
2	Q	217	PRO	3.2
1	M	73	LYS	3.2
2	C	76	LYS	3.2
2	Q	134	SER	3.2
3	O	181	SER	3.2
3	K	177	TYR	3.2
3	D	135	ALA	3.2
3	O	216	CYS	3.2
3	L	194	ARG	3.2
2	H	216	GLU	3.2
2	N	182	LEU	3.2
1	P	238	HIS	3.2
3	G	187	PRO	3.2
2	C	187	THR	3.2
3	O	186	THR	3.2
1	I	221	SER	3.2
3	O	212	ALA	3.2
3	O	164	VAL	3.2
3	R	33	ASN	3.2
2	F	212	ASP	3.2
2	N	148	ASP	3.2
3	G	191	LYS	3.2
1	M	392	GLU	3.2
2	H	127	PRO	3.2
2	J	164	THR	3.2
3	G	167	THR	3.2
3	D	109	THR	3.2
3	O	152	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
3	G	160	VAL	3.2
3	O	89	PHE	3.2
2	H	163	LEU	3.2
3	G	169	PRO	3.2
3	O	118	PRO	3.2
3	O	193	HIS	3.2
1	E	341	THR	3.2
3	G	190	TRP	3.2
3	O	12	GLY	3.2
2	F	132	SER	3.2
2	F	140	ALA	3.2
2	N	132	SER	3.2
2	N	134	SER	3.2
2	F	203	ASN	3.1
1	I	283	CYS	3.1
1	M	381	GLY	3.1
2	F	158	TRP	3.1
2	F	161	GLY	3.1
2	Q	161	GLY	3.1
3	G	112	GLY	3.1
3	G	155	ALA	3.1
3	R	148	ALA	3.1
2	H	124	SER	3.1
2	H	154	VAL	3.1
2	F	150	PHE	3.1
3	L	33	ASN	3.1
3	O	136	THR	3.1
1	E	379	GLY	3.1
2	C	122	GLY	3.1
1	B	239	ALA	3.1
3	G	141	ILE	3.1
2	H	156	VAL	3.1
3	R	157	SER	3.1
1	I	266	LYS	3.1
2	N	205	LYS	3.1
2	F	168	HIS	3.1
3	G	83	GLU	3.1
2	F	175	GLN	3.1
1	E	381	GLY	3.1
2	H	200	CYS	3.1
2	H	126	PHE	3.1
3	D	161	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
3	R	191	LYS	3.1
2	H	202	VAL	3.1
2	J	177	SER	3.1
2	J	11	LEU	3.1
1	E	382	ASP	3.1
2	F	148	ASP	3.1
3	O	129	GLU	3.1
1	M	329	PRO	3.1
1	E	191	GLY	3.1
3	G	210	THR	3.1
1	E	343	ALA	3.1
1	P	328	ALA	3.1
3	K	68	LYS	3.1
2	H	128	LEU	3.0
2	J	86	LEU	3.0
3	G	140	LEU	3.0
1	E	392	GLU	3.0
1	I	392	GLU	3.0
3	O	107	HIS	3.0
1	E	162	ASP	3.0
1	E	189	ASP	3.0
3	D	124	PRO	3.0
2	F	205	LYS	3.0
1	M	14	GLY	3.0
1	M	222	GLY	3.0
3	K	70	GLY	3.0
3	O	147	GLY	3.0
2	H	162	ALA	3.0
3	L	152	ALA	3.0
2	H	185	VAL	3.0
1	M	195	ILE	3.0
1	P	220	GLY	3.0
2	C	164	THR	3.0
1	E	239	ALA	3.0
3	G	162	ALA	3.0
2	C	142	LEU	3.0
2	H	168	HIS	3.0
2	N	159	ASN	3.0
3	D	125	PRO	3.0
3	O	131	GLN	3.0
3	O	68	LYS	3.0
1	P	166	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
2	N	195	THR	3.0
3	G	201	THR	3.0
2	N	172	ALA	3.0
3	O	155	ALA	3.0
1	B	344	VAL	3.0
2	N	150	PHE	3.0
2	H	153	PRO	3.0
1	A	272	ASN	3.0
3	O	177	TYR	3.0
2	H	194	GLY	3.0
2	F	164	THR	3.0
3	K	168	THR	3.0
3	O	167	THR	3.0
1	B	342	ALA	3.0
2	C	172	ALA	3.0
2	N	97	ALA	3.0
2	C	130	PRO	2.9
3	L	131	GLN	2.9
2	H	199	ILE	2.9
3	O	103	GLY	2.9
2	J	115	VAL	2.9
2	N	215	VAL	2.9
3	G	137	LEU	2.9
1	E	199	GLU	2.9
2	H	210	LYS	2.9
2	H	119	SER	2.9
2	J	124	SER	2.9
3	G	27	SER	2.9
3	G	126	SER	2.9
3	G	181	SER	2.9
1	E	372	GLY	2.9
1	I	327	GLY	2.9
3	D	162	ALA	2.9
2	H	188	VAL	2.9
1	E	171	GLU	2.9
2	F	121	LYS	2.9
2	F	160	SER	2.9
2	F	183	SER	2.9
2	N	192	SER	2.9
1	B	192	ASN	2.9
2	Q	195	THR	2.9
3	O	106	THR	2.9

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Mol	Chain	Res	Type	RSRZ
3	D	132	ALA	2.9
1	I	344	VAL	2.9
3	G	211	VAL	2.9
1	E	221	SER	2.9
1	P	221	SER	2.9
2	Q	208	ASN	2.9
3	D	33	ASN	2.9
2	H	138	GLY	2.9
3	G	166	THR	2.9
1	P	343	ALA	2.9
2	N	86	LEU	2.9
3	G	116	ALA	2.9
3	G	118	PRO	2.8
3	O	169	PRO	2.8
1	E	305	SER	2.8
3	D	27	SER	2.8
3	O	192	SER	2.8
1	E	18	GLY	2.8
1	B	338	ASP	2.8
2	C	194	GLY	2.8
3	D	143	ASP	2.8
1	I	245	LEU	2.8
2	Q	142	LEU	2.8
3	D	130	LEU	2.8
2	J	154	VAL	2.8
3	G	205	SER	2.8
2	F	213	LYS	2.8
2	H	135	THR	2.8
2	C	162	ALA	2.8
2	N	164	THR	2.8
2	H	2	VAL	2.8
2	F	167	VAL	2.8
3	L	83	GLU	2.8
3	O	128	GLU	2.8
2	C	217	PRO	2.8
3	K	114	PRO	2.8
3	G	134	LYS	2.8
3	G	195	SER	2.8
1	A	14	GLY	2.8
1	B	166	GLY	2.8
3	L	130	LEU	2.8
3	O	70	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	189	ASP	2.8
1	M	380	THR	2.8
1	I	15	VAL	2.8
3	G	114	PRO	2.8
3	O	187	PRO	2.8
2	Q	136	SER	2.8
3	G	153	TRP	2.8
3	K	173	SER	2.8
1	E	290	LEU	2.8
1	M	276	LEU	2.8
2	N	194	GLY	2.8
1	A	239	ALA	2.8
1	E	380	THR	2.8
1	B	241	THR	2.8
1	P	178	ALA	2.8
2	N	2	VAL	2.8
3	O	211	VAL	2.8
2	H	171	PRO	2.7
2	C	144	CYS	2.7
2	J	200	CYS	2.7
2	N	76	LYS	2.7
2	C	128	LEU	2.7
3	G	119	SER	2.7
2	F	143	GLY	2.7
2	J	161	GLY	2.7
1	M	83	ALA	2.7
2	F	195	THR	2.7
3	G	208	GLU	2.7
3	G	123	PHE	2.7
2	H	130	PRO	2.7
2	F	180	TYR	2.7
3	L	196	TYR	2.7
3	O	213	PRO	2.7
2	F	200	CYS	2.7
2	J	65	LYS	2.7
1	M	349	LEU	2.7
2	C	136	SER	2.7
1	E	81	HIS	2.7
1	I	88	GLY	2.7
1	I	191	GLY	2.7
1	I	219	SER	2.7
3	L	127	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	13	GLU	2.7
2	H	197	THR	2.7
3	D	160	VAL	2.7
3	O	88	TYR	2.7
2	C	166	GLY	2.7
2	N	207	SER	2.7
3	G	204	GLY	2.7
1	E	240	ALA	2.7
1	M	341	THR	2.7
2	H	155	THR	2.7
1	E	326	LYS	2.7
3	O	114	PRO	2.7
3	R	114	PRO	2.7
3	D	131	GLN	2.7
1	E	30	CYS	2.7
3	L	90	CYS	2.7
3	O	90	CYS	2.7
1	I	16	HIS	2.7
2	F	49	SER	2.7
2	F	172	ALA	2.7
3	D	207	VAL	2.7
1	E	37	ASP	2.7
1	E	267	ASP	2.7
1	E	175	TYR	2.6
2	F	112	LEU	2.6
1	M	129	GLU	2.6
1	M	200	LYS	2.6
1	M	303	LYS	2.6
2	N	176	SER	2.6
2	N	203	ASN	2.6
3	K	154	LYS	2.6
3	K	161	LYS	2.6
1	A	344	VAL	2.6
1	B	221	SER	2.6
2	N	112	LEU	2.6
2	F	8	GLY	2.6
2	J	13	LYS	2.6
3	D	30	GLU	2.6
1	I	342	ALA	2.6
1	M	345	ASN	2.6
2	J	185	VAL	2.6
3	R	175	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	288	SER	2.6
2	H	158	TRP	2.6
2	F	153	PRO	2.6
2	N	106	THR	2.6
2	N	151	PRO	2.6
2	N	11	LEU	2.6
3	G	194	ARG	2.6
3	L	123	PHE	2.6
3	D	117	ALA	2.6
1	B	95	THR	2.6
1	B	295	THR	2.6
2	H	191	SER	2.6
2	Q	139	THR	2.6
1	M	51	ASP	2.6
1	M	302	ASP	2.6
3	R	156	ASP	2.6
1	M	204	ILE	2.6
3	G	177	TYR	2.6
2	Q	216	GLU	2.6
3	D	188	GLU	2.6
2	N	144	CYS	2.6
2	F	190	SER	2.5
2	J	190	SER	2.5
2	N	119	SER	2.5
3	K	143	ASP	2.5
1	M	263	ARG	2.5
2	N	149	TYR	2.5
2	C	62	GLU	2.5
1	P	327	GLY	2.5
2	C	211	VAL	2.5
1	B	187	ALA	2.5
1	B	358	THR	2.5
1	M	241	THR	2.5
2	F	134	SER	2.5
3	G	192	SER	2.5
3	D	195	SER	2.5
1	M	10	ASP	2.5
1	A	326	LYS	2.5
3	R	111	LEU	2.5
1	A	392	GLU	2.5
3	O	208	GLU	2.5
3	O	215	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	222	GLY	2.5
1	E	17	GLY	2.5
2	N	122	GLY	2.5
1	M	334	VAL	2.5
2	F	173	VAL	2.5
1	I	240	ALA	2.5
1	M	343	ALA	2.5
2	N	196	GLN	2.5
3	O	1	GLN	2.5
1	A	95	THR	2.5
2	F	169	THR	2.5
2	F	197	THR	2.5
2	F	191	SER	2.5
3	L	195	SER	2.5
3	O	67	SER	2.5
1	B	162	ASP	2.5
1	P	200	LYS	2.5
2	N	78	LEU	2.5
1	M	79	GLU	2.5
1	P	150	GLU	2.5
3	G	30	GLU	2.5
2	N	161	GLY	2.5
2	N	185	VAL	2.5
1	M	259	THR	2.5
1	M	330	CYS	2.5
3	D	171	LYS	2.5
3	O	44	LYS	2.5
1	E	374	SER	2.5
1	M	207	ARG	2.5
2	H	183	SER	2.5
2	N	181	SER	2.5
3	O	184	SER	2.5
1	E	166	GLY	2.5
1	M	194	TYR	2.5
1	M	223	GLY	2.5
1	M	333	PRO	2.5
2	Q	198	TYR	2.5
1	I	27	GLN	2.5
2	Q	215	VAL	2.5
1	M	342	ALA	2.5
3	L	161	LYS	2.4
3	O	134	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	N	114	THR	2.4
1	E	271	ASN	2.4
1	I	30	CYS	2.4
2	H	96	CYS	2.4
2	H	134	SER	2.4
3	D	126	SER	2.4
3	O	157	SER	2.4
3	O	170	SER	2.4
1	E	270	ASP	2.4
3	L	156	ASP	2.4
1	B	55	GLU	2.4
1	A	279	GLY	2.4
2	C	149	TYR	2.4
1	M	130	VAL	2.4
3	O	149	VAL	2.4
1	P	243	ARG	2.4
3	D	168	THR	2.4
1	M	135	ILE	2.4
2	H	182	LEU	2.4
2	C	199	ILE	2.4
2	H	181	SER	2.4
2	J	85	SER	2.4
3	L	126	SER	2.4
3	L	192	SER	2.4
3	K	27	SER	2.4
3	K	69	SER	2.4
3	O	158	SER	2.4
3	R	197	SER	2.4
1	M	189	ASP	2.4
2	H	161	GLY	2.4
3	L	112	GLY	2.4
2	Q	13	LYS	2.4
2	C	215	VAL	2.4
3	G	149	VAL	2.4
3	K	160	VAL	2.4
1	M	371	PHE	2.4
1	P	170	ALA	2.4
2	C	140	ALA	2.4
1	E	301	THR	2.4
2	C	169	THR	2.4
3	D	96	THR	2.4
1	I	153	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	305	SER	2.4
2	Q	165	SER	2.4
3	L	11	SER	2.4
3	L	180	SER	2.4
3	O	13	SER	2.4
3	R	27	SER	2.4
1	E	268	GLU	2.4
3	R	83	GLU	2.4
2	N	14	PRO	2.4
3	D	115	LYS	2.4
2	C	161	GLY	2.4
3	G	132	ALA	2.4
2	N	197	THR	2.4
3	G	168	THR	2.4
1	M	359	ASN	2.4
1	I	55	GLU	2.4
1	P	329	PRO	2.4
3	G	124	PRO	2.4
2	H	196	GLN	2.4
1	I	243	ARG	2.4
1	M	356	ALA	2.4
2	N	140	ALA	2.4
3	O	144	PHE	2.4
3	D	196	TYR	2.3
3	R	186	THR	2.3
1	B	298	LYS	2.3
2	N	186	VAL	2.3
2	J	179	LEU	2.3
3	R	178	ALA	2.3
1	M	137	TYR	2.3
3	K	62	ASN	2.3
3	O	203	GLU	2.3
3	R	161	LYS	2.3
1	A	162	ASP	2.3
1	B	357	SER	2.3
1	M	374	SER	2.3
2	H	49	SER	2.3
3	G	217	SER	2.3
1	B	20	TRP	2.3
2	H	189	PRO	2.3
2	Q	189	PRO	2.3
3	L	159	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	327	GLY	2.3
1	I	300	CYS	2.3
2	F	170	PHE	2.3
2	C	174	LEU	2.3
3	O	29	ILE	2.3
3	G	202	HIS	2.3
1	E	291	THR	2.3
1	B	341	THR	2.3
1	M	304	MET	2.3
3	G	115	LYS	2.3
3	O	85	GLU	2.3
1	A	270	ASP	2.3
1	I	162	ASP	2.3
1	M	167	SER	2.3
2	J	184	SER	2.3
2	H	42	GLY	2.3
2	H	142	LEU	2.3
2	N	4	LEU	2.3
2	Q	96	CYS	2.3
1	M	346	LYS	2.3
3	D	150	THR	2.3
3	O	19	THR	2.3
3	O	161	LYS	2.3
2	N	180	TYR	2.3
1	A	199	GLU	2.3
1	E	55	GLU	2.3
2	F	152	GLU	2.3
3	O	83	GLU	2.3
3	O	165	GLU	2.3
2	J	208	ASN	2.3
2	Q	192	SER	2.3
3	D	142	SER	2.3
3	R	194	ARG	2.3
1	E	378	VAL	2.3
1	B	363	VAL	2.3
1	B	343	ALA	2.2
1	M	332	ILE	2.2
2	C	96	CYS	2.2
2	N	162	ALA	2.2
3	D	178	ALA	2.2
3	O	94	ALA	2.2
3	O	141	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	81	HIS	2.2
3	L	193	HIS	2.2
1	I	200	LYS	2.2
1	E	19	THR	2.2
3	D	210	THR	2.2
1	A	55	GLU	2.2
3	D	182	TYR	2.2
1	E	8	ASP	2.2
2	H	136	SER	2.2
2	N	157	SER	2.2
2	N	115	VAL	2.2
2	N	174	LEU	2.2
3	L	190	TRP	2.2
2	H	211	VAL	2.2
2	C	154	VAL	2.2
2	C	167	VAL	2.2
1	E	280	HIS	2.2
1	P	298	LYS	2.2
3	K	18	ILE	2.2
3	R	98	ILE	2.2
1	M	3	CYS	2.2
1	M	30	CYS	2.2
1	M	375	TYR	2.2
1	A	57	ARG	2.2
1	E	153	ASN	2.2
1	P	207	ARG	2.2
3	K	159	PRO	2.2
1	M	176	GLY	2.2
1	M	305	SER	2.2
2	J	25	SER	2.2
3	O	59	GLY	2.2
3	G	183	LEU	2.2
1	E	303	LYS	2.2
1	M	209	TRP	2.2
2	J	43	LYS	2.2
2	N	121	LYS	2.2
2	H	150	PHE	2.2
1	E	163	ALA	2.2
3	D	212	ALA	2.2
2	H	195	THR	2.2
3	L	186	THR	2.2
3	R	210	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	243	ARG	2.2
2	N	214	ARG	2.2
1	A	271	ASN	2.2
3	L	28	ASN	2.2
3	G	189	GLN	2.2
1	B	278	GLY	2.2
1	E	167	SER	2.2
1	E	357	SER	2.2
1	I	87	ASP	2.2
1	M	338	ASP	2.2
1	P	245	LEU	2.2
2	N	43	LYS	2.2
2	N	138	GLY	2.2
2	Q	44	GLY	2.2
2	C	191	SER	2.2
3	K	127	SER	2.2
3	O	47	LYS	2.2
3	O	119	SER	2.2
1	E	299	MET	2.2
1	P	344	VAL	2.2
2	F	2	VAL	2.2
3	K	151	VAL	2.2
3	R	160	VAL	2.2
1	E	2	HIS	2.2
2	C	40	ALA	2.2
1	A	241	THR	2.2
1	M	185	GLN	2.2
1	A	18	GLY	2.2
1	M	379	GLY	2.2
1	P	18	GLY	2.2
2	N	143	GLY	2.2
3	G	156	ASP	2.2
1	I	296	SER	2.2
2	F	12	VAL	2.2
3	G	138	VAL	2.2
3	D	21	SER	2.2
1	I	74	CYS	2.1
1	M	102	GLY	2.1
3	D	112	GLY	2.1
1	B	219	SER	2.1
1	P	282	SER	2.1
2	F	64	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	185	VAL	2.1
3	G	54	SER	2.1
3	G	158	SER	2.1
3	R	10	VAL	2.1
3	R	205	SER	2.1
2	F	216	GLU	2.1
3	G	203	GLU	2.1
1	M	154	THR	2.1
2	J	123	PRO	2.1
1	B	283	CYS	2.1
2	N	22	CYS	2.1
3	G	139	CYS	2.1
3	D	111	LEU	2.1
3	D	175	ASN	2.1
3	O	113	GLN	2.1
1	M	292	LEU	2.1
1	A	191	GLY	2.1
1	I	5	GLY	2.1
2	F	194	GLY	2.1
1	E	131	ASP	2.1
2	C	202	VAL	2.1
3	D	211	VAL	2.1
1	E	288	SER	2.1
2	C	25	SER	2.1
3	G	61	SER	2.1
3	D	17	SER	2.1
3	O	116	ALA	2.1
1	P	181	GLU	2.1
2	J	62	GLU	2.1
3	O	194	ARG	2.1
3	O	5	THR	2.1
2	N	213	LYS	2.1
2	J	151	PRO	2.1
1	P	74	CYS	2.1
3	K	145	TYR	2.1
2	J	12	VAL	2.1
2	J	156	VAL	2.1
1	I	8	ASP	2.1
1	P	382	ASP	2.1
1	E	219	SER	2.1
2	N	117	SER	2.1
3	G	9	SER	2.1

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Mol	Chain	Res	Type	RSRZ
3	K	11	SER	2.1
3	O	176	LYS	2.1
2	N	209	THR	2.1
2	Q	197	THR	2.1
1	M	325	PRO	2.1
2	F	171	PRO	2.1
3	R	146	PRO	2.1
1	B	299	MET	2.1
2	J	83	MET	2.1
1	M	388	GLN	2.1
1	I	381	GLY	2.1
3	L	26	GLY	2.1
3	R	147	GLY	2.1
1	I	43	ILE	2.1
1	I	130	VAL	2.1
1	M	205	VAL	2.1
2	C	146	VAL	2.1
1	M	162	ASP	2.0
3	G	128	GLU	2.0
3	G	129	GLU	2.0
2	F	63	SER	2.0
2	J	131	SER	2.0
2	N	165	SER	2.0
3	D	184	SER	2.0
3	K	162	ALA	2.0
3	K	191	LYS	2.0
2	C	171	PRO	2.0
3	O	80	LEU	2.0
3	G	28	ASN	2.0
1	P	381	GLY	2.0
2	F	137	GLY	2.0
2	C	10	GLY	2.0
2	J	199	ILE	2.0
3	D	204	GLY	2.0
1	P	30	CYS	2.0
1	P	283	CYS	2.0
2	Q	144	CYS	2.0
3	L	177	TYR	2.0
1	M	8	ASP	2.0
1	P	199	GLU	2.0
1	P	392	GLU	2.0
2	H	170	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
3	R	173	SER	2.0
2	H	106	THR	2.0
3	G	25	THR	2.0
3	D	206	THR	2.0
1	I	340	LEU	2.0
1	M	340	LEU	2.0
3	L	185	LEU	2.0
1	B	242	ILE	2.0
3	L	120	VAL	2.0
3	D	149	VAL	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.