



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:18 PM UTC

PDB ID : 1EAK / pdb_00001eak
Title : Catalytic domain of proMMP-2 E404Q mutant
Authors : Bergmann, U.; Tuuttila, A.; Tryggvason, K.; Morgunova, E.
Deposited on : 2001-07-12
Resolution : 2.66 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:

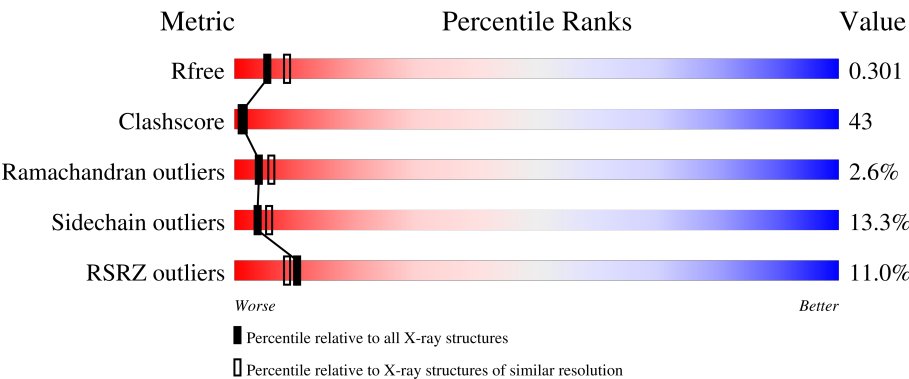
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.66 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	421	12% 45% 41% 13%
1	B	421	6% 46% 43% 9% .
1	C	421	8% 46% 45% 8% ..
1	D	421	15% 40% 43% 14% .
2	P	8	100% 25% 25% 50%

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Mol	Chain	Length	Quality of chain
2	R	8	100% 12% 50% 38%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	C	850	-	-	X	-
3	SO4	D	857	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13504 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 72 KDA TYPE IV COLLAGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3330	2110	553	644	23			
1	B	419	Total	C	N	O	S	0	0	0
			3313	2100	551	639	23			
1	C	418	Total	C	N	O	S	0	0	0
			3305	2096	550	636	23			
1	D	419	Total	C	N	O	S	0	0	0
			3313	2100	551	639	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	404	GLN	GLU	engineered mutation	UNP P08253
B	404	GLN	GLU	engineered mutation	UNP P08253
C	404	GLN	GLU	engineered mutation	UNP P08253
D	404	GLN	GLU	engineered mutation	UNP P08253

- Molecule 2 is a protein called INHIBITOR PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	8	Total	C	N	O	0	0	0
			44	27	8	9			
2	R	8	Total	C	N	O	0	0	0
			44	27	8	9			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	B	2	Total	Zn	0	0
			2	2		
4	C	2	Total	Zn	0	0
			2	2		
4	D	2	Total	Zn	0	0
			2	2		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Ca 2 2	0	0
5	B	2	Total Ca 2 2	0	0
5	C	2	Total Ca 2 2	0	0
5	D	2	Total Ca 2 2	0	0

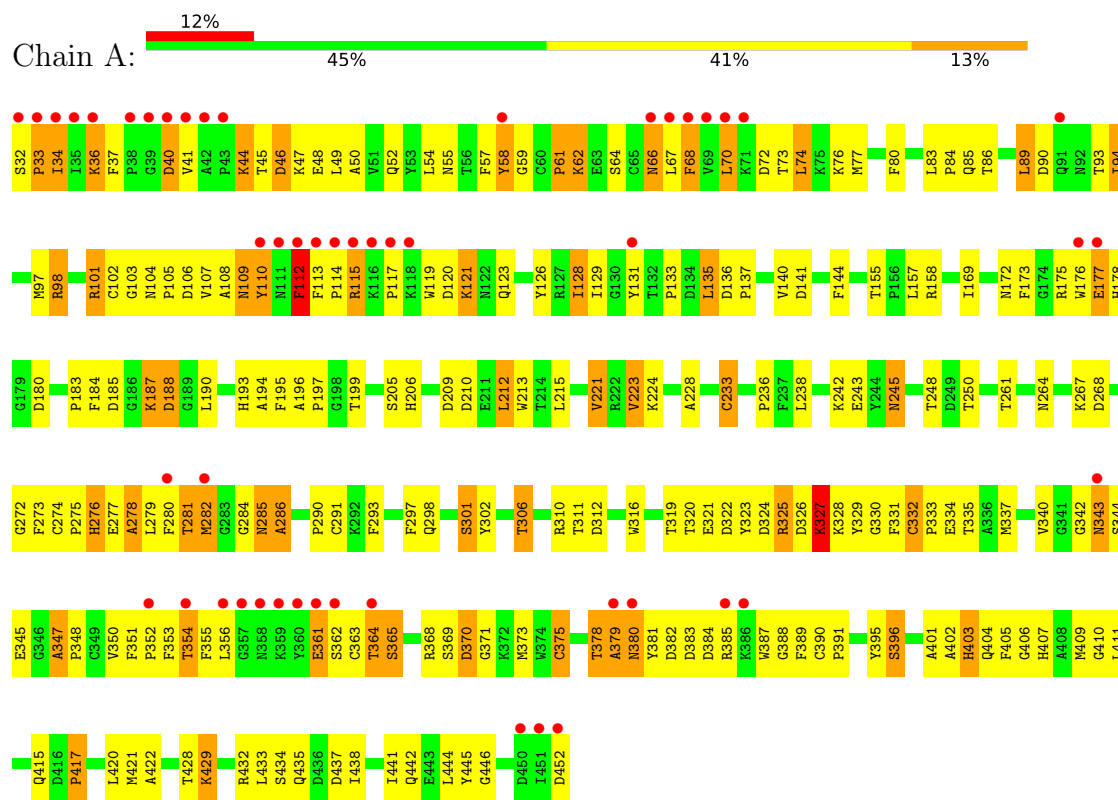
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	34	Total O 34 34	0	0
6	B	36	Total O 36 36	0	0
6	C	27	Total O 27 27	0	0
6	D	12	Total O 12 12	0	0

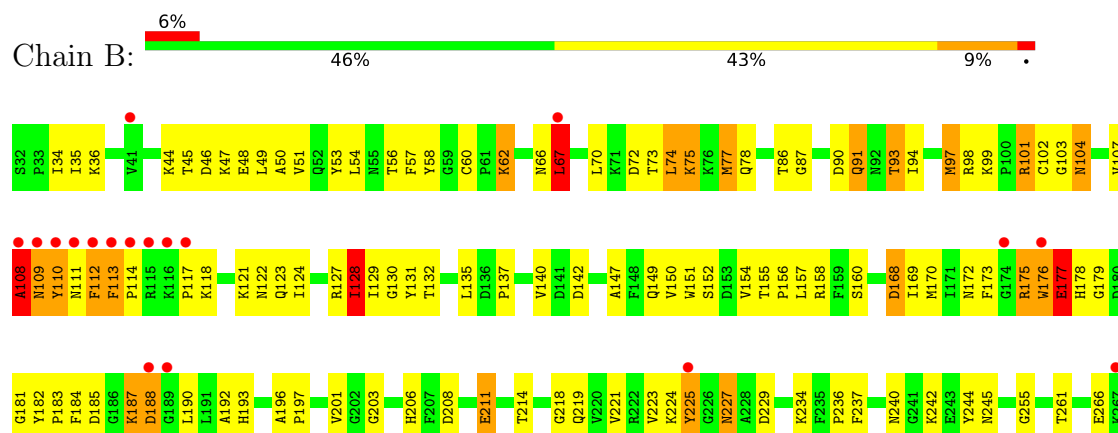
3 Residue-property plots

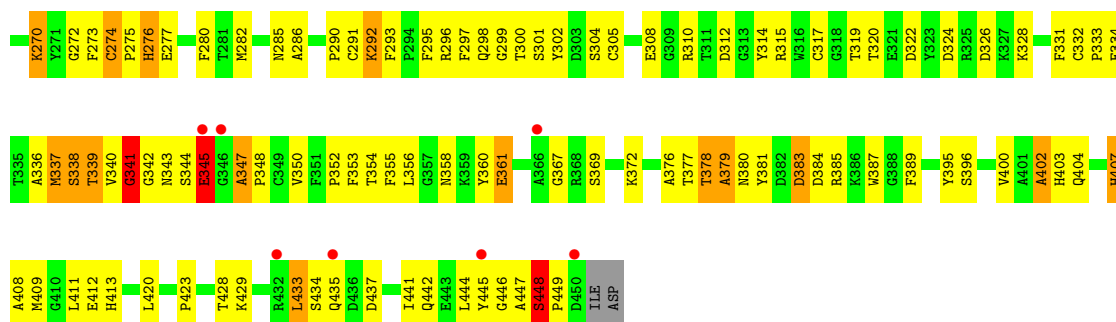
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 72 KDA TYPE IV COLLAGENASE

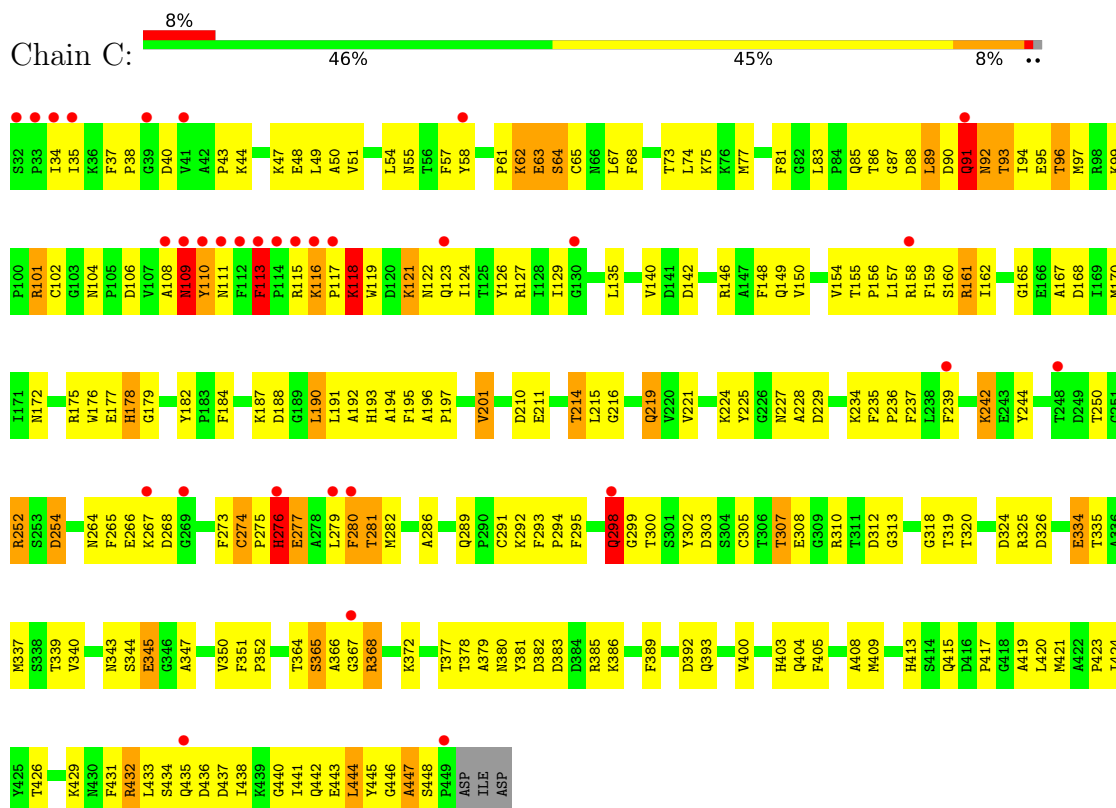


• Molecule 1: 72 KDA TYPE IV COLLAGENASE

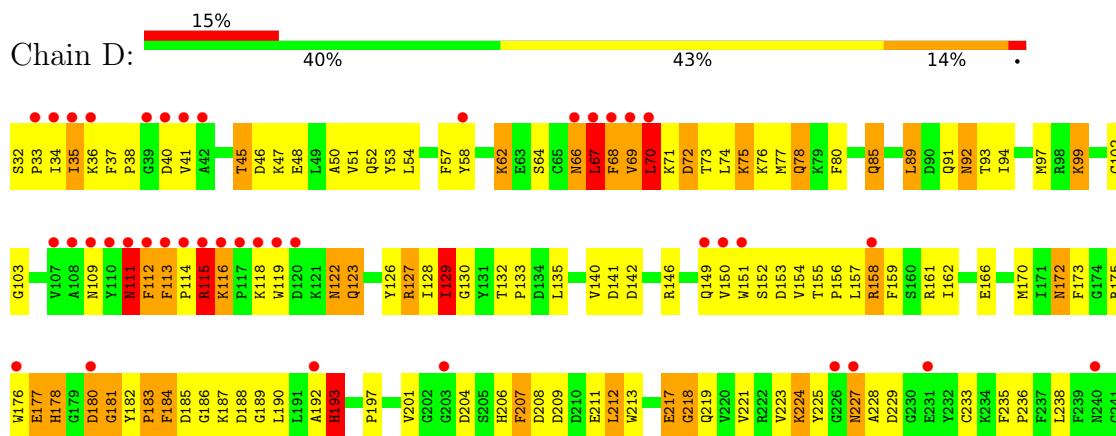


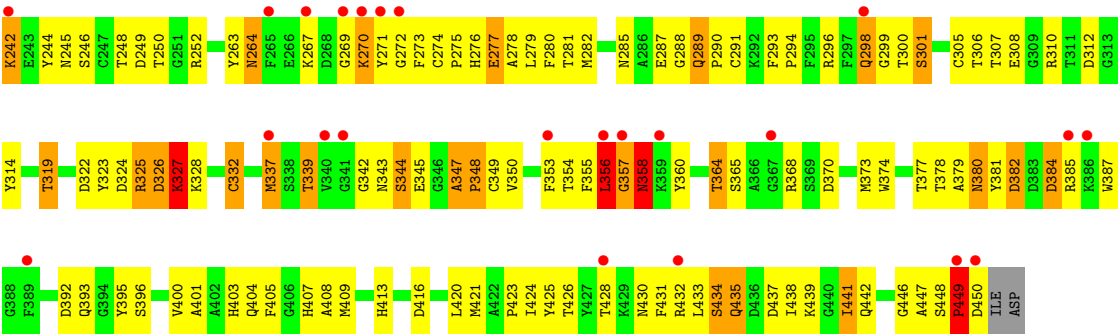


● Molecule 1: 72 KDA TYPE IV COLLAGENASE

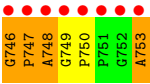
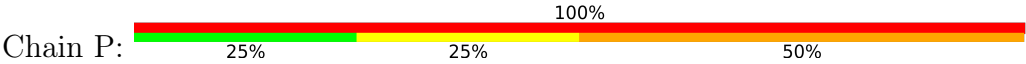


● Molecule 1: 72 KDA TYPE IV COLLAGENASE

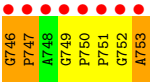




● Molecule 2: INHIBITOR PEPTIDE



● Molecule 2: INHIBITOR PEPTIDE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.67Å 166.15Å 170.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.58 – 2.66 35.58 – 2.66	Depositor EDS
% Data completeness (in resolution range)	80.2 (35.58-2.66) 80.5 (35.58-2.66)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 2.65Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.271 , 0.303 0.270 , 0.301	Depositor DCC
R_{free} test set	3899 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	13504	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SO4, ZN

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	0.61	2/3431 (0.1%)	1.30	28/4646 (0.6%)
1	B	0.66	0/3414	1.37	32/4624 (0.7%)
1	C	0.63	1/3406 (0.0%)	1.35	40/4613 (0.9%)
1	D	0.64	4/3414 (0.1%)	1.37	36/4624 (0.8%)
2	P	25.75	1/46 (2.2%)	1.62	2/62 (3.2%)
2	R	37.99	2/46 (4.3%)	1.54	0/62
All	All	2.73	10/13757 (0.1%)	1.35	138/18631 (0.7%)

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	1
1	B	0	1
1	D	0	3
All	All	0	5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	753	ALA	C-OXT	257.55	6.38	1.23
2	P	753	ALA	C-OXT	174.54	4.72	1.23
1	D	449	PRO	C-N	12.86	1.51	1.33
1	C	435	GLN	CB-CG	-7.83	1.28	1.52
1	A	417	PRO	N-CD	7.54	1.58	1.47
1	A	112	PHE	C-O	-6.73	1.15	1.24
1	D	348	PRO	N-CD	6.10	1.56	1.47
1	D	449	PRO	N-CD	5.39	1.55	1.47
2	R	746	GLY	N-CA	5.34	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	213	TRP	N-CA	5.10	1.52	1.46

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	449	PRO	O-C-N	-25.49	88.23	122.64
1	D	193	HIS	CA-CB-CG	23.60	137.40	113.80
1	C	435	GLN	CB-CG-CD	16.92	141.37	112.60
1	A	112	PHE	CA-CB-CG	13.13	126.93	113.80
1	A	112	PHE	CA-C-O	-10.98	104.81	120.51
1	C	435	GLN	OE1-CD-NE2	-9.87	112.73	122.60
1	B	435	GLN	OE1-CD-NE2	-9.84	112.76	122.60
1	D	435	GLN	OE1-CD-NE2	-9.84	112.76	122.60
1	D	149	GLN	OE1-CD-NE2	-9.82	112.78	122.60
1	C	91	GLN	OE1-CD-NE2	-9.77	112.83	122.60
1	A	435	GLN	OE1-CD-NE2	-9.73	112.87	122.60
1	D	289	GLN	OE1-CD-NE2	-9.70	112.90	122.60
1	C	298	GLN	OE1-CD-NE2	-9.69	112.91	122.60
1	B	91	GLN	OE1-CD-NE2	-9.67	112.93	122.60
1	C	219	GLN	OE1-CD-NE2	-9.65	112.95	122.60
1	C	435	GLN	CA-CB-CG	9.32	132.75	114.10
1	C	149	GLN	OE1-CD-NE2	-9.27	113.33	122.60
1	D	123	GLN	OE1-CD-NE2	-9.27	113.33	122.60
1	D	347	ALA	CA-C-N	9.15	129.09	119.85
1	D	347	ALA	C-N-CA	9.15	129.09	119.85
1	B	182	TYR	CA-C-N	8.34	128.27	119.85
1	B	182	TYR	C-N-CA	8.34	128.27	119.85
1	A	332	CYS	CA-C-N	8.29	127.93	119.56
1	A	332	CYS	C-N-CA	8.29	127.93	119.56
2	P	746	GLY	O-C-N	-8.27	109.77	123.00
1	A	403	HIS	CA-CB-CG	8.01	121.81	113.80
1	B	280	PHE	CA-CB-CG	7.58	121.38	113.80
1	A	129	ILE	CA-C-O	7.46	128.53	120.47
1	A	278	ALA	N-CA-C	-7.42	104.22	113.28
1	A	115	ARG	O-C-N	7.28	131.72	123.27
1	A	59	GLY	N-CA-C	7.24	125.64	115.43
2	P	746	GLY	N-CA-C	-7.22	92.35	113.30
1	C	447	ALA	N-CA-C	7.18	119.24	110.41
1	D	69	VAL	N-CA-C	-7.17	106.15	113.10
1	B	175	ARG	NE-CZ-NH1	-6.92	114.58	121.50
1	C	307	THR	N-CA-C	-6.92	103.23	113.61
1	C	443	GLU	N-CA-C	-6.90	104.61	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	191	LEU	N-CA-C	-6.86	105.44	113.88
1	D	289	GLN	CG-CD-NE2	6.84	126.66	116.40
1	C	276	HIS	CA-CB-CG	6.82	120.62	113.80
1	D	435	GLN	CG-CD-NE2	6.71	126.47	116.40
1	D	149	GLN	CG-CD-NE2	6.71	126.46	116.40
1	B	345	GLU	CA-C-N	6.70	134.55	121.41
1	B	345	GLU	C-N-CA	6.70	134.55	121.41
1	C	435	GLN	CG-CD-NE2	6.70	126.45	116.40
1	B	435	GLN	CG-CD-NE2	6.69	126.44	116.40
1	C	149	GLN	CG-CD-NE2	6.68	126.42	116.40
1	C	274	CYS	CA-C-N	6.67	127.06	119.92
1	C	274	CYS	C-N-CA	6.67	127.06	119.92
1	A	435	GLN	CG-CD-NE2	6.67	126.40	116.40
1	C	91	GLN	CG-CD-NE2	6.65	126.37	116.40
1	C	298	GLN	CG-CD-NE2	6.64	126.36	116.40
1	D	382	ASP	CA-CB-CG	-6.62	105.97	112.60
1	C	113	PHE	N-CA-C	-6.62	101.72	109.93
1	A	417	PRO	N-CA-CB	6.61	109.48	103.20
1	D	212	LEU	CA-C-N	-6.60	112.15	121.72
1	D	212	LEU	C-N-CA	-6.60	112.15	121.72
1	A	33	PRO	CB-CA-C	-6.60	102.44	111.21
1	D	67	LEU	CA-C-O	-6.59	113.42	121.06
1	B	91	GLN	CG-CD-NE2	6.58	126.28	116.40
1	C	219	GLN	CG-CD-NE2	6.54	126.21	116.40
1	D	449	PRO	CA-C-N	6.53	133.46	121.70
1	D	449	PRO	C-N-CA	6.53	133.46	121.70
1	A	105	PRO	CB-CA-C	-6.53	100.13	110.96
1	D	242	LYS	CA-C-N	-6.52	113.48	122.93
1	D	242	LYS	C-N-CA	-6.52	113.48	122.93
1	A	58	TYR	CB-CA-C	6.51	119.57	109.03
1	D	358	ASN	N-CA-C	6.50	117.71	108.74
1	B	108	ALA	O-C-N	6.36	131.05	122.59
1	C	347	ALA	CA-C-N	6.35	127.22	120.11
1	C	347	ALA	C-N-CA	6.35	127.22	120.11
1	D	288	GLY	N-CA-C	-6.34	106.32	115.27
1	D	123	GLN	CG-CD-NE2	6.33	125.90	116.40
1	D	181	GLY	CA-C-O	6.32	126.15	119.07
1	C	403	HIS	CA-CB-CG	6.25	120.05	113.80
1	D	287	GLU	O-C-N	6.23	130.27	122.55
1	C	305	CYS	CA-C-O	-6.17	115.08	121.87
1	B	227	ASN	N-CA-C	-6.14	104.96	112.88
1	A	417	PRO	N-CA-C	-6.12	106.01	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	VAL	CA-C-N	6.09	131.04	121.17
1	A	41	VAL	C-N-CA	6.09	131.04	121.17
1	D	115	ARG	O-C-N	6.00	130.70	122.72
1	B	67	LEU	O-C-N	-6.00	114.61	122.59
1	B	175	ARG	NE-CZ-NH2	5.99	124.59	119.20
1	A	375	CYS	N-CA-CB	-5.99	102.09	111.56
1	B	345	GLU	O-C-N	5.98	130.54	122.59
1	A	188	ASP	CB-CA-C	5.88	122.11	110.42
1	B	274	CYS	CA-C-N	5.86	125.88	119.90
1	B	274	CYS	C-N-CA	5.86	125.88	119.90
1	C	118	LYS	CA-C-N	-5.83	112.47	121.56
1	C	118	LYS	C-N-CA	-5.83	112.47	121.56
1	A	286	ALA	N-CA-C	5.79	120.08	113.19
1	D	70	LEU	N-CA-C	-5.74	106.62	113.97
1	B	128	ILE	CA-CB-CG2	5.69	120.18	110.50
1	B	225	TYR	N-CA-C	5.69	119.52	112.58
1	D	122	ASN	N-CA-C	-5.68	106.99	114.04
1	D	225	TYR	CA-CB-CG	5.67	124.11	113.90
1	A	347	ALA	CA-C-N	5.65	125.58	119.76
1	A	347	ALA	C-N-CA	5.65	125.58	119.76
1	D	184	PHE	CA-C-O	-5.64	114.56	121.78
1	C	277	GLU	N-CA-C	-5.63	106.41	113.28
1	C	318	GLY	N-CA-C	-5.62	103.90	111.54
1	C	182	TYR	CA-C-N	5.59	125.56	120.03
1	C	182	TYR	C-N-CA	5.59	125.56	120.03
1	A	406	GLY	N-CA-C	-5.59	106.03	112.73
1	A	115	ARG	N-CA-C	5.56	117.85	109.23
1	D	356	LEU	N-CA-CB	5.50	119.79	110.49
1	C	109	ASN	CB-CG-ND2	5.49	124.63	116.40
1	C	109	ASN	OD1-CG-ND2	-5.49	117.11	122.60
1	C	448	SER	N-CA-CB	5.46	120.42	109.28
1	B	338	SER	N-CA-C	-5.45	107.00	113.97
1	D	129	ILE	N-CA-C	-5.44	105.06	113.16
1	C	367	GLY	O-C-N	-5.41	116.00	122.33
1	D	133	PRO	CB-CA-C	-5.39	103.30	111.44
1	B	255	GLY	N-CA-C	-5.38	107.62	115.63
1	B	402	ALA	N-CA-C	-5.38	105.53	111.71
1	C	444	LEU	CA-C-N	5.34	130.63	122.24
1	C	444	LEU	C-N-CA	5.34	130.63	122.24
1	D	68	PHE	O-C-N	5.28	127.53	121.88
1	D	416	ASP	CA-C-N	5.19	124.36	118.97
1	D	416	ASP	C-N-CA	5.19	124.36	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	448	SER	CA-C-N	5.17	125.11	119.78
1	B	448	SER	C-N-CA	5.17	125.11	119.78
1	B	168	ASP	N-CA-C	-5.17	105.55	111.14
1	C	334	GLU	CA-C-N	-5.16	115.88	123.00
1	C	334	GLU	C-N-CA	-5.16	115.88	123.00
1	B	99	LYS	N-CA-C	5.15	116.56	110.07
1	B	60	CYS	CA-C-N	5.09	125.09	119.90
1	B	60	CYS	C-N-CA	5.09	125.09	119.90
1	B	332	CYS	O-C-N	5.09	125.50	121.17
1	C	298	GLN	CB-CA-C	5.07	120.50	110.42
1	B	175	ARG	CD-NE-CZ	-5.06	117.31	124.40
1	C	68	PHE	N-CA-C	5.05	118.21	111.75
1	A	378	THR	N-CA-CB	-5.03	102.79	111.55
1	B	177	GLU	CA-C-N	5.02	130.98	122.79
1	B	177	GLU	C-N-CA	5.02	130.98	122.79
1	A	58	TYR	O-C-N	-5.01	115.65	122.36
1	A	233	CYS	N-CA-C	-5.00	103.55	110.35

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	PHE	Mainchain
1	B	341	GLY	Mainchain
1	D	183	PRO	Mainchain
1	D	357	GLY	Mainchain
1	D	449	PRO	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	3330	0	3066	318	0
1	B	3313	0	3048	231	2
1	C	3305	0	3045	281	0
1	D	3313	0	3049	303	1
2	P	44	0	39	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	44	0	39	22	0
3	A	5	0	0	0	0
3	B	10	0	0	2	0
3	C	10	0	0	3	0
3	D	5	0	0	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	34	0	0	4	0
6	B	36	0	0	6	0
6	C	27	0	0	7	1
6	D	12	0	0	2	1
All	All	13504	0	12286	1104	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 43.

All (1104) 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:A:112:PHE:CE1	1:A:115:ARG:NH1	1.81	1.48
1:C:58:TYR:OH	1:C:77:MET:CG	1.72	1.36
1:A:176:TRP:CZ2	1:C:325:ARG:HA	1.61	1.32
1:A:176:TRP:CH2	1:C:325:ARG:HG3	1.64	1.31
1:A:176:TRP:CZ2	1:C:325:ARG:CB	2.16	1.28
1:B:107:VAL:O	1:B:109:ASN:N	1.71	1.23
1:D:184:PHE:HB3	1:D:208:ASP:OD2	1.36	1.22
1:A:176:TRP:CZ2	1:C:325:ARG:CA	2.22	1.22
1:A:112:PHE:CZ	1:A:115:ARG:NH1	1.99	1.20
1:A:175:ARG:HG2	1:C:298:GLN:OE1	1.36	1.20
1:D:176:TRP:CZ3	1:D:185:ASP:HA	1.56	1.18
1:D:152:SER:HA	1:D:155:THR:OG1	1.39	1.17
1:D:426:THR:HA	6:D:2012:HOH:O	1.43	1.17
1:C:58:TYR:CZ	1:C:77:MET:HB2	1.78	1.17
1:C:275:PRO:HA	1:C:280:PHE:CZ	1.80	1.15
1:A:276:HIS:HE2	2:P:748:ALA:C	1.54	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:HIS:NE2	2:P:747:PRO:O	1.78	1.15
1:B:187:LYS:O	1:B:188:ASP:OD1	1.64	1.15
1:A:112:PHE:HE1	1:A:115:ARG:CZ	1.36	1.14
1:C:58:TYR:CZ	1:C:77:MET:CB	2.31	1.13
1:A:58:TYR:CZ	1:A:77:MET:HA	1.83	1.13
1:C:276:HIS:CD2	1:C:335:THR:HG23	1.82	1.13
1:B:296:ARG:NH2	2:R:753:ALA:HB2	1.63	1.12
1:C:299:GLY:HA3	2:P:753:ALA:O	1.46	1.12
1:C:58:TYR:OH	1:C:77:MET:HG2	0.96	1.12
1:D:209:ASP:OD2	2:R:753:ALA:HB1	1.50	1.10
1:A:176:TRP:CH2	1:C:325:ARG:HA	1.85	1.10
1:B:286:ALA:HA	6:B:2022:HOH:O	1.53	1.09
1:A:176:TRP:HZ2	1:C:325:ARG:HB2	1.13	1.08
1:A:278:ALA:HB1	2:P:746:GLY:N	1.67	1.08
1:A:112:PHE:HE1	1:A:115:ARG:NH1	1.32	1.07
1:A:276:HIS:CE1	2:P:747:PRO:O	2.08	1.07
1:A:114:PRO:HB2	1:A:115:ARG:HE	1.20	1.06
1:C:58:TYR:CZ	1:C:77:MET:CG	2.39	1.06
1:B:299:GLY:HA2	2:R:753:ALA:HB3	1.09	1.06
1:D:176:TRP:CZ3	1:D:185:ASP:CA	2.29	1.05
1:A:176:TRP:CZ2	1:C:325:ARG:HB2	1.84	1.04
1:D:327:LYS:HE3	1:D:327:LYS:H	1.15	1.03
1:B:187:LYS:C	1:B:188:ASP:OD1	2.01	1.03
1:D:223:VAL:HG11	1:D:272:GLY:HA3	1.39	1.03
1:C:123:GLN:HG3	1:C:158:ARG:HH12	1.21	1.02
1:A:117:PRO:CB	1:A:197:PRO:HD2	1.89	1.02
1:A:293:PHE:CE2	2:P:750:PRO:CG	2.42	1.02
1:D:67:LEU:O	1:D:68:PHE:CD2	2.13	1.02
1:A:322:ASP:HB3	1:A:325:ARG:HH21	1.25	1.01
1:A:176:TRP:CH2	1:C:325:ARG:CG	2.44	1.00
1:D:112:PHE:O	1:D:113:PHE:O	1.79	0.99
1:B:320:THR:HG21	1:B:326:ASP:HB2	1.45	0.99
1:A:176:TRP:CE2	1:C:325:ARG:HA	1.98	0.99
1:D:276:HIS:HE1	2:R:749:GLY:HA2	1.27	0.98
1:A:113:PHE:HB2	1:A:114:PRO:HD3	1.45	0.98
1:A:293:PHE:CE2	2:P:750:PRO:HG2	1.99	0.98
1:C:58:TYR:CE1	1:C:77:MET:HB2	1.98	0.97
1:C:438:ILE:O	1:C:442:GLN:HG2	1.64	0.96
1:D:32:SER:N	1:D:33:PRO:HD3	1.79	0.96
1:C:89:LEU:HD21	1:C:97:MET:HE1	1.46	0.96
1:A:58:TYR:CE1	1:A:77:MET:HA	2.01	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:GLY:CA	2:R:753:ALA:HB3	1.96	0.95
1:A:177:GLU:OE1	1:A:177:GLU:HA	1.65	0.95
1:C:109:ASN:ND2	1:C:113:PHE:CE2	2.35	0.94
1:A:175:ARG:HG2	1:C:298:GLN:CD	1.93	0.93
1:B:54:LEU:HD11	1:B:74:LEU:HD13	1.49	0.93
1:C:299:GLY:CA	2:P:753:ALA:O	2.15	0.93
1:D:54:LEU:HD12	1:D:70:LEU:HD12	1.51	0.93
1:C:54:LEU:HA	1:C:58:TYR:HD2	1.32	0.92
1:D:111:ASN:HD22	1:D:111:ASN:H	1.15	0.92
1:A:176:TRP:CD1	1:C:324:ASP:HB3	2.05	0.92
1:A:175:ARG:CG	1:C:298:GLN:OE1	2.17	0.91
1:C:214:THR:HG22	1:C:216:GLY:H	1.34	0.91
1:D:176:TRP:CE3	1:D:185:ASP:HA	2.04	0.91
1:A:176:TRP:CZ2	1:C:325:ARG:CG	2.53	0.91
1:A:68:PHE:HD1	1:A:68:PHE:O	1.54	0.91
1:B:296:ARG:HH21	2:R:753:ALA:HB2	1.30	0.91
1:A:378:THR:HG21	1:A:384:ASP:HB2	1.52	0.90
1:D:112:PHE:CD2	1:D:113:PHE:HD1	1.90	0.90
1:A:293:PHE:CE2	2:P:750:PRO:HG3	2.02	0.90
1:D:112:PHE:O	1:D:113:PHE:C	2.10	0.90
1:D:111:ASN:HD22	1:D:111:ASN:N	1.70	0.90
1:A:112:PHE:HZ	1:A:115:ARG:NH1	1.70	0.89
1:B:245:ASN:N	3:B:853:SO4:O4	2.05	0.89
1:C:58:TYR:OH	1:C:77:MET:CB	2.20	0.89
1:C:264:ASN:HB3	1:C:267:LYS:HG2	1.55	0.89
1:D:276:HIS:CE1	2:R:749:GLY:HA2	2.07	0.89
1:A:188:ASP:OD1	1:A:395:TYR:OH	1.91	0.88
1:A:157:LEU:HD13	1:A:409:MET:HE2	1.54	0.88
1:A:176:TRP:CZ2	1:C:325:ARG:HG3	2.09	0.88
1:C:62:LYS:H	1:C:62:LYS:HD2	1.38	0.87
1:D:177:GLU:OE1	1:D:177:GLU:HA	1.70	0.87
1:A:176:TRP:HH2	1:C:325:ARG:HG3	1.01	0.87
1:D:62:LYS:H	1:D:62:LYS:HD3	1.40	0.87
1:D:221:VAL:HB	1:D:233:CYS:SG	2.15	0.86
1:A:117:PRO:HB3	1:A:197:PRO:HD2	1.58	0.85
1:A:187:LYS:HZ1	1:A:212:LEU:H	1.21	0.84
1:D:113:PHE:HD2	1:D:115:ARG:HG3	1.43	0.84
1:A:112:PHE:HZ	1:A:115:ARG:HH11	1.21	0.84
1:A:337:MET:HE3	1:A:340:VAL:HG22	1.59	0.84
1:C:50:ALA:CB	1:C:89:LEU:HD11	2.08	0.84
1:D:355:PHE:HB3	1:D:360:TYR:CE2	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:432:ARG:HH11	1:C:432:ARG:HB3	1.41	0.83
1:D:327:LYS:HE3	1:D:327:LYS:N	1.93	0.83
1:B:341:GLY:C	1:B:345:GLU:OE2	2.21	0.83
1:A:57:PHE:HZ	1:A:190:LEU:HD22	1.43	0.83
1:D:355:PHE:HB3	1:D:360:TYR:HE2	1.43	0.83
1:B:341:GLY:CA	1:B:345:GLU:OE2	2.27	0.83
1:C:57:PHE:HZ	1:C:190:LEU:HD22	1.43	0.83
1:A:176:TRP:HZ2	1:C:325:ARG:CB	1.70	0.83
1:D:223:VAL:CG1	1:D:272:GLY:HA3	2.08	0.82
1:D:112:PHE:HD2	1:D:113:PHE:CD1	1.97	0.82
1:D:276:HIS:NE2	2:R:747:PRO:O	2.12	0.82
1:A:112:PHE:CE1	1:A:115:ARG:CZ	2.26	0.82
1:A:70:LEU:HD11	1:A:74:LEU:HD22	1.61	0.82
1:C:279:LEU:HB2	1:C:280:PHE:HD1	1.45	0.82
1:A:117:PRO:HB2	1:A:197:PRO:HD2	1.60	0.82
1:A:322:ASP:CB	1:A:325:ARG:HH21	1.92	0.81
1:A:276:HIS:CE1	2:P:749:GLY:HA2	2.15	0.81
1:B:62:LYS:HE3	1:B:62:LYS:H	1.45	0.81
1:C:123:GLN:HG3	1:C:158:ARG:NH1	1.94	0.81
1:A:285:ASN:HD21	1:A:329:TYR:H	1.26	0.81
1:D:71:LYS:O	1:D:75:LYS:HG2	1.81	0.81
1:D:184:PHE:CB	1:D:208:ASP:OD2	2.26	0.81
1:A:57:PHE:HZ	1:A:190:LEU:CD2	1.94	0.81
1:C:54:LEU:HA	1:C:58:TYR:CD2	2.15	0.81
1:A:223:VAL:CG1	1:A:272:GLY:HA3	2.10	0.80
1:A:223:VAL:HG11	1:A:272:GLY:HA3	1.62	0.80
1:A:327:LYS:H	1:A:327:LYS:HD2	1.45	0.80
1:A:280:PHE:HD1	1:A:281:THR:O	1.62	0.80
1:C:88:ASP:OD1	6:C:2004:HOH:O	1.99	0.80
1:C:116:LYS:HD2	1:C:117:PRO:HD2	1.63	0.80
1:D:242:LYS:HD3	1:D:244:TYR:CZ	2.16	0.80
1:A:58:TYR:CZ	1:A:77:MET:CA	2.65	0.80
1:A:175:ARG:N	1:C:298:GLN:OE1	2.14	0.80
1:A:176:TRP:CH2	1:C:325:ARG:CA	2.56	0.80
1:A:114:PRO:HB2	1:A:115:ARG:NE	1.96	0.80
1:B:297:PHE:HB3	1:B:302:TYR:HE2	1.46	0.79
1:A:325:ARG:O	1:A:327:LYS:HE3	1.83	0.79
1:A:278:ALA:CB	2:P:746:GLY:N	2.46	0.79
1:D:356:LEU:HD13	1:D:382:ASP:CG	2.08	0.79
1:B:157:LEU:HD13	1:B:409:MET:HE2	1.65	0.79
1:C:154:VAL:HG23	1:C:155:THR:HG23	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:PHE:CD2	1:D:113:PHE:CD1	2.70	0.79
1:C:277:GLU:HB2	1:C:291:CYS:SG	2.22	0.79
1:C:109:ASN:O	1:C:111:ASN:N	2.16	0.78
1:B:128:ILE:HD12	1:B:130:GLY:H	1.48	0.78
1:B:341:GLY:O	1:B:345:GLU:OE2	2.01	0.78
1:D:277:GLU:HG2	1:D:305:CYS:SG	2.24	0.78
1:C:58:TYR:HH	1:C:77:MET:HG2	0.95	0.77
1:C:58:TYR:CZ	1:C:77:MET:HG2	2.08	0.77
1:A:193:HIS:CD2	1:A:206:HIS:HB2	2.19	0.77
1:B:172:ASN:ND2	1:B:173:PHE:H	1.81	0.77
1:B:178:HIS:HB3	1:D:298:GLN:OE1	1.84	0.77
1:D:32:SER:N	1:D:33:PRO:CD	2.48	0.77
1:B:90:ASP:CG	6:B:2006:HOH:O	2.27	0.77
1:C:432:ARG:HB3	1:C:432:ARG:NH1	2.00	0.77
1:D:176:TRP:CZ2	1:D:186:GLY:HA3	2.20	0.76
1:D:356:LEU:HB2	1:D:382:ASP:OD1	1.86	0.76
1:C:58:TYR:HH	1:C:77:MET:CG	1.78	0.76
1:D:209:ASP:OD2	2:R:753:ALA:CB	2.30	0.75
1:C:276:HIS:HD2	1:C:335:THR:HG23	1.49	0.75
1:A:50:ALA:HB2	1:A:97:MET:HE1	1.66	0.75
1:A:353:PHE:HA	1:A:379:ALA:O	1.86	0.74
1:C:444:LEU:HB3	1:C:445:TYR:CD1	2.22	0.74
1:C:298:GLN:NE2	1:C:324:ASP:CG	2.45	0.74
1:C:40:ASP:OD2	1:C:368:ARG:NH2	2.21	0.74
1:D:449:PRO:O	1:D:450:ASP:OD1	2.04	0.74
1:B:129:ILE:HD13	1:B:170:MET:HE3	1.67	0.74
1:C:58:TYR:CE1	1:C:77:MET:CB	2.66	0.74
1:A:117:PRO:HG2	1:A:196:ALA:HB1	1.70	0.73
1:A:276:HIS:NE2	2:P:748:ALA:C	2.39	0.73
1:A:58:TYR:OH	1:A:77:MET:HA	1.87	0.73
1:A:432:ARG:NH1	1:A:433:LEU:O	2.22	0.73
1:D:282:MET:HE3	1:D:282:MET:HA	1.71	0.73
1:A:68:PHE:CD1	1:A:68:PHE:C	2.65	0.73
1:C:313:GLY:HA2	6:C:2021:HOH:O	1.89	0.73
1:C:252:ARG:HG3	1:C:252:ARG:HH11	1.54	0.73
1:D:66:ASN:CG	1:D:67:LEU:H	1.97	0.73
1:A:344:SER:HB3	1:A:347:ALA:HB3	1.71	0.73
1:C:441:ILE:O	1:C:444:LEU:HB2	1.89	0.73
1:B:118:LYS:HE2	1:B:444:LEU:O	1.89	0.73
1:C:320:THR:HG21	1:C:326:ASP:HB2	1.70	0.73
1:B:35:ILE:HD11	1:B:356:LEU:HD21	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:PHE:HZ	1:D:190:LEU:HD21	1.52	0.72
1:C:275:PRO:CA	1:C:280:PHE:CZ	2.68	0.72
1:B:181:GLY:O	1:B:183:PRO:HD3	1.89	0.72
1:B:121:LYS:NZ	1:B:168:ASP:OD1	2.21	0.72
1:C:57:PHE:CZ	1:C:101:ARG:HD2	2.24	0.72
1:A:411:LEU:HB2	1:A:421:MET:HE2	1.71	0.72
1:B:299:GLY:HA2	2:R:752:GLY:O	1.88	0.72
1:A:236:PRO:HB3	1:A:245:ASN:OD1	1.89	0.72
1:A:361:GLU:CD	1:A:361:GLU:H	1.97	0.72
1:D:111:ASN:H	1:D:111:ASN:ND2	1.88	0.72
1:A:115:ARG:HD2	1:A:115:ARG:N	2.04	0.72
1:A:293:PHE:CZ	2:P:750:PRO:HG2	2.25	0.71
1:B:277:GLU:HB2	1:B:291:CYS:SG	2.30	0.71
1:A:68:PHE:HD1	1:A:68:PHE:C	1.98	0.71
1:B:157:LEU:HD21	1:B:445:TYR:CD1	2.25	0.71
1:A:209:ASP:OD2	2:P:753:ALA:HB3	1.91	0.71
1:A:285:ASN:ND2	1:A:329:TYR:H	1.89	0.71
1:A:177:GLU:OE1	1:A:177:GLU:CA	2.38	0.71
1:C:252:ARG:HH21	1:C:273:PHE:HZ	1.36	0.71
1:B:224:LYS:O	1:B:273:PHE:HB2	1.91	0.71
1:B:297:PHE:HB3	1:B:302:TYR:CE2	2.24	0.71
1:C:116:LYS:HD2	1:C:117:PRO:CD	2.21	0.71
1:D:58:TYR:OH	1:D:77:MET:HG2	1.90	0.71
1:A:322:ASP:HB3	1:A:325:ARG:NH2	2.03	0.71
1:B:206:HIS:NE2	6:B:2014:HOH:O	2.24	0.71
1:C:122:ASN:ND2	1:C:156:PRO:HB2	2.06	0.71
1:A:112:PHE:CG	1:A:115:ARG:HB2	2.25	0.70
1:B:310:ARG:HH21	1:B:312:ASP:CG	1.99	0.70
1:B:130:GLY:HA3	1:B:172:ASN:ND2	2.06	0.70
1:C:113:PHE:HD1	1:C:113:PHE:N	1.88	0.70
1:B:380:ASN:HB3	1:B:383:ASP:OD1	1.89	0.70
1:C:89:LEU:CD2	1:C:97:MET:HE1	2.22	0.70
1:C:340:VAL:O	1:C:389:PHE:HB2	1.91	0.70
1:D:37:PHE:HE2	1:D:368:ARG:HG2	1.57	0.70
1:D:113:PHE:CD2	1:D:115:ARG:HG3	2.26	0.70
1:A:276:HIS:NE2	2:P:748:ALA:O	2.25	0.70
1:B:57:PHE:HZ	1:B:190:LEU:HD21	1.56	0.70
1:C:188:ASP:N	1:C:211:GLU:OE2	2.25	0.69
1:B:112:PHE:HD1	1:B:112:PHE:N	1.90	0.69
1:D:299:GLY:HA3	3:D:857:SO4:O2	1.91	0.69
1:A:70:LEU:HD12	1:A:74:LEU:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:GLY:O	1:C:444:LEU:HD23	1.92	0.69
1:A:114:PRO:C	1:A:115:ARG:HD2	2.18	0.69
1:A:429:LYS:NZ	1:A:429:LYS:HB2	2.08	0.68
1:A:47:LYS:NZ	6:A:2001:HOH:O	2.26	0.68
1:C:58:TYR:CE1	1:C:77:MET:HA	2.29	0.68
1:C:156:PRO:HD3	1:C:446:GLY:O	1.93	0.68
1:D:227:ASN:HB3	1:D:270:LYS:HA	1.75	0.68
1:A:337:MET:CE	1:A:340:VAL:HG22	2.23	0.68
1:C:58:TYR:CE1	1:C:77:MET:CA	2.77	0.68
1:B:35:ILE:CD1	1:B:356:LEU:HD21	2.24	0.68
1:B:62:LYS:H	1:B:62:LYS:CE	2.07	0.68
1:B:121:LYS:NZ	1:B:168:ASP:CG	2.50	0.68
1:C:62:LYS:HD2	1:C:62:LYS:N	2.07	0.68
1:A:306:THR:HG23	1:C:300:THR:HG21	1.75	0.68
1:B:50:ALA:HB2	1:B:97:MET:HE1	1.74	0.68
1:B:227:ASN:HD21	1:B:270:LYS:HA	1.58	0.68
1:A:131:TYR:O	2:P:753:ALA:OXT	2.11	0.67
1:C:157:LEU:HD13	1:C:409:MET:HE2	1.76	0.67
1:D:152:SER:CA	1:D:155:THR:OG1	2.30	0.67
1:D:154:VAL:HG23	1:D:155:THR:HG23	1.75	0.67
1:D:156:PRO:HD3	1:D:446:GLY:O	1.95	0.67
1:B:122:ASN:ND2	1:B:156:PRO:HB2	2.10	0.67
1:C:62:LYS:H	1:C:62:LYS:CD	2.00	0.67
1:D:327:LYS:HD3	6:D:2009:HOH:O	1.93	0.67
1:A:172:ASN:ND2	1:A:173:PHE:H	1.91	0.67
1:A:114:PRO:CB	1:A:115:ARG:HE	2.04	0.67
1:A:285:ASN:HD22	1:A:286:ALA:N	1.93	0.67
1:C:54:LEU:O	1:C:58:TYR:HB2	1.94	0.67
1:C:178:HIS:HD1	1:C:178:HIS:H	1.41	0.67
1:D:355:PHE:O	1:D:356:LEU:C	2.37	0.67
2:R:752:GLY:O	2:R:753:ALA:CB	2.42	0.67
1:C:299:GLY:CA	3:C:850:SO4:O1	2.42	0.67
1:D:35:ILE:HG13	1:D:36:LYS:H	1.58	0.67
1:A:184:PHE:O	6:A:2009:HOH:O	2.11	0.67
1:A:187:LYS:HG2	1:A:210:ASP:O	1.95	0.67
1:B:176:TRP:CZ3	1:B:185:ASP:HA	2.30	0.67
1:A:193:HIS:NE2	1:A:206:HIS:HB2	2.10	0.66
1:B:117:PRO:HB2	1:B:196:ALA:HB1	1.77	0.66
1:D:279:LEU:O	1:D:290:PRO:HG3	1.95	0.66
1:D:129:ILE:HD11	1:D:170:MET:HE3	1.77	0.66
1:D:342:GLY:HA2	1:D:387:TRP:CH2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:PHE:HD1	1:B:112:PHE:H	1.44	0.66
1:C:127:ARG:NH1	1:C:165:GLY:H	1.93	0.66
1:D:54:LEU:CD1	1:D:70:LEU:HD12	2.24	0.66
1:A:50:ALA:CB	1:A:97:MET:HE1	2.25	0.66
1:A:278:ALA:HB3	2:P:746:GLY:O	1.96	0.66
1:C:101:ARG:HD3	1:C:102:CYS:O	1.96	0.66
1:C:298:GLN:NE2	1:C:324:ASP:OD1	2.28	0.66
1:D:50:ALA:HB2	1:D:89:LEU:HD11	1.78	0.66
1:A:280:PHE:CD1	1:A:281:THR:O	2.47	0.66
1:C:276:HIS:NE2	1:C:335:THR:HG23	2.10	0.66
1:D:152:SER:HB3	1:D:157:LEU:HD12	1.77	0.66
1:C:109:ASN:ND2	1:C:113:PHE:CZ	2.64	0.66
1:C:279:LEU:HB2	1:C:280:PHE:CD1	2.30	0.66
2:R:752:GLY:O	2:R:753:ALA:HB3	1.96	0.66
1:A:334:GLU:HG3	1:A:335:THR:N	2.11	0.66
1:B:413:HIS:CG	1:B:423:PRO:HG3	2.31	0.66
1:A:80:PHE:HA	1:A:415:GLN:HE21	1.61	0.65
1:A:157:LEU:CD1	1:A:409:MET:HE2	2.25	0.65
1:C:113:PHE:N	1:C:113:PHE:CD1	2.60	0.65
1:D:119:TRP:CD2	1:D:197:PRO:HB3	2.31	0.65
1:D:327:LYS:H	1:D:327:LYS:CE	2.01	0.65
1:A:62:LYS:H	1:A:62:LYS:HD2	1.60	0.65
1:B:107:VAL:O	1:B:108:ALA:C	2.34	0.65
1:C:224:LYS:HE3	1:C:282:MET:HE2	1.78	0.65
1:C:302:TYR:OH	1:C:308:GLU:HG2	1.96	0.65
1:D:123:GLN:HB3	1:D:158:ARG:HH11	1.61	0.65
1:A:403:HIS:ND1	1:A:420:LEU:O	2.30	0.65
1:D:264:ASN:HB3	1:D:267:LYS:HB2	1.78	0.65
1:B:112:PHE:N	1:B:112:PHE:CD1	2.61	0.65
1:D:37:PHE:CE2	1:D:368:ARG:HG2	2.32	0.65
1:D:127:ARG:HG2	1:D:162:ILE:O	1.96	0.65
1:C:225:TYR:N	1:C:229:ASP:HB2	2.13	0.64
1:D:337:MET:HA	1:D:337:MET:HE2	1.80	0.64
1:D:57:PHE:HZ	1:D:190:LEU:CD2	2.11	0.64
1:C:242:LYS:HE2	1:C:244:TYR:CE1	2.32	0.64
1:D:188:ASP:OD1	1:D:395:TYR:OH	2.07	0.64
1:A:176:TRP:CE2	1:C:325:ARG:CA	2.70	0.64
1:C:275:PRO:HA	1:C:280:PHE:HZ	1.56	0.64
1:A:172:ASN:HD22	1:A:173:PHE:H	1.44	0.64
1:A:368:ARG:NH2	1:A:389:PHE:HZ	1.96	0.64
1:A:380:ASN:OD1	1:A:383:ASP:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:TRP:CE3	1:D:184:PHE:O	2.51	0.64
1:A:54:LEU:HD12	1:A:70:LEU:HD13	1.80	0.63
1:A:301:SER:OG	1:C:303:ASP:HB3	1.99	0.63
1:D:176:TRP:HZ3	1:D:185:ASP:HA	1.51	0.63
1:A:119:TRP:C	1:A:121:LYS:H	2.05	0.63
1:A:58:TYR:CE1	1:A:77:MET:CA	2.81	0.63
1:A:276:HIS:HE2	2:P:749:GLY:N	1.96	0.63
1:C:277:GLU:N	1:C:277:GLU:OE1	2.31	0.63
1:D:75:LYS:HA	1:D:78:GLN:CG	2.29	0.63
1:D:201:VAL:HA	1:D:204:ASP:OD2	1.98	0.63
1:D:276:HIS:HB3	1:D:279:LEU:HD12	1.81	0.63
1:D:281:THR:HG22	1:D:289:GLN:O	1.99	0.63
1:A:84:PRO:O	1:A:86:THR:HG23	1.99	0.63
1:B:344:SER:CB	1:B:377:THR:HG21	2.29	0.63
1:B:176:TRP:O	1:B:177:GLU:C	2.41	0.63
1:B:434:SER:HB3	1:B:437:ASP:OD2	1.97	0.63
1:D:57:PHE:CZ	1:D:190:LEU:HD21	2.33	0.63
1:D:75:LYS:HA	1:D:78:GLN:HG2	1.81	0.62
1:D:122:ASN:O	1:D:157:LEU:HA	1.99	0.62
1:D:344:SER:HB3	1:D:347:ALA:HB3	1.80	0.62
1:D:53:TYR:CE2	1:D:97:MET:HA	2.34	0.62
1:B:101:ARG:HD3	1:B:102:CYS:O	1.99	0.62
1:C:313:GLY:CA	6:C:2021:HOH:O	2.46	0.62
1:D:344:SER:CB	1:D:377:THR:HG21	2.29	0.62
1:B:109:ASN:OD1	1:B:110:TYR:N	2.32	0.62
1:D:356:LEU:CB	1:D:382:ASP:OD1	2.47	0.62
1:B:107:VAL:C	1:B:109:ASN:N	2.57	0.62
1:C:118:LYS:HD2	1:C:444:LEU:O	1.99	0.62
1:C:405:PHE:O	1:C:409:MET:HG2	2.00	0.62
1:D:45:THR:HG22	1:D:48:GLU:HB2	1.82	0.62
1:D:277:GLU:HB3	1:D:291:CYS:SG	2.39	0.62
1:A:355:PHE:CD1	1:A:356:LEU:HD13	2.35	0.62
1:B:178:HIS:CB	1:D:298:GLN:OE1	2.46	0.62
1:D:285:ASN:OD1	1:D:328:LYS:HD2	2.00	0.62
1:A:276:HIS:CE1	2:P:749:GLY:CA	2.83	0.61
1:B:187:LYS:HZ1	1:B:340:VAL:HG11	1.65	0.61
1:D:322:ASP:CG	1:D:325:ARG:HB2	2.25	0.61
1:A:334:GLU:CG	1:A:335:THR:N	2.63	0.61
1:B:117:PRO:HB2	1:B:197:PRO:HD2	1.81	0.61
1:C:242:LYS:HE2	1:C:244:TYR:CZ	2.35	0.61
2:P:747:PRO:O	2:P:748:ALA:C	2.43	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ILE:HD11	1:A:369:SER:HB2	1.82	0.61
1:C:101:ARG:NH2	1:C:106:ASP:OD2	2.34	0.61
1:C:320:THR:OG1	1:C:326:ASP:OD2	2.18	0.61
1:B:409:MET:HE3	1:B:445:TYR:OH	2.01	0.61
1:C:101:ARG:HH22	1:C:106:ASP:CG	2.08	0.61
1:C:188:ASP:OD2	1:C:372:LYS:HE2	2.00	0.61
1:A:176:TRP:HH2	1:C:325:ARG:CG	1.93	0.61
1:A:176:TRP:C	1:A:184:PHE:H	2.09	0.61
1:A:429:LYS:HB2	1:A:429:LYS:HZ2	1.65	0.61
1:A:37:PHE:CE2	1:A:368:ARG:HD3	2.36	0.61
1:B:172:ASN:HD22	1:B:173:PHE:H	1.47	0.61
1:D:354:THR:HB	1:D:380:ASN:ND2	2.15	0.61
2:P:746:GLY:O	2:P:747:PRO:O	2.19	0.61
1:C:298:GLN:HE22	1:C:324:ASP:CG	2.08	0.61
1:B:62:LYS:HE3	1:B:62:LYS:N	2.16	0.60
1:D:193:HIS:C	1:D:404:GLN:OE1	2.44	0.60
1:D:238:LEU:HB2	1:D:263:TYR:CE1	2.36	0.60
1:A:285:ASN:HD21	1:A:329:TYR:N	1.99	0.60
1:A:175:ARG:CG	1:C:298:GLN:CD	2.71	0.60
1:C:178:HIS:HD1	1:C:178:HIS:N	2.00	0.60
1:D:177:GLU:OE1	1:D:177:GLU:CA	2.46	0.60
1:D:356:LEU:HD13	1:D:382:ASP:OD2	2.01	0.60
1:B:34:ILE:HD12	1:B:369:SER:HB3	1.83	0.60
1:A:40:ASP:OD2	1:A:368:ARG:NH2	2.34	0.60
1:B:128:ILE:HD11	1:B:131:TYR:CE1	2.36	0.60
1:D:219:GLN:HE22	1:D:337:MET:H	1.49	0.60
1:B:225:TYR:OH	1:B:282:MET:HE1	2.01	0.60
1:B:275:PRO:HG2	1:B:334:GLU:OE1	2.01	0.60
1:B:299:GLY:C	2:R:753:ALA:OXT	2.36	0.60
1:D:38:PRO:HD2	1:D:381:TYR:OH	2.01	0.60
1:D:356:LEU:HA	1:D:382:ASP:OD2	2.00	0.60
1:A:40:ASP:OD2	1:A:368:ARG:CZ	2.50	0.60
1:A:276:HIS:HE1	2:P:749:GLY:HA2	1.61	0.60
1:A:221:VAL:HG13	1:A:233:CYS:HB2	1.83	0.60
1:A:284:GLY:N	6:A:2021:HOH:O	2.31	0.60
1:A:324:ASP:O	1:A:327:LYS:HE2	2.01	0.60
1:B:355:PHE:HB3	1:B:360:TYR:CE1	2.37	0.60
1:A:310:ARG:HD2	1:A:316:TRP:CD1	2.36	0.59
1:B:340:VAL:O	1:B:389:PHE:HB2	2.02	0.59
1:D:72:ASP:O	1:D:76:LYS:HG3	2.02	0.59
1:D:154:VAL:O	1:D:448:SER:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:CYS:SG	1:B:317:CYS:HB3	2.41	0.59
1:C:124:ILE:O	1:C:159:PHE:HA	2.02	0.59
1:C:142:ASP:OD2	1:C:146:ARG:HD3	2.03	0.59
1:D:342:GLY:HA2	1:D:387:TRP:CZ2	2.37	0.59
1:B:236:PRO:HB3	1:B:245:ASN:OD1	2.02	0.59
1:C:122:ASN:HA	1:C:157:LEU:HD23	1.84	0.59
1:A:343:ASN:OD1	1:A:343:ASN:C	2.45	0.59
1:A:45:THR:OG1	1:A:48:GLU:HG2	2.03	0.59
1:A:57:PHE:CZ	1:A:101:ARG:HD2	2.37	0.59
1:A:350:VAL:HG11	1:A:379:ALA:HA	1.83	0.59
1:D:343:ASN:O	1:D:345:GLU:N	2.35	0.59
1:B:54:LEU:HD22	1:B:73:THR:HG22	1.85	0.59
1:C:299:GLY:C	3:C:850:SO4:O1	2.46	0.59
1:D:312:ASP:CG	1:D:314:TYR:HD1	2.11	0.59
1:A:306:THR:HG23	1:C:300:THR:CG2	2.33	0.59
1:D:227:ASN:HB2	1:D:271:TYR:CD1	2.37	0.59
1:D:58:TYR:CZ	1:D:77:MET:CB	2.86	0.59
1:D:326:ASP:O	1:D:328:LYS:N	2.33	0.59
1:B:286:ALA:C	6:B:2022:HOH:O	2.43	0.58
1:D:219:GLN:NE2	1:D:337:MET:H	2.01	0.58
1:D:276:HIS:NE2	2:R:747:PRO:C	2.61	0.58
1:A:285:ASN:HD22	1:A:285:ASN:C	2.10	0.58
1:D:187:LYS:NZ	1:D:211:GLU:OE1	2.35	0.58
1:C:409:MET:O	1:C:445:TYR:OH	2.17	0.58
1:A:108:ALA:O	1:A:110:TYR:N	2.34	0.58
1:A:381:TYR:CD1	1:A:385:ARG:HA	2.38	0.58
1:A:405:PHE:O	1:A:409:MET:HG2	2.03	0.58
1:C:419:ALA:HA	1:C:434:SER:HB3	1.86	0.58
1:A:223:VAL:HG13	1:A:272:GLY:HA3	1.86	0.58
1:B:172:ASN:ND2	1:B:173:PHE:N	2.51	0.58
1:C:413:HIS:CE1	1:C:423:PRO:HB3	2.38	0.58
1:D:66:ASN:CG	1:D:67:LEU:N	2.58	0.58
1:C:177:GLU:OE2	1:C:179:GLY:N	2.35	0.58
1:D:235:PHE:CE1	1:D:246:SER:HA	2.38	0.58
1:B:103:GLY:HA2	1:B:190:LEU:HD22	1.83	0.58
1:C:94:ILE:HA	1:C:97:MET:HE3	1.85	0.58
1:D:176:TRP:CZ2	1:D:186:GLY:CA	2.86	0.58
1:B:47:LYS:O	1:B:51:VAL:HG23	2.03	0.58
1:B:310:ARG:NH2	1:B:312:ASP:OD2	2.37	0.58
1:A:293:PHE:CD2	2:P:750:PRO:HG3	2.39	0.57
1:D:69:VAL:HG12	1:D:69:VAL:O	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:SER:O	1:D:155:THR:N	2.38	0.57
1:D:435:GLN:O	1:D:439:LYS:HG3	2.04	0.57
1:C:57:PHE:CZ	1:C:190:LEU:HD22	2.32	0.57
1:A:58:TYR:CE2	1:A:77:MET:CG	2.87	0.57
1:B:214:THR:O	1:B:396:SER:HA	2.04	0.57
1:D:40:ASP:HB3	1:D:387:TRP:HH2	1.69	0.57
1:D:396:SER:O	1:D:400:VAL:HG23	2.03	0.57
1:A:68:PHE:O	1:A:68:PHE:CD1	2.44	0.57
1:B:324:ASP:HB2	1:D:175:ARG:NH1	2.19	0.57
1:C:178:HIS:N	1:C:178:HIS:ND1	2.52	0.57
1:D:70:LEU:O	1:D:74:LEU:HB2	2.04	0.57
1:D:180:ASP:CG	1:D:182:TYR:H	2.12	0.57
1:C:444:LEU:CB	1:C:445:TYR:CD1	2.87	0.57
1:D:277:GLU:OE1	2:R:750:PRO:HD2	2.04	0.57
1:D:150:VAL:HG12	1:D:150:VAL:O	2.04	0.57
1:A:331:PHE:O	1:A:333:PRO:HD3	2.05	0.57
1:A:403:HIS:HE1	1:A:422:ALA:O	1.87	0.57
1:B:224:LYS:HE3	1:B:282:MET:SD	2.45	0.57
1:C:58:TYR:HE1	1:C:77:MET:HA	1.68	0.57
1:D:155:THR:HG21	1:D:441:ILE:HG12	1.86	0.57
1:A:411:LEU:CB	1:A:421:MET:HE2	2.35	0.57
1:C:83:LEU:CD1	1:C:93:THR:HA	2.35	0.57
1:D:172:ASN:ND2	1:D:173:PHE:H	2.03	0.57
1:D:180:ASP:OD1	1:D:181:GLY:N	2.38	0.57
1:A:364:THR:OG1	1:A:365:SER:N	2.38	0.56
1:B:344:SER:O	1:B:345:GLU:C	2.48	0.56
1:D:54:LEU:HD12	1:D:70:LEU:CD1	2.31	0.56
1:A:58:TYR:CE2	1:A:77:MET:HG2	2.40	0.56
1:B:157:LEU:HD21	1:B:445:TYR:CE1	2.39	0.56
1:A:334:GLU:HG3	1:A:335:THR:H	1.69	0.56
1:B:301:SER:HB2	2:R:751:PRO:HB2	1.85	0.56
1:C:117:PRO:HG2	1:C:196:ALA:HB1	1.87	0.56
1:D:67:LEU:O	1:D:68:PHE:CG	2.57	0.56
1:C:299:GLY:HA2	2:P:753:ALA:H	1.71	0.56
1:D:420:LEU:HB2	1:D:431:PHE:HZ	1.70	0.56
1:A:32:SER:N	1:A:33:PRO:CD	2.67	0.56
1:A:57:PHE:CZ	1:A:190:LEU:HD22	2.33	0.56
1:D:58:TYR:CZ	1:D:77:MET:HB2	2.40	0.56
1:A:188:ASP:OD1	1:A:395:TYR:CE2	2.59	0.56
1:B:312:ASP:OD2	1:B:314:TYR:HD2	1.88	0.56
1:C:54:LEU:HD23	1:C:58:TYR:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:747:PRO:O	2:P:749:GLY:N	2.39	0.56
1:B:442:GLN:O	1:B:446:GLY:N	2.36	0.56
1:C:50:ALA:HB2	1:C:89:LEU:HD21	1.88	0.56
1:C:157:LEU:HD11	1:C:445:TYR:CD2	2.40	0.56
1:D:238:LEU:HG	1:D:242:LYS:O	2.06	0.56
1:B:187:LYS:NZ	1:B:340:VAL:HG11	2.21	0.56
1:D:119:TRP:CE2	1:D:197:PRO:HB3	2.41	0.56
1:D:152:SER:C	1:D:154:VAL:N	2.63	0.56
1:A:101:ARG:HH22	1:A:106:ASP:CG	2.14	0.56
1:B:57:PHE:CZ	1:B:190:LEU:HD21	2.38	0.56
1:D:45:THR:CG2	1:D:48:GLU:H	2.18	0.56
1:A:102:CYS:SG	1:A:103:GLY:N	2.79	0.55
1:B:214:THR:HG22	1:B:219:GLN:HA	1.88	0.55
1:D:38:PRO:HG3	1:D:385:ARG:HB3	1.88	0.55
1:B:350:VAL:HG22	1:B:376:ALA:O	2.06	0.55
1:A:285:ASN:HD21	1:A:328:LYS:HA	1.71	0.55
1:A:342:GLY:HA3	1:A:388:GLY:HA2	1.87	0.55
1:B:221:VAL:HA	1:B:334:GLU:OE2	2.07	0.55
1:A:117:PRO:CG	1:A:196:ALA:HB1	2.35	0.55
1:A:194:ALA:HB2	1:A:205:SER:HA	1.86	0.55
1:B:127:ARG:HG2	1:B:129:ILE:HG23	1.89	0.55
1:C:109:ASN:C	1:C:111:ASN:N	2.64	0.55
1:A:380:ASN:HD21	1:A:382:ASP:HB2	1.72	0.55
1:C:123:GLN:HG2	1:C:158:ARG:HH22	1.72	0.55
1:B:225:TYR:H	1:B:229:ASP:HB2	1.71	0.55
1:C:378:THR:O	1:C:379:ALA:C	2.47	0.55
1:D:45:THR:HG22	1:D:48:GLU:H	1.71	0.55
1:D:152:SER:C	1:D:155:THR:H	2.13	0.55
1:B:442:GLN:HG2	1:B:447:ALA:HA	1.88	0.55
1:D:45:THR:HG22	1:D:48:GLU:CB	2.36	0.55
1:D:58:TYR:CE1	1:D:77:MET:HA	2.42	0.55
1:A:58:TYR:O	1:A:107:VAL:HG21	2.07	0.55
1:A:188:ASP:OD1	1:A:395:TYR:CZ	2.58	0.55
1:A:310:ARG:NH1	1:A:312:ASP:OD2	2.40	0.55
1:C:313:GLY:N	6:C:2021:HOH:O	2.38	0.55
1:A:83:LEU:CD1	1:A:93:THR:HA	2.37	0.55
1:A:187:LYS:NZ	1:A:212:LEU:H	2.02	0.55
1:C:344:SER:CB	1:C:377:THR:HG21	2.36	0.55
1:A:74:LEU:HD21	1:A:89:LEU:HD12	1.89	0.55
1:A:176:TRP:CZ3	1:C:325:ARG:HA	2.39	0.55
1:C:61:PRO:O	1:C:65:CYS:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:THR:OG1	1:C:97:MET:HE2	2.05	0.55
1:C:118:LYS:O	1:C:119:TRP:C	2.48	0.55
1:C:310:ARG:NH1	1:C:312:ASP:OD2	2.40	0.55
1:C:415:GLN:O	1:C:417:PRO:HD3	2.07	0.55
1:C:89:LEU:CD2	1:C:94:ILE:HG12	2.37	0.54
1:C:126:TYR:O	1:C:161:ARG:HA	2.06	0.54
1:D:70:LEU:O	1:D:74:LEU:CB	2.55	0.54
1:D:227:ASN:HB2	1:D:271:TYR:H	1.71	0.54
1:A:104:ASN:OD1	1:A:193:HIS:HB2	2.07	0.54
1:A:128:ILE:HD12	1:A:144:PHE:HD2	1.73	0.54
1:C:54:LEU:HD23	1:C:58:TYR:CE2	2.41	0.54
1:A:34:ILE:CD1	1:A:369:SER:HB2	2.38	0.54
1:C:91:GLN:HE21	1:C:95:GLU:HG3	1.71	0.54
1:A:57:PHE:CZ	1:A:190:LEU:CD2	2.84	0.54
1:B:299:GLY:O	2:R:753:ALA:OXT	2.25	0.54
1:B:350:VAL:HG21	1:B:378:THR:C	2.32	0.54
1:D:192:ALA:HB3	1:D:404:GLN:NE2	2.23	0.54
1:B:350:VAL:HG23	1:B:350:VAL:O	2.07	0.54
1:C:378:THR:HG23	1:C:380:ASN:O	2.07	0.54
1:D:40:ASP:HB3	1:D:387:TRP:CH2	2.42	0.54
1:D:433:LEU:HD11	1:D:437:ASP:CB	2.37	0.54
1:A:276:HIS:O	1:A:279:LEU:HB2	2.08	0.54
1:B:381:TYR:O	1:B:385:ARG:N	2.40	0.54
1:C:219:GLN:NE2	1:C:337:MET:H	2.05	0.54
1:D:252:ARG:NH1	1:D:273:PHE:HZ	2.06	0.54
1:A:52:GLN:HE21	1:A:52:GLN:HA	1.72	0.54
1:A:155:THR:OG1	1:A:157:LEU:HB2	2.08	0.54
1:B:237:PHE:CE2	1:B:244:TYR:HB2	2.42	0.54
1:C:176:TRP:O	1:C:178:HIS:ND1	2.40	0.53
1:D:197:PRO:HG3	1:D:408:ALA:O	2.08	0.53
1:D:404:GLN:O	1:D:407:HIS:HB2	2.09	0.53
1:C:252:ARG:HG3	1:C:252:ARG:NH1	2.22	0.53
1:D:339:THR:HB	1:D:347:ALA:O	2.08	0.53
1:D:343:ASN:OD1	1:D:344:SER:N	2.41	0.53
1:A:119:TRP:O	1:A:121:LYS:N	2.42	0.53
1:A:157:LEU:O	1:A:158:ARG:NH1	2.41	0.53
1:D:285:ASN:OD1	1:D:328:LYS:HA	2.07	0.53
1:A:176:TRP:O	1:A:184:PHE:N	2.42	0.53
1:A:177:GLU:OE1	1:A:178:HIS:N	2.39	0.53
1:A:415:GLN:O	1:A:417:PRO:HD3	2.09	0.53
1:B:147:ALA:HB1	1:B:402:ALA:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ALA:CA	6:B:2022:HOH:O	2.31	0.53
1:C:214:THR:HG21	1:C:393:GLN:O	2.08	0.53
1:C:433:LEU:HD22	1:C:437:ASP:CB	2.39	0.53
1:A:73:THR:O	1:A:76:LYS:N	2.40	0.53
1:B:49:LEU:HD21	1:B:98:ARG:HG2	1.89	0.53
1:C:146:ARG:O	1:C:150:VAL:HG23	2.09	0.53
1:A:275:PRO:HA	1:A:280:PHE:CE2	2.44	0.53
1:B:45:THR:OG1	1:B:48:GLU:HG3	2.09	0.53
1:B:75:LYS:HG2	1:B:87:GLY:HA2	1.91	0.53
1:B:292:LYS:O	1:B:295:PHE:HB3	2.09	0.53
1:C:58:TYR:CE2	1:C:77:MET:HG3	2.44	0.53
1:A:101:ARG:NH2	1:A:106:ASP:OD2	2.41	0.53
1:B:154:VAL:HG23	1:B:155:THR:HG23	1.91	0.53
1:D:157:LEU:HD12	1:D:157:LEU:O	2.09	0.53
1:D:278:ALA:HB1	2:R:746:GLY:O	2.09	0.53
1:A:34:ILE:HG13	1:A:368:ARG:O	2.08	0.53
1:A:77:MET:HE3	1:A:97:MET:HG2	1.91	0.53
1:A:297:PHE:HB3	1:A:302:TYR:CE1	2.44	0.53
1:D:356:LEU:HD22	1:D:382:ASP:OD1	2.09	0.53
1:A:58:TYR:CZ	1:A:77:MET:CB	2.92	0.53
1:A:128:ILE:HD12	1:A:144:PHE:CD2	2.43	0.53
1:A:285:ASN:ND2	1:A:285:ASN:C	2.67	0.53
1:B:175:ARG:HD3	1:D:298:GLN:HA	1.91	0.53
1:B:341:GLY:HA2	1:B:345:GLU:OE2	2.07	0.52
1:B:66:ASN:O	1:B:67:LEU:C	2.53	0.52
1:B:75:LYS:HA	1:B:78:GLN:OE1	2.09	0.52
1:C:58:TYR:CE2	1:C:77:MET:CG	2.91	0.52
1:D:129:ILE:HD12	1:D:170:MET:HB3	1.92	0.52
1:D:150:VAL:HG11	1:D:431:PHE:HE2	1.74	0.52
1:A:40:ASP:OD2	1:A:368:ARG:NH1	2.43	0.52
1:A:140:VAL:O	1:A:141:ASP:C	2.52	0.52
1:B:223:VAL:HG21	1:B:272:GLY:HA3	1.90	0.52
1:A:113:PHE:CB	1:A:114:PRO:HD3	2.25	0.52
1:A:310:ARG:HD2	1:A:316:TRP:HD1	1.74	0.52
1:C:38:PRO:HG3	1:C:385:ARG:NH2	2.24	0.52
1:C:47:LYS:O	1:C:51:VAL:HG23	2.09	0.52
1:C:292:LYS:HB3	1:C:320:THR:O	2.09	0.52
1:D:322:ASP:OD2	1:D:325:ARG:HB2	2.09	0.52
1:D:420:LEU:HB2	1:D:431:PHE:CZ	2.44	0.52
1:B:344:SER:HB3	1:B:377:THR:HG21	1.89	0.52
1:B:378:THR:O	1:B:380:ASN:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ILE:HG13	1:D:36:LYS:N	2.24	0.52
1:A:45:THR:HG23	1:A:48:GLU:OE2	2.09	0.52
1:A:278:ALA:CB	2:P:746:GLY:O	2.58	0.52
1:B:107:VAL:O	1:B:109:ASN:CA	2.56	0.52
1:B:137:PRO:HD3	1:B:333:PRO:O	2.09	0.52
1:D:187:LYS:HZ3	1:D:212:LEU:H	1.57	0.52
1:C:441:ILE:O	1:C:445:TYR:HD1	1.93	0.52
1:D:296:ARG:HG2	1:D:296:ARG:HH11	1.75	0.52
1:A:58:TYR:CZ	1:A:77:MET:HG2	2.46	0.51
1:A:293:PHE:HE2	2:P:750:PRO:CG	2.14	0.51
1:B:285:ASN:OD1	1:B:285:ASN:C	2.53	0.51
1:B:409:MET:HE3	1:B:445:TYR:CZ	2.44	0.51
1:D:58:TYR:CZ	1:D:77:MET:CG	2.93	0.51
1:D:207:PHE:CD1	1:D:207:PHE:N	2.78	0.51
1:D:276:HIS:CE1	2:R:749:GLY:CA	2.88	0.51
1:D:306:THR:HG23	1:D:308:GLU:H	1.73	0.51
1:A:113:PHE:HB2	1:A:114:PRO:CD	2.31	0.51
1:A:310:ARG:HH21	1:A:331:PHE:HZ	1.58	0.51
1:B:175:ARG:O	1:B:176:TRP:C	2.50	0.51
1:C:50:ALA:HA	1:C:97:MET:SD	2.51	0.51
1:C:109:ASN:C	1:C:111:ASN:H	2.18	0.51
1:D:324:ASP:O	1:D:327:LYS:HE2	2.10	0.51
1:D:142:ASP:O	1:D:146:ARG:HG3	2.11	0.51
1:A:62:LYS:H	1:A:62:LYS:CD	2.21	0.51
1:C:175:ARG:HB2	1:C:210:ASP:OD2	2.10	0.51
1:C:219:GLN:HE22	1:C:337:MET:H	1.58	0.51
1:A:172:ASN:ND2	1:A:173:PHE:N	2.59	0.51
1:B:312:ASP:CG	1:B:314:TYR:HD2	2.19	0.51
1:C:61:PRO:HB2	1:C:64:SER:HB3	1.92	0.51
1:D:47:LYS:O	1:D:51:VAL:HG23	2.11	0.51
1:C:110:TYR:HA	1:C:113:PHE:HB2	1.93	0.51
1:D:448:SER:OG	1:D:450:ASP:OD2	2.26	0.51
1:A:381:TYR:CE1	1:A:385:ARG:HA	2.45	0.51
1:B:175:ARG:C	1:B:176:TRP:O	2.51	0.51
1:C:63:GLU:CD	1:C:63:GLU:H	2.18	0.51
1:D:310:ARG:NH2	1:D:312:ASP:OD2	2.36	0.51
1:C:162:ILE:HD11	1:C:167:ALA:HB2	1.93	0.51
1:D:115:ARG:O	1:D:116:LYS:HG3	2.11	0.51
1:A:428:THR:O	1:A:429:LYS:C	2.53	0.51
1:A:176:TRP:O	1:A:183:PRO:HA	2.11	0.50
1:B:169:ILE:HG23	1:B:203:GLY:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:ALA:O	1:B:193:HIS:HB3	2.11	0.50
1:D:122:ASN:O	1:D:157:LEU:CA	2.59	0.50
1:D:289:GLN:HB2	1:D:319:THR:HG21	1.94	0.50
1:A:228:ALA:CB	1:A:261:THR:HG21	2.42	0.50
1:D:122:ASN:O	1:D:157:LEU:CB	2.59	0.50
1:D:185:ASP:OD2	1:D:189:GLY:HA3	2.10	0.50
1:A:243:GLU:CD	1:D:91:GLN:HG2	2.36	0.50
1:A:361:GLU:CD	1:A:361:GLU:N	2.65	0.50
1:B:117:PRO:CB	1:B:196:ALA:HB1	2.41	0.50
1:D:432:ARG:NH1	1:D:434:SER:HA	2.27	0.50
1:C:58:TYR:CZ	1:C:77:MET:CA	2.93	0.50
1:C:81:PHE:HZ	1:C:101:ARG:HH21	1.59	0.50
1:C:298:GLN:NE2	1:C:324:ASP:OD2	2.44	0.50
1:D:152:SER:HA	1:D:155:THR:HG1	1.66	0.50
1:A:282:MET:HE3	1:A:282:MET:O	2.12	0.50
1:C:224:LYS:HE3	1:C:282:MET:CE	2.41	0.50
1:C:292:LYS:O	1:C:295:PHE:HB3	2.11	0.50
1:D:378:THR:HG21	1:D:384:ASP:HB2	1.93	0.50
1:A:112:PHE:CZ	1:A:115:ARG:HG2	2.44	0.50
1:B:57:PHE:HZ	1:B:190:LEU:CD2	2.24	0.50
1:B:434:SER:O	1:B:437:ASP:N	2.44	0.50
1:C:433:LEU:HD22	1:C:437:ASP:HB3	1.93	0.50
1:D:275:PRO:HA	1:D:280:PHE:CZ	2.46	0.50
1:B:227:ASN:O	1:B:270:LYS:HE2	2.11	0.50
1:B:286:ALA:CB	1:B:319:THR:HG21	2.41	0.50
1:C:119:TRP:HD1	1:C:409:MET:CE	2.25	0.50
1:C:444:LEU:HB3	1:C:445:TYR:CE1	2.46	0.50
1:D:296:ARG:HG2	1:D:296:ARG:NH1	2.27	0.50
1:A:275:PRO:O	1:A:276:HIS:HB2	2.12	0.49
1:A:340:VAL:O	1:A:389:PHE:HB2	2.11	0.49
1:C:43:PRO:O	1:C:44:LYS:HE2	2.11	0.49
1:C:157:LEU:HD11	1:C:445:TYR:CE2	2.47	0.49
1:C:197:PRO:HG3	1:C:408:ALA:O	2.12	0.49
1:D:112:PHE:C	1:D:113:PHE:O	2.54	0.49
1:D:193:HIS:CD2	1:D:206:HIS:HB2	2.47	0.49
1:D:353:PHE:HE1	1:D:355:PHE:HB2	1.77	0.49
1:D:438:ILE:O	1:D:442:GLN:HG3	2.12	0.49
1:B:211:GLU:HG3	1:B:395:TYR:CE1	2.48	0.49
1:B:296:ARG:HH21	2:R:753:ALA:CB	2.13	0.49
1:C:350:VAL:HG11	1:C:379:ALA:N	2.27	0.49
1:C:135:LEU:HB2	1:C:140:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:PHE:CE1	1:C:244:TYR:HB2	2.48	0.49
1:A:62:LYS:HD2	1:A:62:LYS:N	2.26	0.49
1:A:279:LEU:C	1:A:290:PRO:HB3	2.37	0.49
1:B:341:GLY:N	1:B:345:GLU:OE2	2.44	0.49
1:C:58:TYR:OH	1:C:77:MET:CA	2.59	0.49
1:D:112:PHE:CG	1:D:113:PHE:N	2.79	0.49
1:D:159:PHE:HZ	1:D:409:MET:HE2	1.78	0.49
1:D:368:ARG:HH12	1:D:370:ASP:CG	2.20	0.49
1:B:298:GLN:N	1:B:324:ASP:OD2	2.33	0.49
1:C:155:THR:HB	1:C:156:PRO:HD2	1.94	0.49
1:B:282:MET:O	1:B:331:PHE:HB2	2.13	0.49
1:C:148:PHE:HB3	1:C:159:PHE:CD2	2.47	0.49
1:A:364:THR:O	1:A:373:MET:HA	2.12	0.49
1:C:50:ALA:HB3	1:C:89:LEU:HD11	1.91	0.49
1:D:111:ASN:N	1:D:111:ASN:ND2	2.44	0.49
1:D:353:PHE:CD1	1:D:353:PHE:C	2.91	0.49
1:A:243:GLU:OE1	1:D:91:GLN:HG2	2.13	0.49
1:A:281:THR:HG21	1:A:330:GLY:HA3	1.94	0.49
1:B:121:LYS:HZ2	1:B:168:ASP:CG	2.16	0.49
1:B:350:VAL:HG21	1:B:379:ALA:N	2.28	0.49
1:A:121:LYS:HD3	1:A:123:GLN:O	2.13	0.49
1:B:77:MET:CE	1:B:93:THR:HB	2.42	0.49
1:C:34:ILE:HG23	1:C:368:ARG:HA	1.95	0.49
1:D:54:LEU:HD22	1:D:73:THR:HG22	1.94	0.49
1:D:350:VAL:HG11	1:D:379:ALA:HA	1.94	0.49
1:A:442:GLN:O	1:A:446:GLY:N	2.40	0.48
1:B:121:LYS:HZ1	1:B:168:ASP:CG	2.13	0.48
1:C:281:THR:OG1	1:C:289:GLN:O	2.22	0.48
1:A:444:LEU:HD23	1:A:445:TYR:CE2	2.48	0.48
1:B:184:PHE:CD2	1:B:208:ASP:HA	2.47	0.48
1:C:123:GLN:CG	1:C:158:ARG:HH22	2.25	0.48
1:A:117:PRO:HB3	1:A:197:PRO:CD	2.37	0.48
1:C:129:ILE:HD11	1:C:172:ASN:HB2	1.95	0.48
1:A:46:ASP:OD1	1:A:94:ILE:HD13	2.12	0.48
1:B:188:ASP:OD2	1:B:372:LYS:NZ	2.43	0.48
1:B:197:PRO:HG3	1:B:408:ALA:O	2.13	0.48
1:C:129:ILE:HG21	1:C:170:MET:HE3	1.95	0.48
1:D:89:LEU:HD13	1:D:94:ILE:HD11	1.95	0.48
1:D:152:SER:O	1:D:153:ASP:C	2.54	0.48
2:P:746:GLY:O	2:P:747:PRO:C	2.52	0.48
1:A:381:TYR:O	1:A:385:ARG:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LYS:HE3	1:B:124:ILE:HD13	1.95	0.48
1:C:299:GLY:N	3:C:850:SO4:O1	2.46	0.48
1:D:102:CYS:SG	1:D:103:GLY:N	2.86	0.48
1:C:117:PRO:HB2	1:C:197:PRO:HD2	1.95	0.48
1:C:420:LEU:HD13	1:C:431:PHE:CZ	2.48	0.48
1:D:300:THR:HG22	1:D:301:SER:N	2.28	0.48
1:D:368:ARG:NH1	1:D:368:ARG:HB3	2.29	0.48
1:A:302:TYR:N	1:A:302:TYR:CD1	2.81	0.48
1:A:354:THR:OG1	1:A:380:ASN:HB2	2.14	0.48
1:B:188:ASP:OD2	1:B:372:LYS:CE	2.61	0.48
1:C:86:THR:HG22	1:C:88:ASP:H	1.79	0.48
1:C:96:THR:HA	1:C:99:LYS:HG3	1.94	0.48
1:D:327:LYS:N	1:D:327:LYS:CE	2.69	0.48
1:A:185:ASP:OD1	1:A:185:ASP:N	2.46	0.48
1:C:90:ASP:OD2	1:C:92:ASN:HB2	2.12	0.48
1:C:381:TYR:CD1	1:C:381:TYR:C	2.92	0.48
1:D:37:PHE:O	1:D:40:ASP:OD1	2.31	0.48
1:D:78:GLN:HG3	1:D:85:GLN:HA	1.96	0.48
1:A:44:LYS:HB2	1:A:48:GLU:HG3	1.96	0.48
1:B:185:ASP:OD2	1:B:190:LEU:HG	2.13	0.48
1:C:308:GLU:HG2	6:C:2020:HOH:O	2.14	0.48
1:D:152:SER:O	1:D:154:VAL:N	2.47	0.48
1:A:37:PHE:CD2	1:A:368:ARG:HD3	2.49	0.48
1:C:155:THR:HB	1:C:156:PRO:CD	2.43	0.48
1:B:90:ASP:O	1:B:93:THR:N	2.47	0.47
1:B:127:ARG:HG2	1:B:129:ILE:CG2	2.43	0.47
1:B:339:THR:HB	1:B:347:ALA:O	2.14	0.47
1:C:381:TYR:O	1:C:385:ARG:N	2.38	0.47
1:D:357:GLY:C	1:D:358:ASN:CG	2.82	0.47
1:A:36:LYS:O	1:A:36:LYS:HG2	2.14	0.47
1:A:119:TRP:HD1	1:A:409:MET:HE3	1.79	0.47
1:B:35:ILE:CG2	1:B:36:LYS:N	2.76	0.47
1:B:227:ASN:ND2	1:B:270:LYS:HA	2.28	0.47
1:D:151:TRP:CE3	1:D:441:ILE:HD13	2.50	0.47
1:B:57:PHE:CZ	1:B:101:ARG:HD2	2.49	0.47
1:C:409:MET:HE3	1:C:445:TYR:OH	2.14	0.47
1:B:193:HIS:C	1:B:193:HIS:CD2	2.90	0.47
1:C:55:ASN:OD1	1:C:62:LYS:HG3	2.14	0.47
1:D:127:ARG:HD2	1:D:129:ILE:HG13	1.96	0.47
1:A:175:ARG:O	1:A:176:TRP:C	2.57	0.47
1:B:175:ARG:O	1:B:176:TRP:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:TYR:OH	1:B:282:MET:CE	2.63	0.47
1:C:77:MET:CE	1:C:97:MET:HG3	2.45	0.47
1:C:83:LEU:HD13	1:C:93:THR:HA	1.97	0.47
1:C:109:ASN:CG	1:C:113:PHE:CZ	2.92	0.47
1:C:275:PRO:CA	1:C:280:PHE:HZ	2.22	0.47
1:D:368:ARG:NH1	1:D:370:ASP:OD1	2.47	0.47
1:A:55:ASN:HD21	1:A:62:LYS:HG3	1.80	0.47
1:A:355:PHE:CE1	1:A:356:LEU:HD13	2.49	0.47
1:A:375:CYS:O	1:A:375:CYS:SG	2.68	0.47
1:B:132:THR:HG23	1:B:132:THR:O	2.15	0.47
1:B:403:HIS:ND1	1:B:420:LEU:O	2.45	0.47
1:C:104:ASN:HD21	1:C:194:ALA:H	1.62	0.47
1:C:279:LEU:CB	1:C:280:PHE:HD1	2.22	0.47
1:D:74:LEU:HD11	1:D:93:THR:HG21	1.96	0.47
1:D:92:ASN:HD22	1:D:92:ASN:HA	1.54	0.47
1:D:211:GLU:OE1	1:D:211:GLU:HA	2.14	0.47
1:D:223:VAL:CG1	1:D:224:LYS:N	2.78	0.47
1:B:90:ASP:O	1:B:91:GLN:C	2.56	0.47
1:D:58:TYR:CE2	1:D:77:MET:HG3	2.50	0.47
1:D:57:PHE:CZ	1:D:190:LEU:CD2	2.94	0.47
1:D:217:GLU:O	1:D:218:GLY:O	2.33	0.47
1:A:407:HIS:O	1:A:410:GLY:N	2.41	0.46
1:C:214:THR:CG2	1:C:216:GLY:H	2.19	0.46
1:D:80:PHE:CD1	1:D:80:PHE:C	2.93	0.46
1:D:123:GLN:HB3	1:D:158:ARG:HD3	1.97	0.46
1:B:343:ASN:OD1	1:B:387:TRP:N	2.49	0.46
1:C:89:LEU:HD23	1:C:94:ILE:HG12	1.96	0.46
1:A:52:GLN:HA	1:A:52:GLN:NE2	2.29	0.46
1:C:117:PRO:O	1:C:118:LYS:HB2	2.15	0.46
1:C:252:ARG:NH2	1:C:273:PHE:CZ	2.79	0.46
1:D:58:TYR:CE2	1:D:77:MET:HB2	2.50	0.46
1:B:74:LEU:O	1:B:78:GLN:HG3	2.16	0.46
1:D:152:SER:CB	1:D:157:LEU:O	2.63	0.46
1:D:235:PHE:CZ	1:D:246:SER:HA	2.51	0.46
1:D:312:ASP:OD1	1:D:314:TYR:HD1	1.98	0.46
1:D:403:HIS:CE1	1:D:421:MET:HA	2.50	0.46
1:C:116:LYS:HA	1:C:117:PRO:HD3	1.76	0.46
1:C:299:GLY:HA2	2:P:753:ALA:O	2.08	0.46
1:A:316:TRP:HA	1:A:331:PHE:HA	1.98	0.46
1:B:121:LYS:NZ	1:B:168:ASP:OD2	2.46	0.46
1:C:221:VAL:HA	1:C:334:GLU:OE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:GLN:CB	1:D:158:ARG:HH11	2.27	0.46
1:D:193:HIS:HD2	1:D:206:HIS:HB2	1.79	0.46
1:B:54:LEU:HD11	1:B:74:LEU:CD1	2.35	0.46
1:B:102:CYS:SG	1:B:104:ASN:HB2	2.56	0.46
1:B:344:SER:HB3	1:B:347:ALA:HB3	1.98	0.46
1:C:109:ASN:HB2	1:C:113:PHE:CG	2.50	0.46
1:C:148:PHE:C	1:C:150:VAL:H	2.24	0.46
1:B:184:PHE:CE2	1:B:208:ASP:HA	2.50	0.46
1:B:336:ALA:O	1:B:337:MET:HE3	2.16	0.46
1:C:35:ILE:HD11	1:C:37:PHE:CE1	2.51	0.46
1:C:129:ILE:CG2	1:C:170:MET:HE3	2.45	0.46
1:C:227:ASN:C	6:C:2012:HOH:O	2.58	0.46
1:D:337:MET:HA	1:D:337:MET:CE	2.44	0.46
1:D:368:ARG:HD2	1:D:374:TRP:CD1	2.50	0.46
1:D:407:HIS:HE2	1:D:413:HIS:CD2	2.34	0.46
1:A:90:ASP:O	1:A:93:THR:HB	2.16	0.46
1:A:117:PRO:HG2	1:A:196:ALA:CB	2.43	0.46
1:A:382:ASP:HA	1:A:385:ARG:HE	1.81	0.46
1:B:77:MET:HG3	1:B:78:GLN:N	2.31	0.46
1:C:121:LYS:NZ	1:C:168:ASP:OD1	2.47	0.46
1:C:122:ASN:HB3	1:C:156:PRO:O	2.16	0.46
1:D:180:ASP:OD1	1:D:182:TYR:N	2.41	0.46
1:A:277:GLU:HB2	1:A:291:CYS:SG	2.56	0.45
1:A:286:ALA:HB2	1:A:319:THR:OG1	2.16	0.45
1:A:401:ALA:O	1:A:402:ALA:C	2.58	0.45
1:B:135:LEU:HB2	1:B:140:VAL:CG2	2.46	0.45
1:B:352:PRO:HB3	1:B:361:GLU:OE2	2.16	0.45
1:C:400:VAL:O	1:C:404:GLN:HG2	2.15	0.45
1:D:152:SER:HB3	1:D:157:LEU:O	2.16	0.45
1:D:350:VAL:O	1:D:353:PHE:HB3	2.16	0.45
1:A:80:PHE:HA	1:A:415:GLN:NE2	2.28	0.45
1:A:248:THR:CG2	1:A:250:THR:HG22	2.46	0.45
1:A:356:LEU:HD12	1:A:382:ASP:OD1	2.16	0.45
1:A:433:LEU:HD22	1:A:437:ASP:CB	2.46	0.45
1:B:157:LEU:CD1	1:B:409:MET:HE2	2.40	0.45
1:D:154:VAL:HB	1:D:442:GLN:NE2	2.31	0.45
1:A:193:HIS:CD2	1:A:193:HIS:C	2.94	0.45
1:B:177:GLU:OE2	1:B:179:GLY:N	2.46	0.45
1:B:234:LYS:O	1:B:237:PHE:HB3	2.16	0.45
1:B:400:VAL:O	1:B:404:GLN:HG2	2.16	0.45
1:C:413:HIS:HA	1:C:421:MET:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:THR:O	1:D:308:GLU:C	2.57	0.45
1:A:176:TRP:CD1	1:C:324:ASP:CB	2.90	0.45
1:A:264:ASN:CG	1:A:267:LYS:HG3	2.41	0.45
1:C:447:ALA:HB1	6:C:2027:HOH:O	2.16	0.45
1:D:176:TRP:HA	1:D:184:PHE:O	2.17	0.45
1:A:74:LEU:HD21	1:A:89:LEU:CD1	2.47	0.45
1:A:113:PHE:N	1:A:114:PRO:CD	2.80	0.45
1:D:62:LYS:H	1:D:62:LYS:CD	2.13	0.45
1:D:78:GLN:NE2	1:D:93:THR:OG1	2.50	0.45
1:D:242:LYS:HD3	1:D:244:TYR:CE2	2.51	0.45
1:D:299:GLY:HA3	3:D:857:SO4:S	2.57	0.45
1:D:312:ASP:CG	1:D:314:TYR:CD1	2.94	0.45
1:B:46:ASP:OD2	1:B:94:ILE:HG21	2.17	0.45
1:B:53:TYR:CD1	1:B:57:PHE:HD2	2.34	0.45
1:B:214:THR:CG2	1:B:219:GLN:HA	2.45	0.45
1:C:307:THR:O	1:C:308:GLU:C	2.60	0.45
1:D:154:VAL:O	1:D:447:ALA:HA	2.17	0.45
1:D:224:LYS:HA	1:D:229:ASP:OD1	2.17	0.45
1:A:438:ILE:O	1:A:442:GLN:HG3	2.17	0.45
1:A:84:PRO:O	1:A:86:THR:N	2.49	0.45
1:B:90:ASP:OD1	1:B:93:THR:CG2	2.64	0.45
1:B:433:LEU:HD23	1:B:433:LEU:HA	1.78	0.45
1:C:57:PHE:HZ	1:C:190:LEU:CD2	2.22	0.45
1:C:73:THR:O	1:C:74:LEU:C	2.58	0.45
1:C:192:ALA:O	1:C:193:HIS:HB3	2.17	0.45
1:D:364:THR:OG1	1:D:365:SER:N	2.49	0.45
1:D:442:GLN:HA	1:D:446:GLY:H	1.82	0.45
1:A:40:ASP:CG	1:A:387:TRP:HH2	2.23	0.45
1:A:172:ASN:HD22	1:A:173:PHE:N	2.14	0.45
1:A:276:HIS:NE2	2:P:747:PRO:C	2.68	0.45
1:B:348:PRO:O	1:B:377:THR:HG22	2.17	0.45
1:D:176:TRP:O	1:D:183:PRO:HA	2.17	0.45
1:B:50:ALA:CB	1:B:97:MET:HE1	2.42	0.45
1:D:176:TRP:CZ2	1:D:186:GLY:N	2.82	0.45
1:D:178:HIS:ND1	1:D:178:HIS:N	2.65	0.45
1:D:228:ALA:HB2	1:D:270:LYS:HB3	1.99	0.45
1:D:448:SER:HG	1:D:450:ASP:CG	2.23	0.45
1:A:324:ASP:HB2	1:C:175:ARG:NH1	2.31	0.44
1:A:347:ALA:HA	1:A:348:PRO:HD3	1.80	0.44
1:A:351:PHE:HA	1:A:352:PRO:HA	1.80	0.44
1:D:128:ILE:HD13	1:D:141:ASP:OD1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:GLU:H	1:D:217:GLU:HG2	1.55	0.44
1:A:58:TYR:OH	1:A:77:MET:HG2	2.16	0.44
1:B:34:ILE:HA	1:B:367:GLY:O	2.17	0.44
1:B:315:ARG:HG3	1:B:315:ARG:HH11	1.81	0.44
1:D:112:PHE:CE2	1:D:113:PHE:HD1	2.33	0.44
1:D:249:ASP:C	1:D:249:ASP:OD1	2.59	0.44
1:A:119:TRP:HD1	1:A:409:MET:CE	2.30	0.44
1:B:130:GLY:HA3	1:B:172:ASN:HD22	1.81	0.44
1:B:181:GLY:C	1:B:183:PRO:HD3	2.43	0.44
1:B:275:PRO:O	1:B:276:HIS:HB2	2.15	0.44
1:C:154:VAL:O	1:C:447:ALA:HA	2.17	0.44
1:C:252:ARG:NH1	1:C:254:ASP:OD1	2.50	0.44
1:D:53:TYR:CD2	1:D:97:MET:HG2	2.52	0.44
1:D:135:LEU:HB2	1:D:140:VAL:HG22	1.99	0.44
1:A:61:PRO:O	1:A:62:LYS:C	2.60	0.44
1:A:126:TYR:HA	1:A:169:ILE:O	2.18	0.44
1:A:368:ARG:NH2	1:A:389:PHE:CZ	2.81	0.44
1:D:74:LEU:O	1:D:78:GLN:HG2	2.17	0.44
1:D:358:ASN:ND2	1:D:358:ASN:N	2.63	0.44
1:A:322:ASP:O	1:A:323:TYR:C	2.61	0.44
1:A:362:SER:OG	1:A:363:CYS:N	2.51	0.44
1:B:274:CYS:HA	1:B:275:PRO:HD3	1.83	0.44
1:C:124:ILE:HB	1:C:159:PHE:CD1	2.53	0.44
1:D:401:ALA:HB1	1:D:405:PHE:CE2	2.53	0.44
1:A:113:PHE:CB	1:A:114:PRO:CD	2.94	0.44
1:C:211:GLU:OE1	1:C:211:GLU:HA	2.18	0.44
1:D:395:TYR:N	1:D:395:TYR:CD1	2.85	0.44
1:A:50:ALA:CA	1:A:97:MET:HE1	2.47	0.44
1:A:128:ILE:HG21	1:A:131:TYR:CE1	2.52	0.44
1:C:54:LEU:CD2	1:C:58:TYR:CD2	3.00	0.44
1:D:154:VAL:HB	1:D:442:GLN:HE21	1.82	0.44
1:A:55:ASN:ND2	1:A:62:LYS:HG3	2.33	0.44
1:A:196:ALA:HB1	1:A:197:PRO:HD2	1.98	0.44
1:B:128:ILE:HD11	1:B:131:TYR:CD1	2.51	0.44
1:B:184:PHE:HB3	1:B:208:ASP:OD2	2.18	0.44
1:B:302:TYR:OH	1:B:308:GLU:HG2	2.18	0.44
1:C:109:ASN:HB2	1:C:113:PHE:CD1	2.53	0.44
1:D:54:LEU:HA	1:D:58:TYR:HD2	1.83	0.44
1:D:271:TYR:CD2	1:D:272:GLY:N	2.85	0.44
1:B:187:LYS:HA	1:B:211:GLU:OE1	2.18	0.44
1:B:380:ASN:CB	1:B:383:ASP:OD1	2.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:TYR:CA	1:C:229:ASP:HB2	2.48	0.44
1:D:413:HIS:HD1	1:D:423:PRO:HG3	1.83	0.44
1:B:86:THR:HG21	6:B:2006:HOH:O	2.17	0.43
1:B:188:ASP:OD2	1:B:372:LYS:HE2	2.17	0.43
1:B:342:GLY:O	1:B:345:GLU:HG2	2.18	0.43
1:D:159:PHE:CZ	1:D:409:MET:HE2	2.53	0.43
1:A:37:PHE:HE2	1:A:368:ARG:HD3	1.78	0.43
1:B:175:ARG:HH11	1:B:175:ARG:HD2	1.49	0.43
1:B:353:PHE:CG	1:B:376:ALA:HB3	2.54	0.43
1:B:404:GLN:O	1:B:407:HIS:HB2	2.18	0.43
1:C:104:ASN:ND2	1:C:193:HIS:HB2	2.33	0.43
1:D:89:LEU:HB3	1:D:94:ILE:HD11	1.99	0.43
1:D:343:ASN:ND2	1:D:385:ARG:O	2.51	0.43
1:D:433:LEU:HD11	1:D:437:ASP:HB2	2.00	0.43
1:A:133:PRO:HG2	2:P:753:ALA:HA	2.01	0.43
1:A:327:LYS:H	1:A:327:LYS:CD	2.24	0.43
1:B:340:VAL:O	1:B:341:GLY:C	2.59	0.43
1:C:239:PHE:CD1	1:C:265:PHE:HD2	2.36	0.43
1:C:420:LEU:HD13	1:C:431:PHE:CE1	2.53	0.43
1:D:152:SER:C	1:D:154:VAL:H	2.26	0.43
1:B:109:ASN:ND2	1:B:110:TYR:CE1	2.86	0.43
1:B:285:ASN:OD1	1:B:328:LYS:HA	2.18	0.43
1:C:63:GLU:CD	1:C:63:GLU:N	2.76	0.43
1:A:136:ASP:O	1:A:140:VAL:HG23	2.18	0.43
1:A:248:THR:HG23	1:A:250:THR:HG22	2.00	0.43
1:A:411:LEU:HD11	1:A:441:ILE:HB	2.01	0.43
1:B:225:TYR:CZ	1:B:282:MET:HE1	2.52	0.43
1:B:322:ASP:OD1	1:B:322:ASP:C	2.61	0.43
1:C:49:LEU:O	1:C:50:ALA:C	2.60	0.43
1:D:248:THR:OG1	1:D:250:THR:HG22	2.18	0.43
1:A:119:TRP:CD1	1:A:409:MET:CE	3.02	0.43
1:A:194:ALA:CB	1:A:205:SER:HA	2.48	0.43
1:B:58:TYR:CE1	1:B:77:MET:HB2	2.54	0.43
1:B:123:GLN:NE2	1:B:158:ARG:HD3	2.33	0.43
1:D:130:GLY:HA3	1:D:172:ASN:ND2	2.34	0.43
1:A:140:VAL:HG12	1:A:144:PHE:CE2	2.54	0.43
1:B:300:THR:OG1	3:B:852:SO4:O1	2.35	0.43
1:D:344:SER:HB3	1:D:377:THR:HG21	2.01	0.43
1:A:73:THR:O	1:A:74:LEU:C	2.61	0.43
1:A:276:HIS:NE2	2:P:749:GLY:CA	2.82	0.43
1:B:261:THR:HG22	1:B:261:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:MET:HE3	1:C:97:MET:HG3	2.01	0.43
1:A:390:CYS:O	1:A:391:PRO:C	2.62	0.43
1:C:239:PHE:HD1	1:C:265:PHE:HD2	1.67	0.43
1:C:392:ASP:OD1	1:C:392:ASP:C	2.62	0.43
1:A:176:TRP:CD2	1:C:325:ARG:HA	2.50	0.43
1:A:378:THR:HG21	1:A:384:ASP:CB	2.37	0.43
1:B:113:PHE:CZ	1:B:114:PRO:CG	2.91	0.43
1:B:298:GLN:NE2	1:B:324:ASP:OD1	2.47	0.43
1:D:115:ARG:C	1:D:116:LYS:HG3	2.44	0.43
1:A:57:PHE:CZ	1:A:190:LEU:HD21	2.54	0.42
1:C:276:HIS:CD2	1:C:335:THR:CG2	2.76	0.42
1:C:364:THR:OG1	1:C:365:SER:N	2.52	0.42
1:D:58:TYR:CZ	1:D:77:MET:HA	2.54	0.42
1:D:176:TRP:HE3	1:D:184:PHE:O	2.01	0.42
1:B:293:PHE:CE1	1:B:304:SER:HA	2.54	0.42
1:C:176:TRP:C	1:C:184:PHE:H	2.28	0.42
1:C:434:SER:OG	1:C:436:ASP:HB3	2.19	0.42
1:C:275:PRO:O	1:C:276:HIS:HB2	2.19	0.42
1:D:54:LEU:O	1:D:58:TYR:HB2	2.19	0.42
1:D:99:LYS:HE3	1:D:99:LYS:HA	2.01	0.42
1:A:135:LEU:HD13	1:A:213:TRP:O	2.19	0.42
1:A:238:LEU:HD12	1:A:242:LYS:O	2.20	0.42
1:A:354:THR:H	1:A:380:ASN:HA	1.83	0.42
1:B:448:SER:HA	1:B:449:PRO:HD3	1.79	0.42
1:C:77:MET:SD	1:C:77:MET:C	3.02	0.42
1:C:126:TYR:CZ	1:C:161:ARG:HB2	2.54	0.42
1:B:70:LEU:O	1:B:74:LEU:HD22	2.19	0.42
1:B:135:LEU:HB2	1:B:140:VAL:HG23	2.01	0.42
1:C:47:LYS:O	1:C:48:GLU:C	2.60	0.42
1:C:437:ASP:O	1:C:441:ILE:HG22	2.19	0.42
1:D:155:THR:HA	1:D:446:GLY:O	2.20	0.42
1:D:293:PHE:HA	1:D:294:PRO:HA	1.83	0.42
1:B:151:TRP:CZ3	1:B:441:ILE:HB	2.55	0.42
1:D:403:HIS:C	1:D:403:HIS:CD2	2.97	0.42
1:A:331:PHE:C	1:A:333:PRO:HD3	2.45	0.42
1:A:355:PHE:O	1:A:356:LEU:HB2	2.19	0.42
1:B:196:ALA:HB1	1:B:197:PRO:HD2	2.01	0.42
1:B:223:VAL:CG2	1:B:272:GLY:HA3	2.49	0.42
1:C:75:LYS:HG3	1:C:87:GLY:HA2	2.00	0.42
1:C:351:PHE:HA	1:C:352:PRO:HA	1.75	0.42
1:D:58:TYR:OH	1:D:77:MET:CG	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:TYR:CE2	1:D:77:MET:CG	3.03	0.42
1:D:350:VAL:HG11	1:D:379:ALA:CA	2.49	0.42
1:B:193:HIS:HD2	1:B:193:HIS:O	2.01	0.42
1:C:50:ALA:HB1	1:C:89:LEU:HD11	1.96	0.42
1:C:150:VAL:HG12	1:C:150:VAL:O	2.20	0.42
1:C:228:ALA:O	1:C:229:ASP:C	2.63	0.42
1:C:343:ASN:OD1	1:C:386:LYS:HA	2.20	0.42
1:D:72:ASP:O	1:D:75:LYS:HG3	2.20	0.42
1:D:263:TYR:CD1	1:D:263:TYR:C	2.97	0.42
1:A:40:ASP:CG	1:A:387:TRP:CH2	2.98	0.42
1:A:321:GLU:HG2	6:A:2027:HOH:O	2.19	0.42
1:B:128:ILE:HD12	1:B:128:ILE:C	2.45	0.42
1:B:149:GLN:HA	1:B:152:SER:OG	2.19	0.42
1:D:53:TYR:CG	1:D:97:MET:HG2	2.55	0.42
1:D:151:TRP:CE3	1:D:151:TRP:HA	2.55	0.42
1:D:350:VAL:CG1	1:D:379:ALA:HA	2.49	0.42
1:A:58:TYR:CE2	1:A:77:MET:CB	3.02	0.42
1:B:292:LYS:HD3	1:B:292:LYS:HA	1.79	0.42
1:B:353:PHE:CD1	1:B:353:PHE:C	2.97	0.42
1:C:81:PHE:HE1	1:C:423:PRO:HG2	1.84	0.42
1:C:108:ALA:HB1	1:C:110:TYR:HD1	1.85	0.42
1:C:195:PHE:CD2	1:C:201:VAL:HG13	2.55	0.42
1:C:343:ASN:OD1	1:C:386:LYS:HD2	2.20	0.42
1:A:101:ARG:HD3	1:A:102:CYS:O	2.20	0.41
1:A:224:LYS:O	1:A:273:PHE:HB2	2.20	0.41
1:A:442:GLN:C	1:A:444:LEU:N	2.77	0.41
1:C:188:ASP:OD2	1:C:372:LYS:CE	2.67	0.41
1:C:286:ALA:CB	1:C:319:THR:HG21	2.50	0.41
1:D:432:ARG:HD3	1:D:432:ARG:O	2.20	0.41
1:B:170:MET:HE3	1:B:170:MET:HB3	1.95	0.41
1:B:344:SER:CB	1:B:377:THR:HG1	2.26	0.41
1:D:235:PHE:CE1	1:D:246:SER:CA	3.03	0.41
1:A:32:SER:HB2	1:D:373:MET:HE1	2.02	0.41
1:A:196:ALA:HB1	1:A:197:PRO:CD	2.49	0.41
1:A:280:PHE:CD1	1:A:280:PHE:C	2.95	0.41
1:B:149:GLN:O	1:B:150:VAL:C	2.63	0.41
1:B:285:ASN:OD1	1:B:328:LYS:HD2	2.20	0.41
1:B:342:GLY:HA2	1:B:387:TRP:CZ2	2.56	0.41
1:C:108:ALA:O	1:C:109:ASN:OD1	2.38	0.41
1:D:89:LEU:HD13	1:D:94:ILE:CD1	2.51	0.41
1:B:35:ILE:HG22	1:B:36:LYS:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:PHE:HB2	1:B:376:ALA:HB3	2.02	0.41
1:C:274:CYS:O	1:C:280:PHE:CE1	2.74	0.41
1:D:274:CYS:HA	1:D:275:PRO:HD3	1.78	0.41
1:D:405:PHE:O	1:D:409:MET:HG2	2.21	0.41
1:B:378:THR:OG1	1:B:384:ASP:OD2	2.38	0.41
1:D:347:ALA:HA	1:D:348:PRO:HD3	1.85	0.41
1:A:176:TRP:CA	1:A:184:PHE:H	2.33	0.41
1:A:215:LEU:C	1:A:396:SER:HB2	2.46	0.41
1:C:119:TRP:CD1	1:C:409:MET:CE	3.03	0.41
1:D:72:ASP:OD1	1:D:72:ASP:N	2.43	0.41
1:D:122:ASN:H	1:D:123:GLN:NE2	2.19	0.41
1:D:178:HIS:CE1	1:D:182:TYR:O	2.73	0.41
1:B:49:LEU:CD2	1:B:98:ARG:HG2	2.51	0.41
1:B:151:TRP:CH2	1:B:411:LEU:CD1	3.03	0.41
1:D:227:ASN:OD1	1:D:269:GLY:O	2.39	0.41
1:D:435:GLN:HG3	1:D:439:LYS:HE3	2.03	0.41
1:A:187:LYS:HE3	1:A:212:LEU:HB2	2.03	0.41
1:B:58:TYR:CZ	1:B:77:MET:HB2	2.55	0.41
1:D:126:TYR:CZ	1:D:161:ARG:HB2	2.56	0.41
1:A:73:THR:HA	1:A:76:LYS:HG3	2.02	0.41
1:A:378:THR:O	1:A:379:ALA:C	2.63	0.41
1:A:434:SER:HB3	1:A:437:ASP:OD2	2.21	0.41
1:B:110:TYR:HB2	1:B:111:ASN:H	1.26	0.41
1:B:227:ASN:OD1	1:B:227:ASN:C	2.63	0.41
1:C:148:PHE:C	1:C:150:VAL:N	2.77	0.41
1:D:276:HIS:CD2	2:R:747:PRO:C	2.99	0.41
1:D:312:ASP:O	1:D:314:TYR:CD1	2.74	0.41
1:A:274:CYS:HA	1:A:275:PRO:HD3	1.91	0.41
1:A:276:HIS:NE2	2:P:749:GLY:N	2.66	0.41
1:A:282:MET:HG2	1:A:333:PRO:HG2	2.02	0.41
1:A:298:GLN:NE2	1:A:324:ASP:OD1	2.53	0.41
1:B:75:LYS:HG2	1:B:87:GLY:CA	2.51	0.41
1:B:123:GLN:OE1	1:B:158:ARG:NH1	2.54	0.41
1:C:92:ASN:HD22	1:C:92:ASN:HA	1.62	0.41
1:D:277:GLU:HG3	1:D:332:CYS:HB3	2.03	0.41
1:D:395:TYR:HD2	1:D:425:TYR:CD2	2.39	0.41
1:A:49:LEU:HD21	1:A:98:ARG:HD2	2.03	0.40
1:A:193:HIS:C	1:A:404:GLN:OE1	2.64	0.40
1:C:365:SER:O	1:C:366:ALA:C	2.63	0.40
1:D:392:ASP:CG	1:D:393:GLN:N	2.77	0.40
1:A:66:ASN:HD22	1:A:66:ASN:HA	1.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:CD1	1:A:74:LEU:HB2	2.48	0.40
1:C:92:ASN:O	1:C:96:THR:HG23	2.22	0.40
1:C:275:PRO:HB2	1:C:334:GLU:O	2.21	0.40
1:C:293:PHE:HA	1:C:294:PRO:HA	1.63	0.40
1:D:227:ASN:CB	1:D:270:LYS:HA	2.48	0.40
1:A:180:ASP:OD2	1:A:195:PHE:HZ	2.04	0.40
1:A:193:HIS:CA	1:A:404:GLN:OE1	2.69	0.40
1:A:320:THR:OG1	1:A:321:GLU:N	2.54	0.40
1:A:433:LEU:HD22	1:A:437:ASP:HB2	2.02	0.40
1:B:45:THR:O	1:B:46:ASP:C	2.62	0.40
1:D:236:PRO:HB3	1:D:245:ASN:OD1	2.22	0.40
2:R:749:GLY:HA2	2:R:750:PRO:HD3	1.94	0.40
1:C:119:TRP:CD1	1:C:409:MET:HE1	2.56	0.40
1:C:124:ILE:HB	1:C:159:PHE:HD1	1.86	0.40
1:C:381:TYR:O	1:C:382:ASP:C	2.63	0.40
1:D:323:TYR:O	1:D:327:LYS:HA	2.21	0.40
1:A:137:PRO:HD3	1:A:333:PRO:O	2.22	0.40
1:B:242:LYS:HD3	1:B:244:TYR:CZ	2.57	0.40
1:C:40:ASP:CG	1:C:368:ARG:NH2	2.80	0.40
1:C:127:ARG:NH1	1:C:165:GLY:N	2.67	0.40
1:C:235:PHE:HA	1:C:236:PRO:HA	1.80	0.40
1:D:151:TRP:O	1:D:155:THR:HG23	2.21	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)
6:C:2007:HOH:O	6:D:2007:HOH:O[4_555]	1.89	0.31
1:B:67:LEU:CD1	1:B:290:PRO:CG[4_465]	2.16	0.04
1:B:361:GLU:O	1:D:68:PHE:CE1[4_465]	2.19	0.01

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	419/421 (100%)	376 (90%)	33 (8%)	10 (2%)	4	7
1	B	417/421 (99%)	374 (90%)	31 (7%)	12 (3%)	3	5
1	C	416/421 (99%)	378 (91%)	31 (8%)	7 (2%)	7	12
1	D	417/421 (99%)	370 (89%)	35 (8%)	12 (3%)	3	5
2	P	6/8 (75%)	4 (67%)	0	2 (33%)	0	0
2	R	6/8 (75%)	1 (17%)	4 (67%)	1 (17%)	0	0
All	All	1681/1700 (99%)	1503 (89%)	134 (8%)	44 (3%)	4	6

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	120	ASP
1	B	67	LEU
1	B	108	ALA
1	B	379	ALA
1	C	110	TYR
1	D	66	ASN
1	D	111	ASN
1	D	113	PHE
1	D	218	GLY
1	D	344	SER
2	P	747	PRO
2	P	748	ALA
1	A	276	HIS
1	B	176	TRP
1	B	177	GLU
1	B	276	HIS
1	B	345	GLU
1	C	118	LYS
1	D	327	LYS
2	R	747	PRO
1	A	327	LYS
1	A	370	ASP
1	B	218	GLY
1	C	85	GLN
1	C	345	GLU
1	A	109	ASN
1	B	113	PHE

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Mol	Chain	Res	Type
1	C	109	ASN
1	C	276	HIS
1	D	112	PHE
1	D	356	LEU
1	A	85	GLN
1	A	379	ALA
1	B	188	ASP
1	C	91	GLN
1	D	85	GLN
1	D	180	ASP
1	B	347	ALA
1	A	61	PRO
1	B	341	GLY
1	A	371	GLY
1	D	114	PRO
1	D	449	PRO

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	351/351 (100%)	301 (86%)	50 (14%)	3	5
1	B	349/351 (99%)	311 (89%)	38 (11%)	6	9
1	C	348/351 (99%)	307 (88%)	41 (12%)	5	7
1	D	349/351 (99%)	292 (84%)	57 (16%)	2	3
2	P	3/3 (100%)	3 (100%)	0	100	100
2	R	3/3 (100%)	3 (100%)	0	100	100
All	All	1403/1410 (100%)	1217 (87%)	186 (13%)	4	6

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ILE
1	A	36	LYS

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Mol	Chain	Res	Type
1	A	40	ASP
1	A	44	LYS
1	A	46	ASP
1	A	62	LYS
1	A	64	SER
1	A	66	ASN
1	A	68	PHE
1	A	70	LEU
1	A	72	ASP
1	A	74	LEU
1	A	89	LEU
1	A	94	ILE
1	A	98	ARG
1	A	101	ARG
1	A	109	ASN
1	A	110	TYR
1	A	121	LYS
1	A	128	ILE
1	A	135	LEU
1	A	177	GLU
1	A	187	LYS
1	A	199	THR
1	A	212	LEU
1	A	221	VAL
1	A	223	VAL
1	A	245	ASN
1	A	268	ASP
1	A	281	THR
1	A	282	MET
1	A	285	ASN
1	A	301	SER
1	A	306	THR
1	A	311	THR
1	A	325	ARG
1	A	326	ASP
1	A	327	LYS
1	A	332	CYS
1	A	343	ASN
1	A	345	GLU
1	A	354	THR
1	A	361	GLU
1	A	364	THR

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Mol	Chain	Res	Type
1	A	365	SER
1	A	370	ASP
1	A	380	ASN
1	A	396	SER
1	A	429	LYS
1	A	452	ASP
1	B	44	LYS
1	B	56	THR
1	B	62	LYS
1	B	72	ASP
1	B	74	LEU
1	B	75	LYS
1	B	77	MET
1	B	93	THR
1	B	97	MET
1	B	101	ARG
1	B	104	ASN
1	B	109	ASN
1	B	110	TYR
1	B	112	PHE
1	B	128	ILE
1	B	142	ASP
1	B	160	SER
1	B	187	LYS
1	B	201	VAL
1	B	211	GLU
1	B	240	ASN
1	B	266	GLU
1	B	270	LYS
1	B	292	LYS
1	B	337	MET
1	B	338	SER
1	B	339	THR
1	B	354	THR
1	B	358	ASN
1	B	361	GLU
1	B	378	THR
1	B	383	ASP
1	B	407	HIS
1	B	412	GLU
1	B	428	THR
1	B	429	LYS

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Mol	Chain	Res	Type
1	B	433	LEU
1	B	448	SER
1	C	62	LYS
1	C	63	GLU
1	C	64	SER
1	C	67	LEU
1	C	89	LEU
1	C	92	ASN
1	C	93	THR
1	C	96	THR
1	C	101	ARG
1	C	113	PHE
1	C	115	ARG
1	C	116	LYS
1	C	121	LYS
1	C	160	SER
1	C	161	ARG
1	C	178	HIS
1	C	187	LYS
1	C	190	LEU
1	C	201	VAL
1	C	214	THR
1	C	215	LEU
1	C	234	LYS
1	C	242	LYS
1	C	250	THR
1	C	252	ARG
1	C	254	ASP
1	C	266	GLU
1	C	268	ASP
1	C	276	HIS
1	C	280	PHE
1	C	281	THR
1	C	298	GLN
1	C	339	THR
1	C	345	GLU
1	C	365	SER
1	C	368	ARG
1	C	383	ASP
1	C	424	ILE
1	C	426	THR
1	C	429	LYS

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Mol	Chain	Res	Type
1	C	432	ARG
1	D	34	ILE
1	D	35	ILE
1	D	41	VAL
1	D	45	THR
1	D	46	ASP
1	D	52	GLN
1	D	62	LYS
1	D	64	SER
1	D	67	LEU
1	D	70	LEU
1	D	72	ASP
1	D	75	LYS
1	D	78	GLN
1	D	89	LEU
1	D	92	ASN
1	D	99	LYS
1	D	109	ASN
1	D	111	ASN
1	D	115	ARG
1	D	116	LYS
1	D	118	LYS
1	D	127	ARG
1	D	129	ILE
1	D	132	THR
1	D	158	ARG
1	D	166	GLU
1	D	172	ASN
1	D	177	GLU
1	D	178	HIS
1	D	193	HIS
1	D	207	PHE
1	D	217	GLU
1	D	224	LYS
1	D	227	ASN
1	D	264	ASN
1	D	270	LYS
1	D	277	GLU
1	D	298	GLN
1	D	301	SER
1	D	319	THR
1	D	325	ARG

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Mol	Chain	Res	Type
1	D	326	ASP
1	D	327	LYS
1	D	332	CYS
1	D	337	MET
1	D	339	THR
1	D	349	CYS
1	D	356	LEU
1	D	358	ASN
1	D	364	THR
1	D	380	ASN
1	D	384	ASP
1	D	424	ILE
1	D	428	THR
1	D	430	ASN
1	D	434	SER
1	D	441	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	55	ASN
1	A	66	ASN
1	A	172	ASN
1	A	264	ASN
1	A	285	ASN
1	A	415	GLN
1	A	442	GLN
1	B	52	GLN
1	B	85	GLN
1	B	122	ASN
1	B	172	ASN
1	B	240	ASN
1	B	264	ASN
1	B	358	ASN
1	B	407	HIS
1	B	415	GLN
1	C	91	GLN
1	C	92	ASN
1	C	104	ASN
1	C	219	GLN
1	C	404	GLN

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Mol	Chain	Res	Type
1	C	407	HIS
1	C	430	ASN
1	C	442	GLN
1	D	55	ASN
1	D	66	ASN
1	D	78	GLN
1	D	85	GLN
1	D	92	ASN
1	D	111	ASN
1	D	123	GLN
1	D	172	ASN
1	D	219	GLN
1	D	227	ASN
1	D	442	GLN

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](#)

Of 22 ligands modelled in this entry, 16 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	B	853	-	4,4,4	1.03	0	6,6,6	0.36	0
3	SO4	B	852	-	4,4,4	0.69	0	6,6,6	0.26	0
3	SO4	C	856	-	4,4,4	0.66	0	6,6,6	0.43	0
3	SO4	A	851	-	4,4,4	0.60	0	6,6,6	0.19	0
3	SO4	D	857	-	4,4,4	0.80	0	6,6,6	0.46	0
3	SO4	C	850	-	4,4,4	0.64	0	6,6,6	0.41	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	853	SO4	1	0
3	B	852	SO4	1	0
3	D	857	SO4	2	0
3	C	850	SO4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	421/421 (100%)	0.64	51 (12%) 8 7	16, 34, 78, 100	0
1	B	419/421 (99%)	0.32	25 (5%) 27 21	15, 31, 60, 100	0
1	C	418/421 (99%)	0.62	32 (7%) 19 14	17, 37, 71, 100	0
1	D	419/421 (99%)	1.02	63 (15%) 5 4	21, 47, 83, 100	0
2	P	8/8 (100%)	8.31	8 (100%) 0 0	78, 81, 90, 94	0
2	R	8/8 (100%)	5.22	8 (100%) 0 0	71, 74, 78, 80	0
All	All	1693/1700 (99%)	0.71	187 (11%) 10 9	15, 38, 78, 100	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	746	GLY	12.8
2	P	753	ALA	10.9
2	P	748	ALA	9.1
2	P	751	PRO	8.6
2	P	747	PRO	8.1
1	D	114	PRO	8.0
1	C	58	TYR	7.8
1	A	176	TRP	7.6
1	A	114	PRO	7.6
1	B	109	ASN	7.3
1	C	110	TYR	6.6
1	C	114	PRO	6.6
1	B	113	PHE	6.6
2	R	751	PRO	6.6
1	D	176	TRP	6.5
1	D	113	PHE	6.5
1	C	112	PHE	6.4
1	B	112	PHE	6.4
1	B	110	TYR	6.2

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Mol	Chain	Res	Type	RSRZ
1	C	113	PHE	6.1
1	B	114	PRO	6.0
1	C	115	ARG	6.0
1	A	280	PHE	5.8
2	P	752	GLY	5.8
2	R	750	PRO	5.7
2	R	752	GLY	5.7
1	A	67	LEU	5.7
2	P	749	GLY	5.7
1	D	66	ASN	5.5
2	P	750	PRO	5.5
2	R	746	GLY	5.5
1	D	356	LEU	5.4
1	C	280	PHE	5.3
1	A	113	PHE	5.2
1	A	110	TYR	5.2
2	R	748	ALA	5.2
1	D	110	TYR	5.2
1	A	451	ILE	5.1
1	A	40	ASP	5.1
2	R	753	ALA	5.1
1	C	35	ILE	5.0
1	B	115	ARG	4.9
1	A	68	PHE	4.7
1	D	67	LEU	4.7
1	A	33	PRO	4.7
1	C	32	SER	4.6
1	D	109	ASN	4.6
1	C	33	PRO	4.5
1	A	39	GLY	4.5
1	A	452	ASP	4.5
1	A	66	ASN	4.5
1	A	116	LYS	4.4
1	D	68	PHE	4.4
1	C	449	PRO	4.4
1	A	32	SER	4.3
1	A	354	THR	4.3
1	D	450	ASP	4.3
1	B	67	LEU	4.3
2	R	747	PRO	4.3
1	D	34	ILE	4.2
1	C	109	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	116	LYS	4.1
1	D	112	PHE	4.1
1	D	151	TRP	4.1
1	A	111	ASN	4.1
1	D	117	PRO	4.0
1	A	118	LYS	4.0
1	C	267	LYS	4.0
1	A	117	PRO	3.9
1	A	112	PHE	3.9
1	C	298	GLN	3.9
1	D	449	PRO	3.8
1	A	362	SER	3.8
1	D	69	VAL	3.8
1	D	150	VAL	3.8
1	A	58	TYR	3.8
1	A	69	VAL	3.8
1	A	385	ARG	3.8
2	R	749	GLY	3.8
1	A	115	ARG	3.7
1	D	111	ASN	3.6
1	B	345	GLU	3.6
1	D	35	ILE	3.6
1	B	111	ASN	3.5
1	B	176	TRP	3.5
1	A	70	LEU	3.4
1	D	115	ARG	3.4
1	C	34	ILE	3.3
1	C	116	LYS	3.3
1	B	445	TYR	3.3
1	D	116	LYS	3.3
1	C	111	ASN	3.3
1	D	385	ARG	3.2
1	C	108	ALA	3.2
1	A	41	VAL	3.2
1	A	357	GLY	3.2
1	B	225	TYR	3.1
1	D	271	TYR	3.1
1	C	91	GLN	3.1
1	D	298	GLN	3.1
1	D	70	LEU	3.0
1	D	149	GLN	3.0
1	D	357	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	432	ARG	2.9
1	A	450	ASP	2.9
1	B	108	ALA	2.9
1	D	36	LYS	2.9
1	C	239	PHE	2.9
1	A	282	MET	2.9
1	A	356	LEU	2.8
1	A	360	TYR	2.8
1	B	188	ASP	2.8
1	D	118	LYS	2.7
1	D	108	ALA	2.7
1	C	276	HIS	2.7
1	D	226	GLY	2.7
1	D	42	ALA	2.7
1	D	265	PHE	2.7
1	A	71	LYS	2.7
1	A	359	LYS	2.7
1	D	158	ARG	2.7
1	D	428	THR	2.7
1	A	34	ILE	2.7
1	A	35	ILE	2.7
1	C	123	GLN	2.6
1	D	386	LYS	2.6
1	D	340	VAL	2.6
1	A	386	LYS	2.6
1	D	242	LYS	2.6
1	C	39	GLY	2.6
1	D	367	GLY	2.6
1	B	41	VAL	2.6
1	D	353	PHE	2.5
1	D	40	ASP	2.5
1	D	180	ASP	2.5
1	C	117	PRO	2.5
1	D	119	TRP	2.5
1	B	432	ARG	2.5
1	A	38	PRO	2.5
1	B	435	GLN	2.5
1	A	379	ALA	2.5
1	B	267	LYS	2.4
1	D	41	VAL	2.4
1	B	346	GLY	2.4
1	D	203	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	120	ASP	2.4
1	A	43	PRO	2.4
1	B	117	PRO	2.4
1	C	158	ARG	2.4
1	B	450	ASP	2.3
1	A	352	PRO	2.3
1	C	279	LEU	2.3
1	C	248	THR	2.3
1	D	227	ASN	2.3
1	C	269	GLY	2.3
1	C	41	VAL	2.3
1	D	389	PHE	2.3
1	D	270	LYS	2.3
1	B	189	GLY	2.3
1	D	39	GLY	2.3
1	D	269	GLY	2.3
1	D	337	MET	2.2
1	D	33	PRO	2.2
1	B	174	GLY	2.2
1	A	42	ALA	2.2
1	A	358	ASN	2.2
1	A	380	ASN	2.2
1	C	367	GLY	2.2
1	D	341	GLY	2.2
1	D	192	ALA	2.2
1	A	361	GLU	2.2
1	D	359	LYS	2.2
1	A	36	LYS	2.1
1	A	131	TYR	2.1
1	D	58	TYR	2.1
1	A	177	GLU	2.1
1	A	364	THR	2.1
1	D	267	LYS	2.1
1	A	91	GLN	2.1
1	D	240	ASN	2.1
1	D	231	GLU	2.1
1	C	130	GLY	2.1
1	D	272	GLY	2.1
1	A	343	ASN	2.0
1	D	107	VAL	2.0
1	B	366	ALA	2.0
1	C	435	GLN	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	D	999	1/1	0.60	0.17	100,100,100,100	0
3	SO4	C	856	5/5	0.70	0.19	75,77,77,79	0
5	CA	B	999	1/1	0.76	0.23	100,100,100,100	0
5	CA	C	999	1/1	0.81	0.15	94,94,94,94	0
5	CA	A	999	1/1	0.81	0.16	76,76,76,76	0
3	SO4	B	853	5/5	0.82	0.16	72,72,74,75	0
3	SO4	B	852	5/5	0.89	0.14	64,65,66,67	0
5	CA	B	998	1/1	0.92	0.05	20,20,20,20	0
3	SO4	A	851	5/5	0.92	0.14	40,41,44,45	0
3	SO4	D	857	5/5	0.94	0.09	46,47,48,49	0
3	SO4	C	850	5/5	0.95	0.08	41,41,43,44	0
5	CA	D	998	1/1	0.96	0.06	34,34,34,34	0
4	ZN	D	996	1/1	0.96	0.05	35,35,35,35	0
5	CA	A	998	1/1	0.97	0.04	20,20,20,20	0
4	ZN	A	996	1/1	0.97	0.04	26,26,26,26	0
5	CA	C	998	1/1	0.97	0.03	30,30,30,30	0
4	ZN	B	997	1/1	0.98	0.05	23,23,23,23	0
4	ZN	D	997	1/1	0.98	0.07	40,40,40,40	0
4	ZN	C	996	1/1	0.99	0.04	32,32,32,32	0
4	ZN	C	997	1/1	0.99	0.05	26,26,26,26	0
4	ZN	B	996	1/1	0.99	0.05	24,24,24,24	0
4	ZN	A	997	1/1	1.00	0.04	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.