



Full wwPDB EM Validation Report ⓘ

Sep 10, 2026 – 03:31 PM EDT

PDB ID : 9ZN8 / pdb_00009zn8
EMDB ID : EMD-74438
Title : Structure of rabbit RyR1 complexed with FKBP12.6 and calmodulin in the presence of ATP, ADP, and Mg²⁺ (mimicking physiological conditions)
Authors : Kim, K.; Clarke, O.B.
Deposited on : 2025-12-12
Resolution : 2.57 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

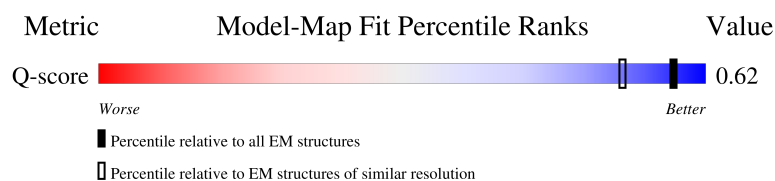
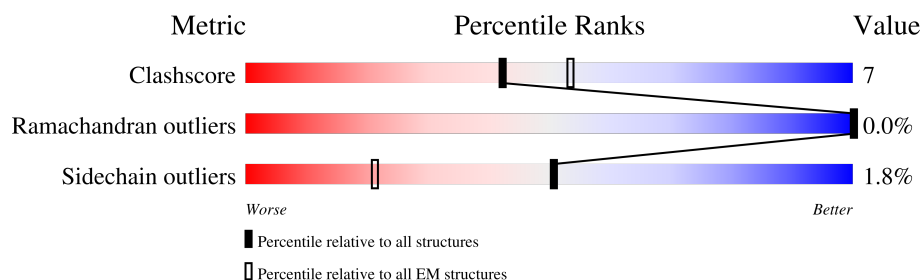
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.57 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.



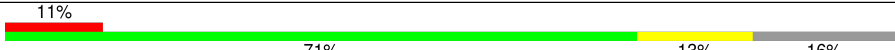
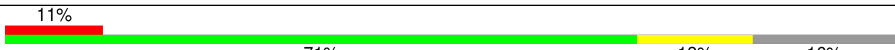
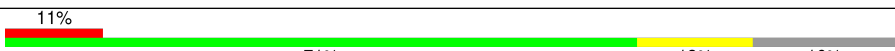
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7615 (2.07 - 3.07)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	I	148	51% 78% 22%
1	J	148	53% 78% 22%
1	K	148	51% 80% 20%
1	L	148	53% 86% 14%

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Mol	Chain	Length	Quality of chain
2	E	107	
2	F	107	
2	G	107	
2	H	107	
3	A	5037	
3	B	5037	
3	C	5037	
3	D	5037	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 146702 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	148	Total	C	N	O	S	0	0
			1017	624	174	213	6		
1	I	148	Total	C	N	O	S	0	0
			1017	624	174	213	6		
1	J	148	Total	C	N	O	S	0	0
			1017	624	174	213	6		
1	K	148	Total	C	N	O	S	0	0
			1017	624	174	213	6		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-1	HIS	-	expression tag	UNP P0DP23
I	-1	HIS	-	expression tag	UNP P0DP23
J	-1	HIS	-	expression tag	UNP P0DP23
K	-1	HIS	-	expression tag	UNP P0DP23

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	H	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	F	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	G	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

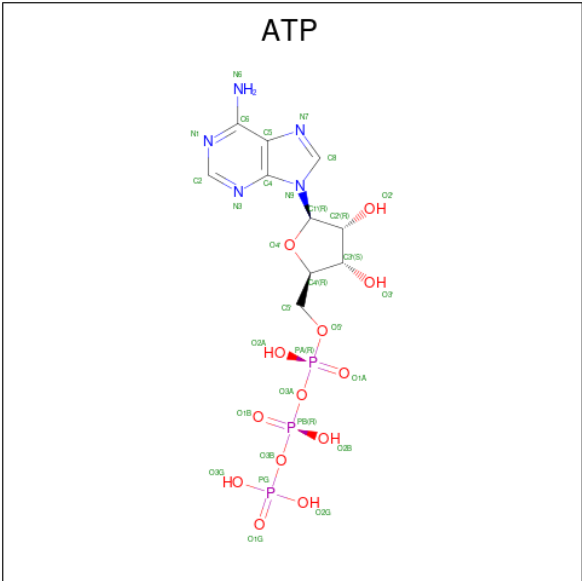
- Molecule 3 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	4249	Total	C	N	O	S	1	0
			33879	21584	5829	6232	234		
3	C	4249	Total	C	N	O	S	1	0
			33879	21584	5829	6232	234		
3	D	4249	Total	C	N	O	S	1	0
			33879	21584	5829	6232	234		
3	B	4249	Total	C	N	O	S	1	0
			33879	21584	5829	6232	234		

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

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	
4	C	1	Total	Zn	0
			1	1	
4	D	1	Total	Zn	0
			1	1	
4	B	1	Total	Zn	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

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Mol	Chain	Residues	Atoms					AltConf
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

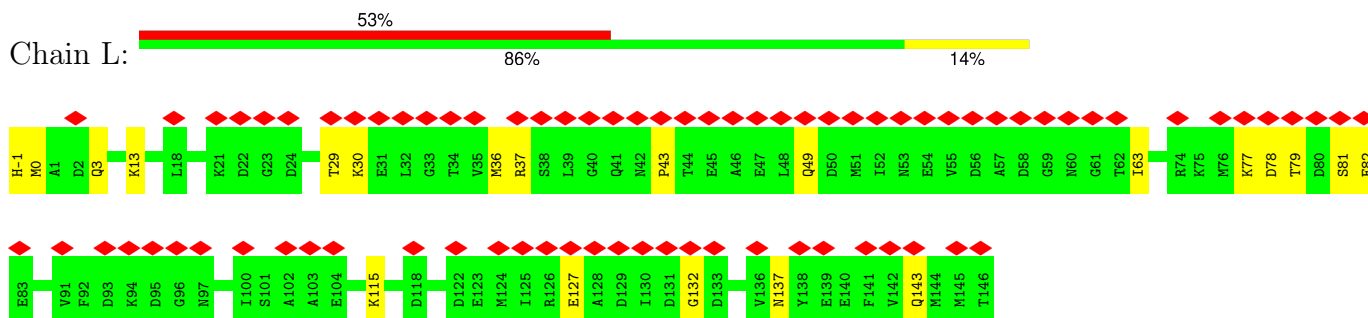
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	L	41	Total	O	0
			41	41	
6	I	41	Total	O	0
			41	41	
6	J	47	Total	O	0
			47	47	
6	K	46	Total	O	0
			46	46	
6	E	15	Total	O	0
			15	15	
6	A	866	Total	O	0
			866	866	
6	C	871	Total	O	0
			871	871	
6	D	868	Total	O	0
			868	868	
6	B	870	Total	O	0
			870	870	
6	H	15	Total	O	0
			15	15	
6	F	16	Total	O	0
			16	16	
6	G	18	Total	O	0
			18	18	

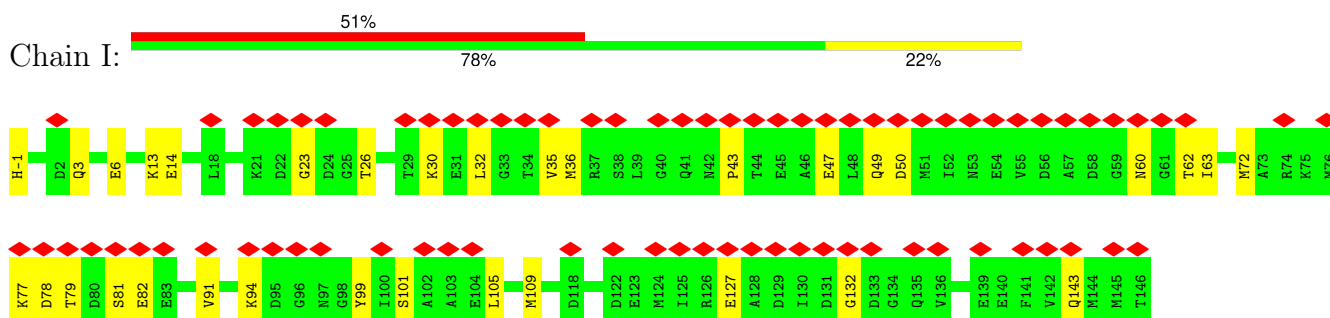
3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

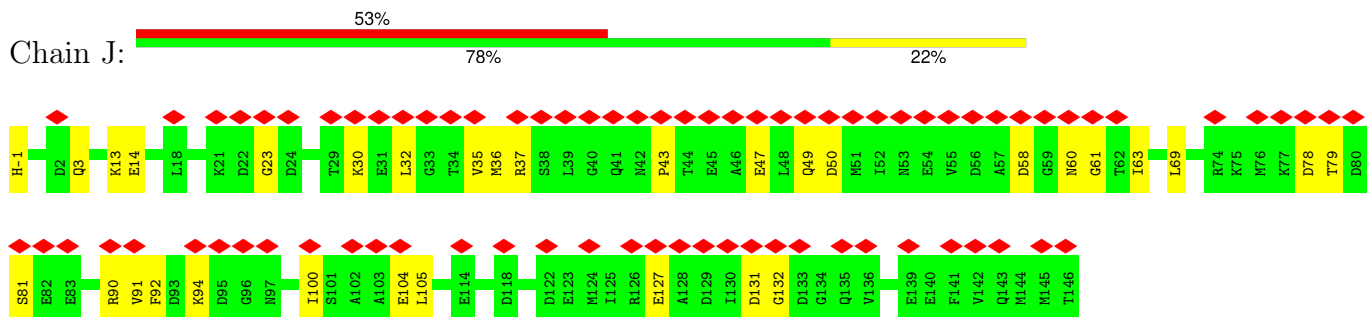
• Molecule 1: Calmodulin-1



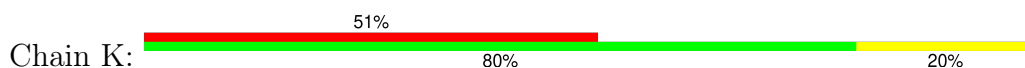
• Molecule 1: Calmodulin-1

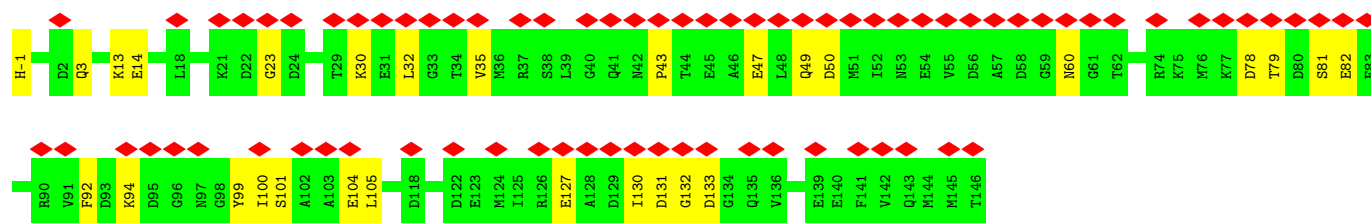


• Molecule 1: Calmodulin-1

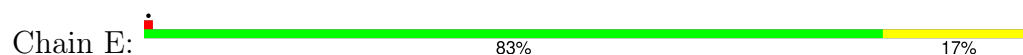


• Molecule 1: Calmodulin-1

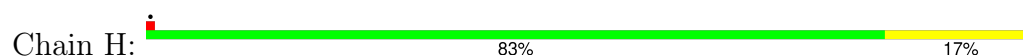




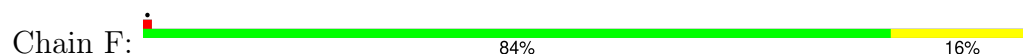
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



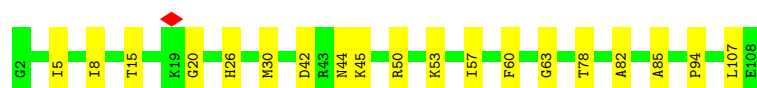
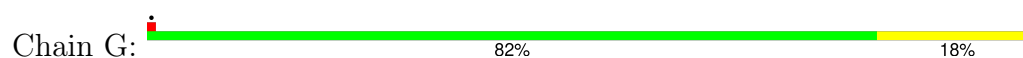
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



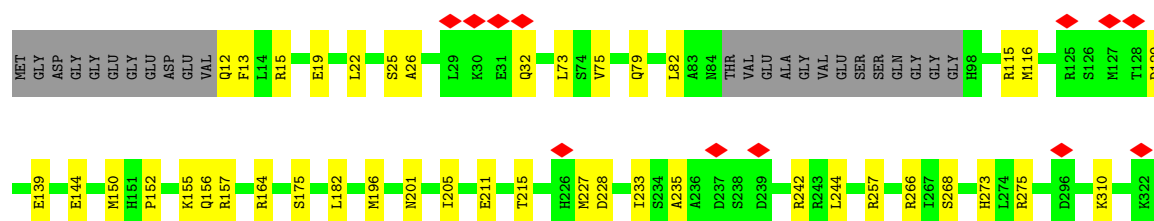
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

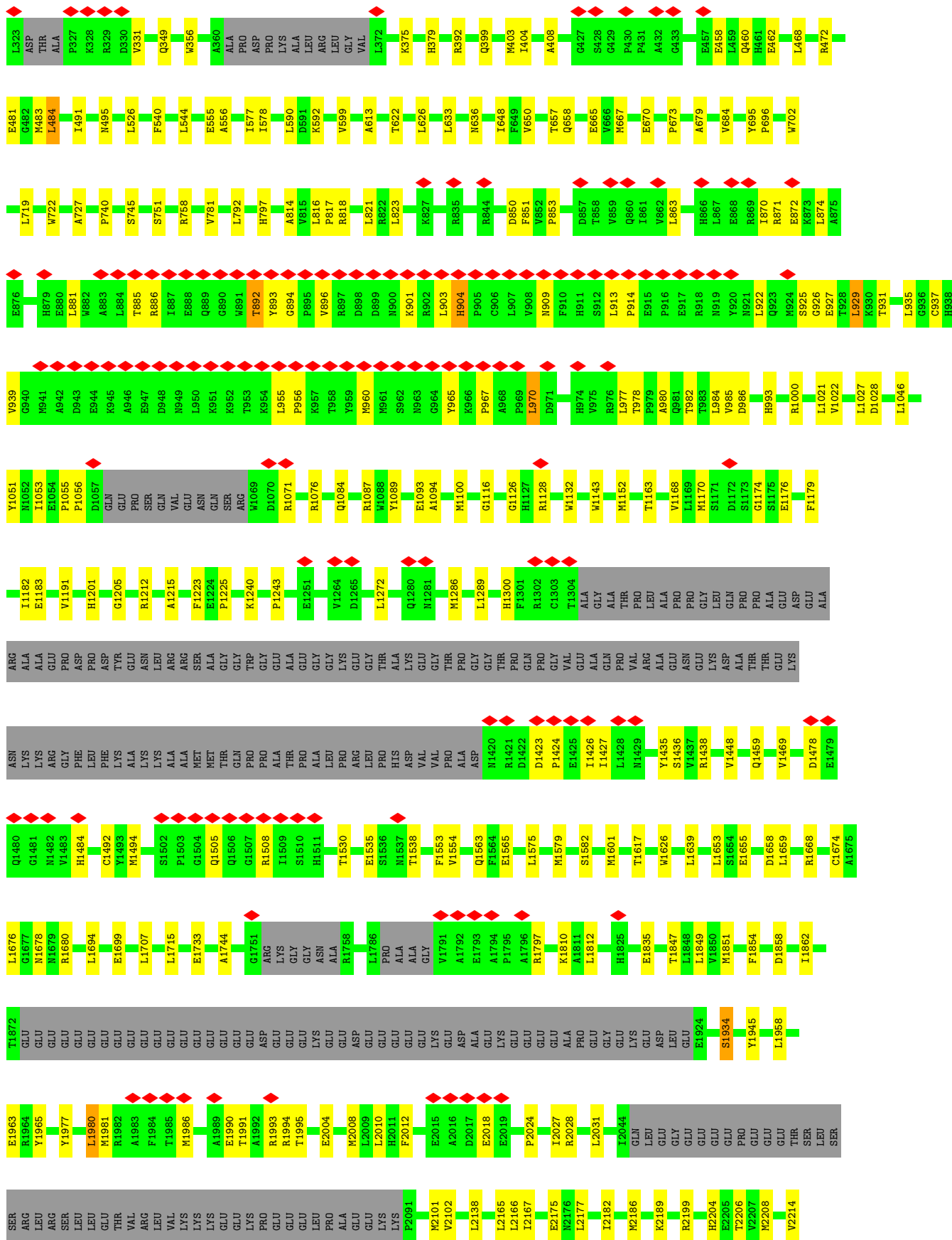


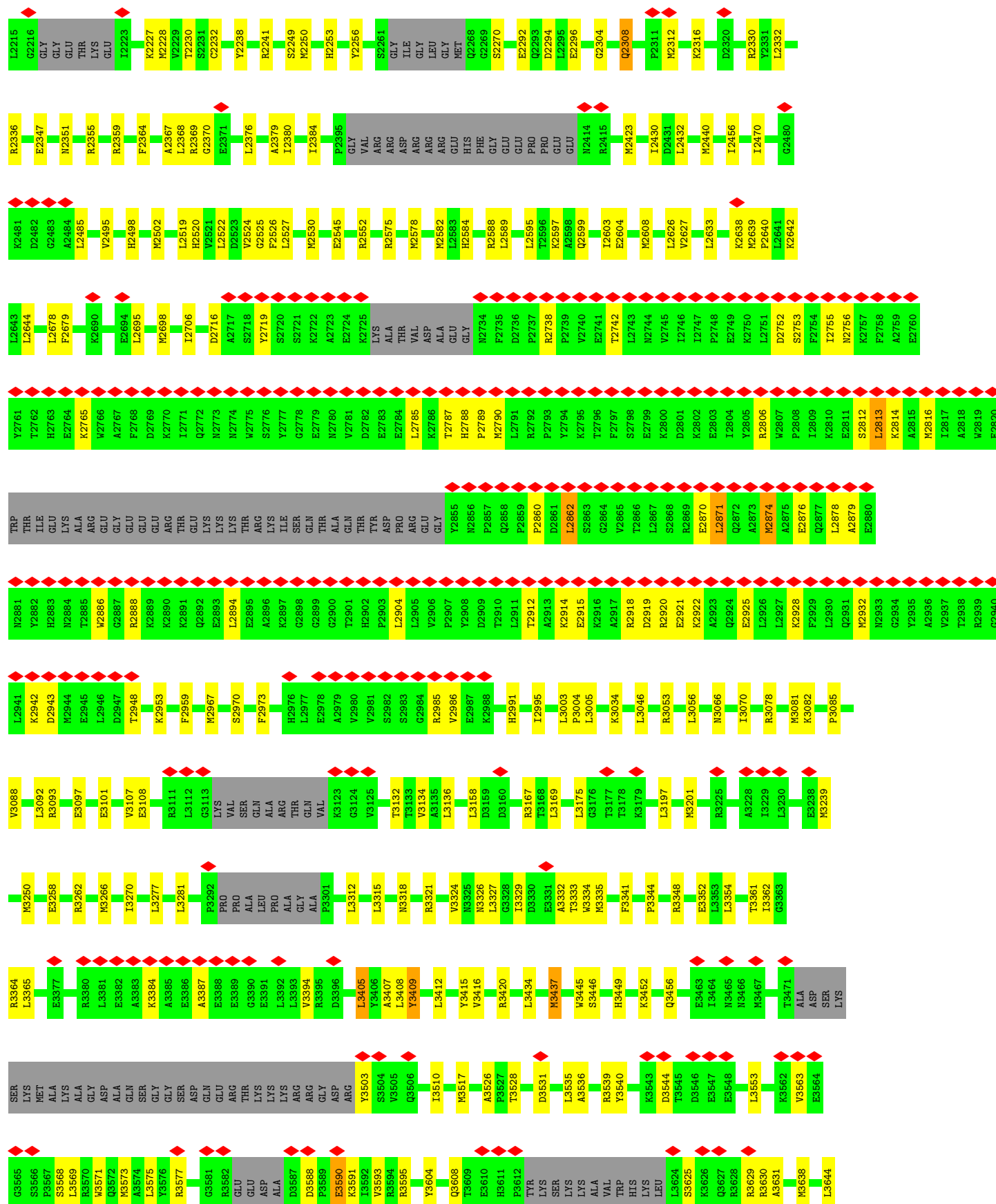
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

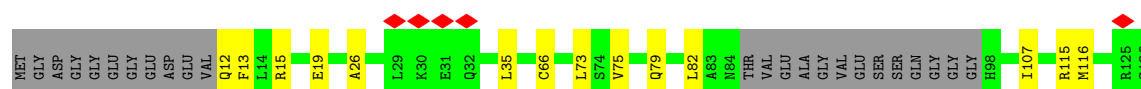


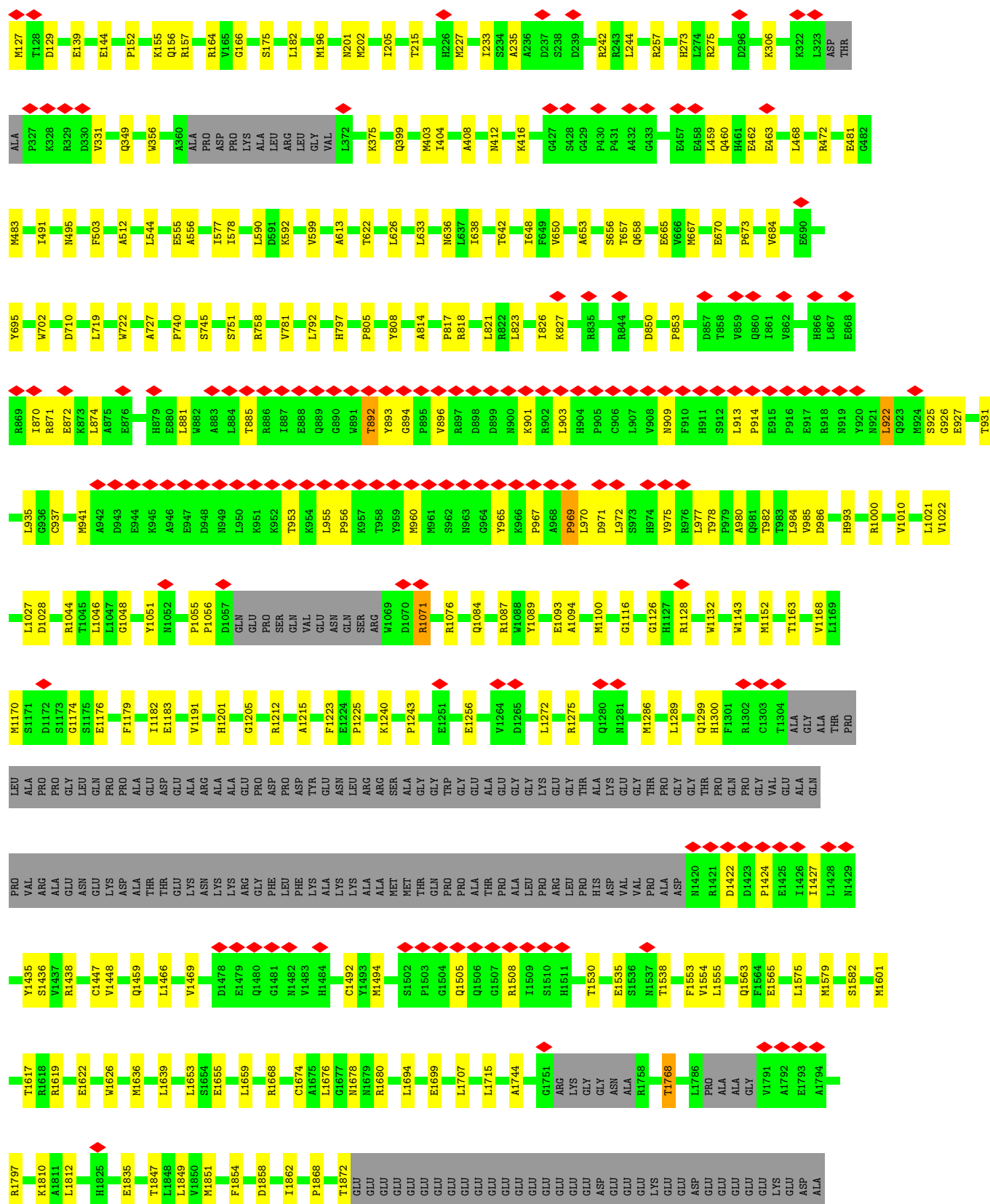
- Molecule 3: Ryanodine receptor 1

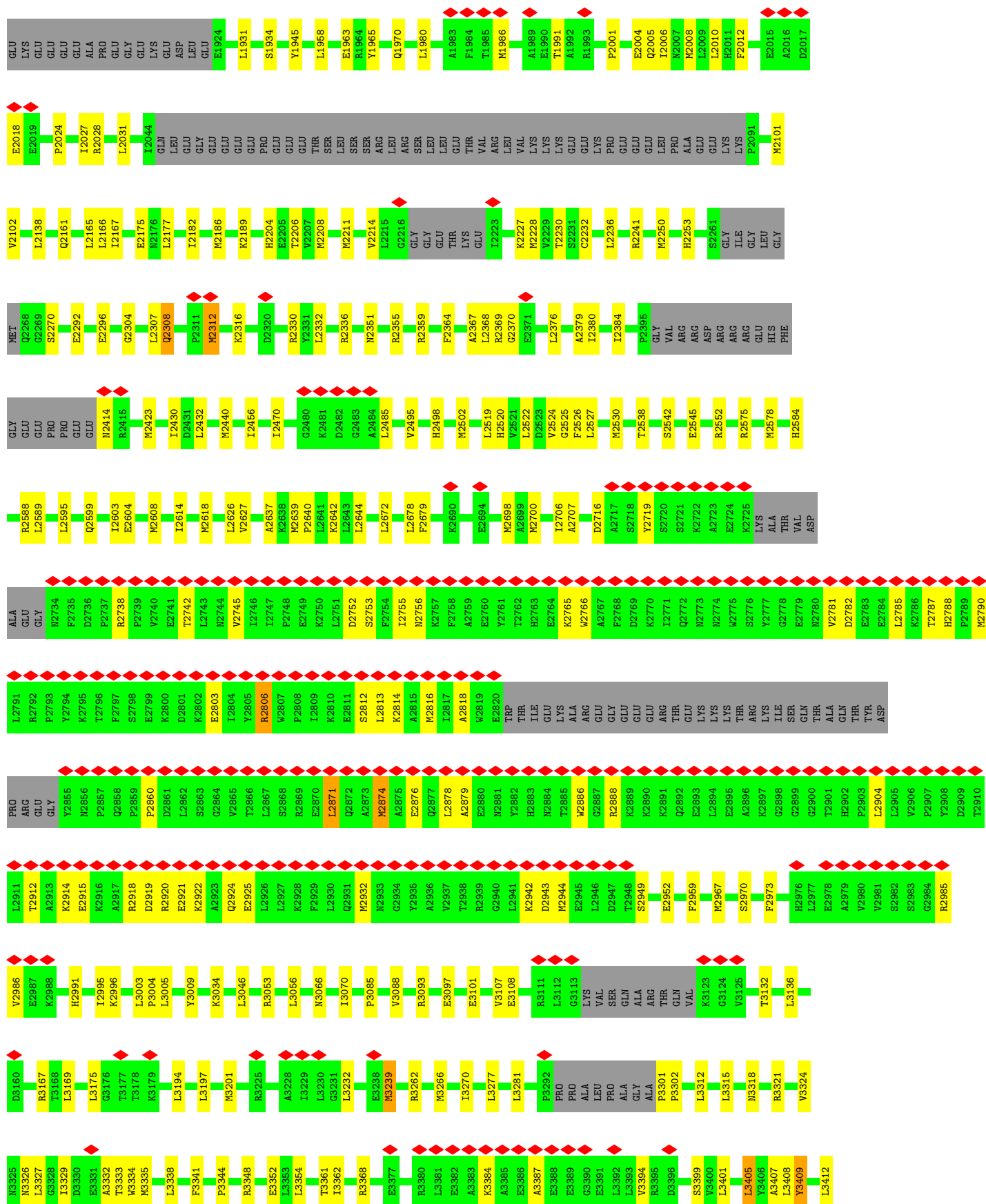










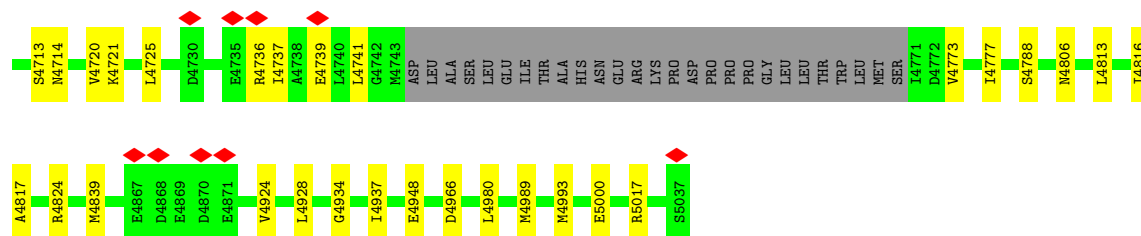




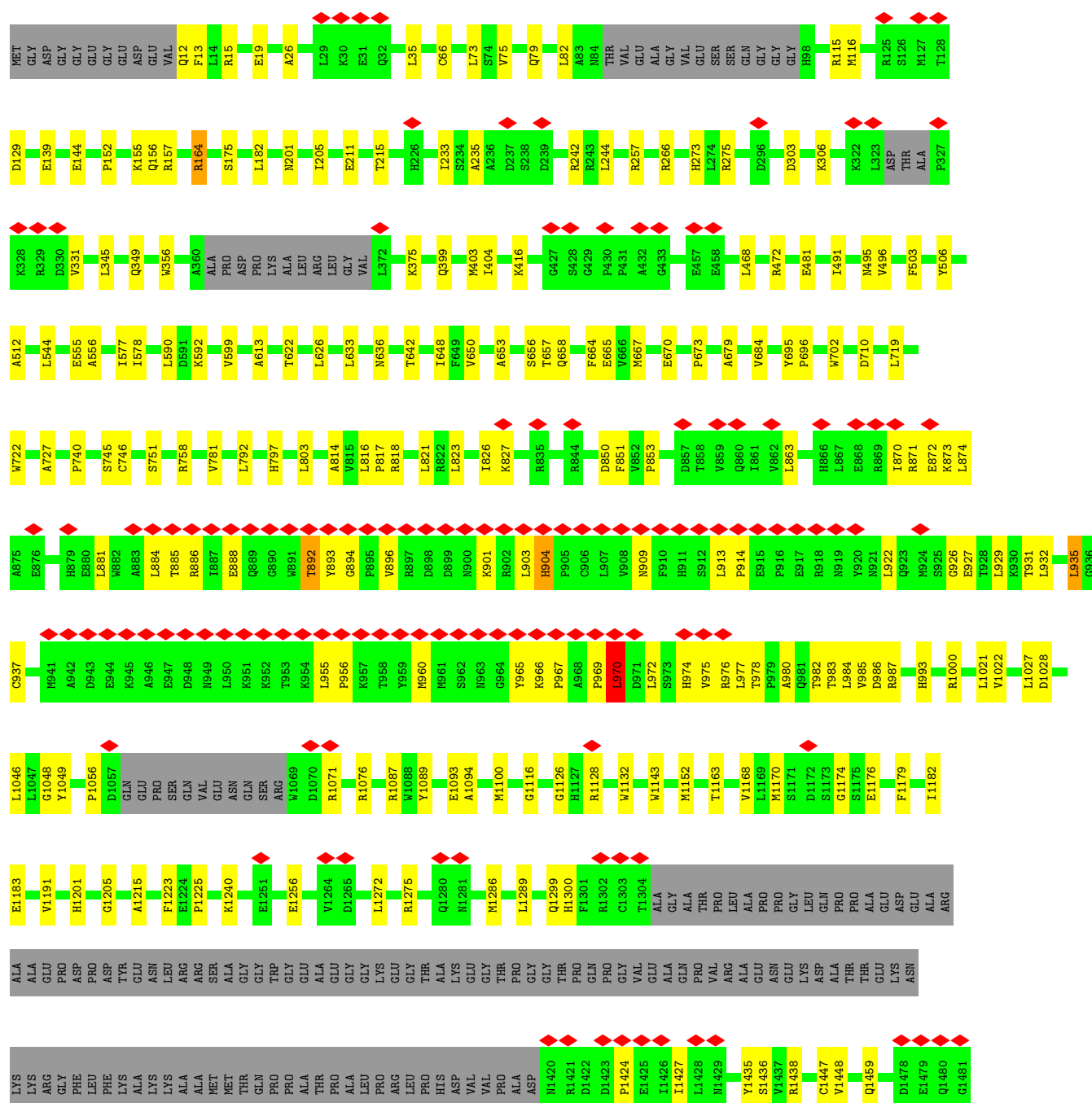






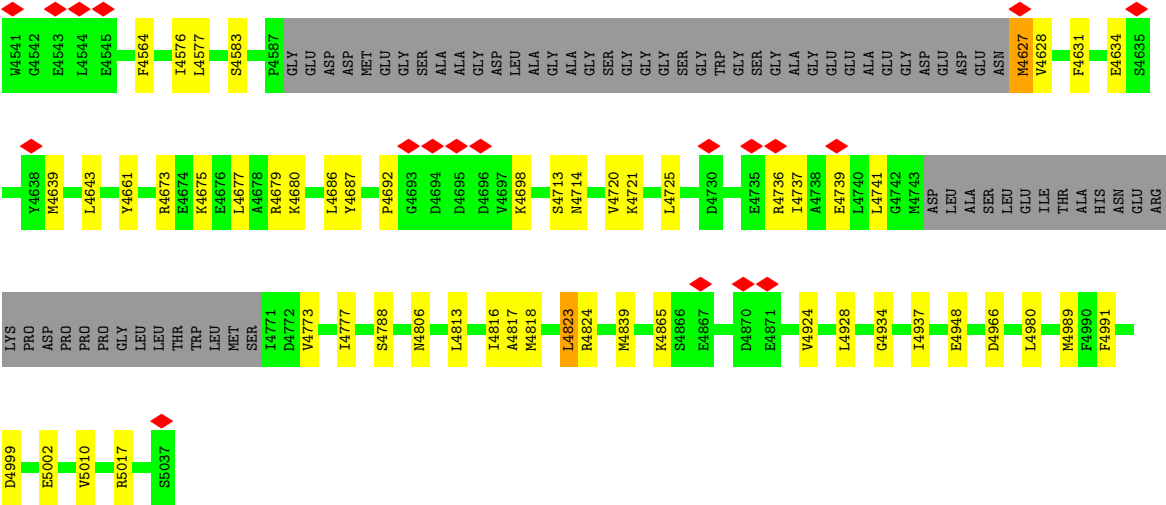


• Molecule 3: Ryanodine receptor 1









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	177312	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.549	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	498.0, 498.0, 498.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, 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	I	0.10	0/1026	0.26	0/1386
1	J	0.11	0/1026	0.25	0/1386
1	K	0.10	0/1026	0.24	0/1386
1	L	0.10	0/1026	0.23	0/1386
2	E	0.15	0/835	0.31	0/1123
2	F	0.15	0/835	0.30	0/1123
2	G	0.14	0/835	0.29	0/1123
2	H	0.14	0/835	0.29	0/1123
3	A	0.16	0/34640	0.32	0/46902
3	B	0.14	0/34640	0.31	0/46902
3	C	0.16	0/34640	0.32	1/46902 (0.0%)
3	D	0.15	0/34640	0.31	2/46902 (0.0%)
All	All	0.15	0/146004	0.31	3/197644 (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
3	A	0	1
3	C	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4062	PHE	CA-CB-CG	6.60	120.40	113.80
3	D	3159	ASP	CA-C-N	5.71	132.46	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3159	ASP	C-N-CA	5.71	132.46	121.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	4137	ARG	Sidechain
3	C	4137	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	I	1017	0	841	32	0
1	J	1017	0	841	36	0
1	K	1017	0	841	33	0
1	L	1017	0	841	21	0
2	E	819	0	821	13	0
2	F	819	0	821	12	0
2	G	819	0	821	12	0
2	H	819	0	821	12	0
3	A	33879	0	33511	431	0
3	B	33879	0	33511	443	0
3	C	33879	0	33511	440	0
3	D	33879	0	33511	435	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	31	0	12	0	0
5	B	31	0	12	0	0
5	C	31	0	12	0	0
5	D	31	0	12	0	0
6	A	866	0	0	62	0
6	B	870	0	0	71	0
6	C	871	0	0	62	0
6	D	868	0	0	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	15	0	0	2	0
6	F	16	0	0	3	0
6	G	18	0	0	3	0
6	H	15	0	0	2	0
6	I	41	0	0	21	0
6	J	47	0	0	27	0
6	K	46	0	0	27	0
6	L	41	0	0	16	0
All	All	146702	0	140740	1897	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 7.

All (1897) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3338:LEU:HD12	6:C:6415:HOH:O	1.28	1.32
1:L:30:LYS:HB3	6:L:219:HOH:O	1.17	1.30
1:L:-1:HIS:HD2	6:L:224:HOH:O	1.13	1.29
1:J:60:ASN:HB3	6:J:205:HOH:O	1.32	1.23
1:J:30:LYS:HB3	6:J:227:HOH:O	1.36	1.21
1:J:58:ASP:HB3	6:J:240:HOH:O	1.37	1.20
3:A:3865:VAL:HG21	6:A:6018:HOH:O	1.42	1.20
1:K:130:ILE:HB	6:K:238:HOH:O	1.37	1.19
1:I:30:LYS:HB3	6:I:226:HOH:O	1.38	1.18
3:B:3865:VAL:HG21	6:B:6168:HOH:O	1.46	1.16
3:C:3865:VAL:HG21	6:C:6188:HOH:O	1.45	1.16
3:D:3865:VAL:HG21	6:D:6129:HOH:O	1.47	1.11
1:K:30:LYS:HB3	6:K:227:HOH:O	1.47	1.11
1:L:0:MET:HB3	6:L:238:HOH:O	1.54	1.07
1:L:37:ARG:HG2	6:L:217:HOH:O	1.56	1.06
3:C:975:VAL:HB	6:C:5767:HOH:O	1.52	1.06
1:J:37:ARG:CG	6:J:220:HOH:O	2.04	1.04
1:K:94:LYS:HG3	6:K:211:HOH:O	1.59	1.03
1:J:127:GLU:HG3	6:J:213:HOH:O	1.62	1.00
1:J:37:ARG:HG2	6:J:220:HOH:O	1.61	0.97
3:C:975:VAL:CB	6:C:5767:HOH:O	2.09	0.96
3:B:416:LYS:NZ	6:B:5703:HOH:O	2.01	0.94
1:L:132:GLY:N	6:L:201:HOH:O	2.01	0.93
1:J:78:ASP:CB	6:J:225:HOH:O	2.17	0.92
3:C:975:VAL:CG1	6:C:5767:HOH:O	2.19	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:37:ARG:CG	6:L:217:HOH:O	2.16	0.90
3:D:416:LYS:NZ	6:D:5707:HOH:O	2.06	0.89
3:B:4066:LEU:HB2	6:B:6440:HOH:O	1.72	0.88
1:I:81:SER:HB3	6:I:228:HOH:O	1.76	0.85
1:J:79:THR:N	6:J:203:HOH:O	2.12	0.82
1:J:-1:HIS:NE2	6:J:202:HOH:O	2.06	0.82
3:D:1668:ARG:CD	6:D:5805:HOH:O	2.28	0.82
1:K:127:GLU:HG3	6:K:228:HOH:O	1.80	0.82
3:C:1668:ARG:CD	6:C:5788:HOH:O	2.29	0.81
1:K:-1:HIS:NE2	6:K:202:HOH:O	2.01	0.80
3:D:1668:ARG:HD3	6:D:5805:HOH:O	1.80	0.80
3:B:1668:ARG:CD	6:B:5805:HOH:O	2.29	0.80
1:J:30:LYS:CB	6:J:227:HOH:O	2.09	0.80
2:H:50:ARG:O	6:H:201:HOH:O	2.00	0.80
3:A:1668:ARG:HD3	6:A:5804:HOH:O	1.82	0.79
3:B:975:VAL:HB	6:B:5732:HOH:O	1.83	0.79
3:A:1668:ARG:CD	6:A:5804:HOH:O	2.28	0.79
2:G:20:GLY:HA2	2:G:50:ARG:HH21	1.47	0.79
3:D:4232:GLU:OE1	6:D:5701:HOH:O	2.00	0.79
3:A:1733:GLU:OE2	6:A:5701:HOH:O	2.01	0.78
6:A:6226:HOH:O	3:D:2456:ILE:HG13	1.83	0.78
3:B:1668:ARG:HD3	6:B:5805:HOH:O	1.82	0.78
1:K:50:ASP:O	6:K:201:HOH:O	2.01	0.78
3:C:850:ASP:OD2	6:C:5701:HOH:O	2.00	0.78
1:L:81:SER:HB3	6:L:225:HOH:O	1.83	0.78
3:B:1733:GLU:OE2	6:B:5702:HOH:O	2.00	0.78
1:K:78:ASP:CB	6:K:222:HOH:O	2.32	0.78
3:D:850:ASP:OD2	6:D:5703:HOH:O	2.01	0.78
3:B:987:ARG:NE	6:B:5720:HOH:O	2.17	0.77
3:D:1713:ASP:OD1	6:D:5704:HOH:O	2.02	0.77
3:A:4188:ARG:NH2	6:A:5719:HOH:O	2.16	0.77
3:C:1668:ARG:HD3	6:C:5788:HOH:O	1.83	0.76
3:C:986:ASP:OD1	6:C:5702:HOH:O	2.04	0.76
3:A:2456:ILE:HG13	6:B:6215:HOH:O	1.85	0.76
3:C:4188:ARG:NH2	6:C:5711:HOH:O	2.16	0.76
3:D:266:ARG:NH2	6:D:5702:HOH:O	2.00	0.76
3:B:3883:ASP:OD2	6:B:5705:HOH:O	2.04	0.76
3:B:1713:ASP:OD1	6:B:5706:HOH:O	2.04	0.76
2:G:82:ALA:O	6:G:201:HOH:O	2.04	0.76
3:C:3338:LEU:CD1	6:C:6415:HOH:O	2.03	0.76
3:A:3984:ARG:NH1	6:A:5722:HOH:O	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3996:PHE:O	3:D:4000:MET:HG3	1.86	0.75
3:B:3329:ILE:HD11	3:B:3332:ALA:HB2	1.68	0.75
3:A:850:ASP:OD2	6:A:5702:HOH:O	2.02	0.75
3:A:3329:ILE:HD11	3:A:3332:ALA:HB2	1.69	0.75
3:D:228:ASP:OD2	6:D:5705:HOH:O	2.04	0.75
3:B:850:ASP:OD2	6:B:5704:HOH:O	2.03	0.75
1:I:50:ASP:O	6:I:201:HOH:O	2.03	0.75
6:C:6203:HOH:O	3:B:2456:ILE:HG13	1.85	0.75
3:C:2627:VAL:HG22	3:C:2678:LEU:HB2	1.70	0.74
3:D:2333:ASP:HA	3:D:2336:ARG:HD3	1.69	0.74
3:C:196:MET:HE2	6:C:6211:HOH:O	1.86	0.74
3:D:331:VAL:O	6:D:5702:HOH:O	2.04	0.74
3:D:3329:ILE:HD11	3:D:3332:ALA:HB2	1.69	0.74
3:D:3644:LEU:O	6:D:5709:HOH:O	2.06	0.74
3:B:986:ASP:OD1	6:B:5708:HOH:O	2.06	0.74
3:B:3996:PHE:O	3:B:4000:MET:HG3	1.86	0.74
3:C:3329:ILE:HD11	3:C:3332:ALA:HB2	1.69	0.74
3:B:2627:VAL:HG22	3:B:2678:LEU:HB2	1.69	0.74
3:C:2456:ILE:HG13	6:D:6247:HOH:O	1.87	0.73
3:A:331:VAL:O	6:A:5704:HOH:O	2.05	0.73
3:D:1658:ASP:OD2	6:D:5708:HOH:O	2.06	0.73
3:D:2627:VAL:HG22	3:D:2678:LEU:HB2	1.69	0.73
3:D:3984:ARG:NH1	6:D:5725:HOH:O	2.21	0.73
3:A:2627:VAL:HG22	3:A:2678:LEU:HB2	1.69	0.73
3:B:2642:LYS:HB2	3:B:2698:MET:HE1	1.70	0.73
3:A:3644:LEU:O	6:A:5705:HOH:O	2.05	0.73
1:I:127:GLU:HG3	6:I:214:HOH:O	1.88	0.73
1:J:50:ASP:OD2	6:J:201:HOH:O	2.06	0.73
3:D:986:ASP:OD1	6:D:5706:HOH:O	2.05	0.72
1:I:30:LYS:CB	6:I:226:HOH:O	2.11	0.72
3:B:679:ALA:O	6:B:5709:HOH:O	2.07	0.72
3:B:3644:LEU:O	6:B:5707:HOH:O	2.05	0.72
3:B:1658:ASP:OD2	6:B:5710:HOH:O	2.07	0.72
3:C:3644:LEU:O	6:C:5703:HOH:O	2.05	0.72
3:A:228:ASP:OD2	6:A:5706:HOH:O	2.06	0.72
3:C:975:VAL:HG12	6:C:5767:HOH:O	1.82	0.72
2:F:82:ALA:O	6:F:201:HOH:O	2.06	0.72
2:G:42:ASP:OD1	6:G:202:HOH:O	2.06	0.72
3:A:960:MET:HE2	3:A:967:PRO:HB3	1.71	0.71
3:C:1459:GLN:HG3	6:C:5905:HOH:O	1.91	0.71
2:F:50:ARG:O	6:F:202:HOH:O	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:990:GLU:OE2	6:D:5711:HOH:O	2.08	0.71
3:C:3984:ARG:NH1	6:C:5721:HOH:O	2.24	0.71
1:I:78:ASP:CB	6:I:222:HOH:O	2.38	0.70
3:A:196:MET:HE2	6:A:6231:HOH:O	1.89	0.70
2:E:50:ARG:O	6:E:201:HOH:O	2.08	0.70
3:D:1459:GLN:HG3	6:D:5918:HOH:O	1.90	0.70
3:B:1459:GLN:HG3	6:B:5906:HOH:O	1.91	0.70
1:K:81:SER:HB3	6:K:229:HOH:O	1.90	0.70
3:D:116:MET:HG2	3:D:139:GLU:HA	1.73	0.70
3:A:1215:ALA:O	6:A:5707:HOH:O	2.08	0.70
3:D:850:ASP:OD1	6:D:5712:HOH:O	2.09	0.70
3:B:4180:ARG:O	6:B:5712:HOH:O	2.09	0.70
1:J:61:GLY:N	6:J:205:HOH:O	2.23	0.70
3:A:116:MET:HG2	3:A:139:GLU:HA	1.72	0.70
3:C:116:MET:HG2	3:C:139:GLU:HA	1.73	0.70
3:C:850:ASP:OD1	6:C:5704:HOH:O	2.08	0.70
1:J:132:GLY:N	6:J:206:HOH:O	2.24	0.69
2:E:42:ASP:OD1	6:E:202:HOH:O	2.10	0.69
2:H:42:ASP:OD1	6:H:202:HOH:O	2.09	0.69
3:C:2904:LEU:HD21	3:C:2915:GLU:HG3	1.73	0.69
3:B:1215:ALA:O	6:B:5711:HOH:O	2.09	0.69
3:A:1459:GLN:HG3	6:A:5907:HOH:O	1.91	0.69
3:D:913:LEU:HD22	3:D:914:PRO:HD2	1.74	0.69
3:D:139:GLU:OE1	6:D:5713:HOH:O	2.10	0.69
1:I:-1:HIS:CD2	6:I:231:HOH:O	2.46	0.69
3:B:116:MET:HG2	3:B:139:GLU:HA	1.73	0.69
3:B:266:ARG:NH2	6:B:5701:HOH:O	2.00	0.69
1:L:-1:HIS:CD2	6:L:224:HOH:O	2.02	0.69
3:A:986:ASP:OD2	6:A:5709:HOH:O	2.09	0.68
3:C:1538:THR:O	6:C:5705:HOH:O	2.11	0.68
3:C:2642:LYS:HB2	3:C:2698:MET:HE1	1.75	0.68
3:A:913:LEU:HD22	3:A:914:PRO:HD2	1.74	0.68
3:A:4180:ARG:O	6:A:5712:HOH:O	2.12	0.68
3:B:913:LEU:HD22	3:B:914:PRO:HD2	1.74	0.68
3:B:331:VAL:O	6:B:5701:HOH:O	2.11	0.68
3:B:3984:ARG:NH1	6:B:5730:HOH:O	2.26	0.68
3:A:139:GLU:OE1	6:A:5711:HOH:O	2.11	0.68
1:L:127:GLU:HG3	6:L:206:HOH:O	1.94	0.68
3:C:1215:ALA:O	6:C:5706:HOH:O	2.12	0.68
3:D:1215:ALA:O	6:D:5714:HOH:O	2.11	0.68
3:D:2230:THR:HG23	3:D:2270:SER:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4180:ARG:O	6:D:5715:HOH:O	2.11	0.68
1:I:23:GLY:O	6:I:202:HOH:O	2.11	0.67
1:J:131:ASP:HA	6:J:238:HOH:O	1.94	0.67
1:I:79:THR:N	6:I:206:HOH:O	2.27	0.67
1:J:23:GLY:O	6:J:204:HOH:O	2.12	0.67
1:K:50:ASP:OD1	6:K:203:HOH:O	2.12	0.67
3:A:25:SER:HB3	3:A:32:GLN:HE22	1.59	0.67
3:A:392[B]:ARG:NH1	6:A:5708:HOH:O	2.27	0.67
3:A:2642:LYS:HB2	3:A:2698:MET:HE1	1.75	0.67
1:K:131:ASP:HA	6:K:233:HOH:O	1.94	0.67
3:B:1655:GLU:OE1	6:B:5713:HOH:O	2.13	0.67
2:F:42:ASP:OD1	6:F:203:HOH:O	2.11	0.67
1:J:3:GLN:HG3	6:J:231:HOH:O	1.94	0.67
3:A:1655:GLU:OE1	6:A:5713:HOH:O	2.13	0.66
3:B:4066:LEU:CB	6:B:6440:HOH:O	2.37	0.66
1:I:50:ASP:OD2	6:I:203:HOH:O	2.12	0.66
1:I:36:MET:HG2	1:I:43:PRO:HG3	1.76	0.66
3:B:1538:THR:O	6:B:5715:HOH:O	2.14	0.66
3:D:2175:GLU:HG3	3:D:2228:MET:HB2	1.78	0.66
3:A:2175:GLU:HG3	3:A:2228:MET:HB2	1.78	0.66
3:C:2230:THR:HG23	3:C:2270:SER:H	1.61	0.66
3:C:4180:ARG:O	6:C:5707:HOH:O	2.14	0.66
3:D:4680:LYS:HD2	3:D:4686:LEU:HD22	1.78	0.66
3:B:2175:GLU:HG3	3:B:2228:MET:HB2	1.77	0.66
3:C:913:LEU:HD22	3:C:914:PRO:HD2	1.76	0.66
3:B:3081:MET:HE3	3:B:3092:LEU:HD23	1.76	0.66
3:B:4034:ASN:OD1	6:B:5714:HOH:O	2.14	0.65
3:A:1538:THR:O	6:A:5714:HOH:O	2.14	0.65
3:C:2440:MET:HA	3:C:2440:MET:HE3	1.79	0.65
1:K:3:GLN:HG3	6:K:230:HOH:O	1.97	0.65
1:K:133:ASP:HA	6:K:238:HOH:O	1.95	0.65
3:C:1655:GLU:OE1	6:C:5708:HOH:O	2.14	0.65
1:K:132:GLY:N	6:K:206:HOH:O	2.29	0.65
3:B:2230:THR:HG23	3:B:2270:SER:H	1.61	0.65
1:K:23:GLY:O	6:K:204:HOH:O	2.15	0.65
3:D:1538:THR:O	6:D:5716:HOH:O	2.13	0.65
3:A:3081:MET:HE3	3:A:3092:LEU:HD23	1.78	0.64
3:A:1986:MET:HG2	3:A:1991:THR:HB	1.79	0.64
3:B:331:VAL:CG2	6:B:6437:HOH:O	2.45	0.64
3:C:870:ILE:HD11	3:C:1051:TYR:CZ	2.33	0.64
3:B:4001:MET:HE2	3:B:4001:MET:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:79:THR:N	6:K:207:HOH:O	2.31	0.64
1:I:94:LYS:HD2	6:I:221:HOH:O	1.96	0.64
3:D:331:VAL:HG23	6:D:6394:HOH:O	1.98	0.64
3:B:2294:ASP:OD2	6:B:5716:HOH:O	2.14	0.64
3:B:233:ILE:HD12	3:B:242:ARG:HB3	1.79	0.64
3:A:679:ALA:O	6:A:5715:HOH:O	2.15	0.63
3:A:1582:SER:HB3	6:A:6535:HOH:O	1.97	0.63
2:G:50:ARG:O	6:G:203:HOH:O	2.15	0.63
1:I:99:TYR:CB	6:I:233:HOH:O	2.46	0.63
3:A:850:ASP:OD1	6:A:5716:HOH:O	2.15	0.63
3:A:2230:THR:HG23	3:A:2270:SER:H	1.62	0.63
3:A:2519:LEU:HD13	3:A:2575:ARG:HG3	1.80	0.63
3:C:2292:GLU:CD	3:C:2292:GLU:H	2.07	0.63
3:A:3722:TYR:HE1	3:A:3778:MET:HE3	1.63	0.63
3:D:986:ASP:HB2	6:D:5833:HOH:O	1.98	0.63
3:A:3540:TYR:HB3	3:A:3604:TYR:CD1	2.34	0.63
3:C:2175:GLU:HG3	3:C:2228:MET:HB2	1.80	0.63
3:A:633:LEU:HD13	3:A:1639:LEU:HD21	1.81	0.63
3:C:986:ASP:HB2	6:C:5825:HOH:O	1.97	0.63
3:D:1655:GLU:OE1	6:D:5717:HOH:O	2.15	0.63
3:D:3722:TYR:HE1	3:D:3778:MET:HE3	1.64	0.63
1:K:30:LYS:CB	6:K:227:HOH:O	2.21	0.63
3:D:155:LYS:O	6:D:5719:HOH:O	2.16	0.63
3:D:2384:ILE:HG13	3:D:2423:MET:HE2	1.81	0.63
1:L:78:ASP:CB	6:L:223:HOH:O	2.46	0.63
3:C:1582:SER:HB3	6:C:6536:HOH:O	1.98	0.63
3:D:235:ALA:HA	3:D:257:ARG:HD3	1.81	0.63
3:D:679:ALA:O	6:D:5718:HOH:O	2.15	0.63
3:D:2519:LEU:HD13	3:D:2575:ARG:HG3	1.81	0.63
3:D:3693:LYS:O	6:D:5720:HOH:O	2.16	0.63
3:B:850:ASP:OD1	6:B:5717:HOH:O	2.16	0.63
3:C:2384:ILE:HG13	3:C:2423:MET:HE2	1.81	0.62
3:C:3630:ARG:HH22	3:C:3861:GLU:HA	1.63	0.62
3:B:1582:SER:HB3	6:B:6535:HOH:O	1.98	0.62
3:B:4054:ASN:O	3:B:4058:ILE:HD12	1.97	0.62
3:D:331:VAL:CG2	6:D:6394:HOH:O	2.46	0.62
3:B:2384:ILE:HG13	3:B:2423:MET:HE2	1.81	0.62
3:A:233:ILE:HD12	3:A:242:ARG:HB3	1.80	0.62
3:D:633:LEU:HD13	3:D:1639:LEU:HD21	1.81	0.62
3:B:2519:LEU:HD13	3:B:2575:ARG:HG3	1.81	0.62
3:D:1168:VAL:HG11	3:D:1176:GLU:HG3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:233:ILE:HD12	3:C:242:ARG:HB3	1.80	0.62
3:C:2470:ILE:HG22	3:C:2525:GLY:HA3	1.82	0.62
1:J:-1:HIS:CD2	6:J:234:HOH:O	2.53	0.62
3:C:2519:LEU:HD13	3:C:2575:ARG:HG3	1.81	0.62
3:A:2294:ASP:OD2	6:A:5717:HOH:O	2.16	0.62
3:A:3384:LYS:H	3:A:3387:ALA:HB3	1.64	0.62
3:C:3722:TYR:HE1	3:C:3778:MET:HE3	1.64	0.62
3:D:233:ILE:HD12	3:D:242:ARG:HB3	1.79	0.62
3:A:235:ALA:HA	3:A:257:ARG:HD3	1.81	0.62
3:C:670:GLU:HA	3:C:740:PRO:HG3	1.81	0.62
3:B:3384:LYS:H	3:B:3387:ALA:HB3	1.65	0.62
3:B:3722:TYR:HE1	3:B:3778:MET:HE3	1.63	0.62
3:B:3395:ARG:HD3	3:B:3453:ARG:HH22	1.65	0.61
3:A:155:LYS:O	6:A:5718:HOH:O	2.16	0.61
3:D:2716:ASP:HB3	3:D:2719:TYR:HB2	1.82	0.61
3:D:3101:GLU:HG3	3:D:3167:ARG:HH22	1.66	0.61
3:A:3630:ARG:HH22	3:A:3861:GLU:HA	1.64	0.61
3:C:235:ALA:HA	3:C:257:ARG:HD3	1.81	0.61
3:C:633:LEU:HD13	3:C:1639:LEU:HD21	1.80	0.61
3:B:670:GLU:HA	3:B:740:PRO:HG3	1.81	0.61
3:B:2716:ASP:HB3	3:B:2719:TYR:HB2	1.83	0.61
3:A:2716:ASP:HB3	3:A:2719:TYR:HB2	1.83	0.61
3:A:4011:GLU:O	3:A:4015:GLU:HG3	2.01	0.61
3:D:3540:TYR:HB3	3:D:3604:TYR:CD1	2.36	0.61
3:C:3384:LYS:H	3:C:3387:ALA:HB3	1.64	0.61
3:D:2470:ILE:HG22	3:D:2525:GLY:HA3	1.82	0.61
3:B:331:VAL:HG23	6:B:6437:HOH:O	2.00	0.61
3:D:1986:MET:HG2	3:D:1991:THR:HB	1.83	0.61
3:A:2384:ILE:HG13	3:A:2423:MET:HE2	1.81	0.61
3:A:2879:ALA:HB1	3:A:2919:ASP:HB3	1.83	0.61
3:D:1582:SER:HB3	6:D:6533:HOH:O	1.99	0.61
3:B:115:ARG:NH1	6:B:5750:HOH:O	2.34	0.61
3:A:115:ARG:NH1	6:A:5748:HOH:O	2.33	0.61
3:A:1699:GLU:HG3	3:A:1810:LYS:HE3	1.83	0.61
3:C:155:LYS:O	6:C:5710:HOH:O	2.16	0.61
3:D:670:GLU:HA	3:D:740:PRO:HG3	1.81	0.61
3:B:633:LEU:HD13	3:B:1639:LEU:HD21	1.82	0.61
3:B:2440:MET:HA	3:B:2440:MET:HE3	1.83	0.61
3:C:115:ARG:NH1	6:C:5740:HOH:O	2.33	0.60
3:B:235:ALA:HA	3:B:257:ARG:HD3	1.81	0.60
3:A:2470:ILE:HG22	3:A:2525:GLY:HA3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1797:ARG:NH2	6:A:5751:HOH:O	2.34	0.60
3:D:4046:ASP:O	3:D:4050:GLU:HG3	2.00	0.60
3:A:2790:MET:HA	3:A:2790:MET:HE3	1.82	0.60
3:C:462:GLU:H	3:C:462:GLU:CD	2.09	0.60
3:B:155:LYS:O	6:B:5718:HOH:O	2.16	0.60
3:A:3101:GLU:HG3	3:A:3167:ARG:HH22	1.66	0.60
3:C:1505:GLN:HG3	3:C:1508:ARG:HH21	1.66	0.60
3:D:115:ARG:NH1	6:D:5753:HOH:O	2.34	0.60
3:D:1699:GLU:HG3	3:D:1810:LYS:HE3	1.82	0.60
3:C:3540:TYR:HB3	3:C:3604:TYR:CD2	2.37	0.60
3:D:2879:ALA:HB1	3:D:2919:ASP:HB3	1.83	0.60
3:D:3384:LYS:H	3:D:3387:ALA:HB3	1.67	0.60
3:D:3630:ARG:HH22	3:D:3861:GLU:HA	1.66	0.60
3:B:1699:GLU:HG3	3:B:1810:LYS:HE3	1.83	0.60
3:B:2879:ALA:HB1	3:B:2919:ASP:HB3	1.84	0.60
1:L:3:GLN:HG3	6:L:212:HOH:O	2.02	0.60
3:A:1658:ASP:OD2	6:A:5720:HOH:O	2.16	0.60
3:D:4075:GLU:HA	3:D:4078:GLN:HB2	1.83	0.60
3:B:506:TYR:OH	6:B:5719:HOH:O	2.17	0.60
3:B:1986:MET:HG2	3:B:1991:THR:HB	1.84	0.60
3:B:2470:ILE:HG22	3:B:2525:GLY:HA3	1.82	0.60
3:B:3630:ARG:HH22	3:B:3861:GLU:HA	1.65	0.60
2:E:5:ILE:HD11	2:E:63:GLY:HA2	1.84	0.60
3:A:2440:MET:HA	3:A:2440:MET:HE3	1.83	0.60
3:A:670:GLU:HA	3:A:740:PRO:HG3	1.82	0.59
3:B:3540:TYR:HB3	3:B:3604:TYR:CD1	2.36	0.59
3:C:201:ASN:OD1	6:C:5709:HOH:O	2.15	0.59
3:D:2440:MET:HA	3:D:2440:MET:HE3	1.83	0.59
3:B:1797:ARG:NH2	6:B:5752:HOH:O	2.34	0.59
3:B:4075:GLU:HA	3:B:4078:GLN:HB2	1.83	0.59
3:C:1163:THR:HG22	3:C:1168:VAL:HA	1.85	0.59
3:D:2642:LYS:HB2	3:D:2698:MET:HE1	1.84	0.59
3:C:3101:GLU:HG3	3:C:3167:ARG:HH22	1.67	0.59
3:B:3834:ALA:O	3:B:3838:THR:HG23	2.02	0.59
1:J:81:SER:HB3	6:J:232:HOH:O	2.02	0.59
3:C:4680:LYS:HD2	3:C:4686:LEU:HD22	1.83	0.59
3:C:2614:ILE:HG23	3:C:2618:MET:HE3	1.85	0.59
3:C:2788:HIS:HB3	3:C:2790:MET:SD	2.42	0.59
3:D:1163:THR:HG22	3:D:1168:VAL:HA	1.85	0.59
3:B:1163:THR:HG22	3:B:1168:VAL:HA	1.84	0.59
3:A:1505:GLN:HG3	3:A:1508:ARG:HH21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4075:GLU:HA	3:A:4078:GLN:HB2	1.83	0.59
3:C:1699:GLU:HG3	3:C:1810:LYS:HE3	1.83	0.59
3:C:4075:GLU:HA	3:C:4078:GLN:HB2	1.83	0.59
3:C:2879:ALA:HB1	3:C:2919:ASP:HB3	1.85	0.59
3:B:1680:ARG:HD3	3:B:1797:ARG:HB2	1.84	0.59
3:B:2116:LEU:O	3:B:2120:MET:HG3	2.02	0.59
1:I:132:GLY:N	6:I:209:HOH:O	2.36	0.58
3:C:894:GLY:HA3	3:C:903:LEU:HD13	1.86	0.58
3:B:3053:ARG:HB3	3:B:3056:LEU:HB2	1.85	0.58
3:C:3053:ARG:HB3	3:C:3056:LEU:HB2	1.85	0.58
3:B:4721:LYS:HD3	3:B:4741:LEU:HB3	1.84	0.58
3:A:201:ASN:OD1	6:A:5721:HOH:O	2.17	0.58
3:A:823:LEU:HB2	3:A:1617:THR:HG21	1.85	0.58
3:A:3834:ALA:O	3:A:3838:THR:HG23	2.03	0.58
3:C:3834:ALA:O	3:C:3838:THR:HG23	2.03	0.58
3:D:1505:GLN:HG3	3:D:1508:ARG:HH21	1.67	0.58
3:D:3834:ALA:O	3:D:3838:THR:HG23	2.03	0.58
3:D:2355:ARG:NH2	6:D:5737:HOH:O	2.26	0.58
3:B:3101:GLU:HG3	3:B:3167:ARG:HH22	1.66	0.58
2:H:5:ILE:HD11	2:H:63:GLY:HA2	1.86	0.58
3:C:1680:ARG:HD3	3:C:1797:ARG:HB2	1.84	0.58
3:A:1163:THR:HG22	3:A:1168:VAL:HA	1.85	0.58
3:C:2639:MET:HE3	3:C:2640:PRO:HD3	1.85	0.58
3:D:3604:TYR:O	3:D:3608:GLN:HG2	2.04	0.58
1:I:49:GLN:CB	6:I:227:HOH:O	2.51	0.58
3:C:1168:VAL:HG11	3:C:1176:GLU:HG3	1.85	0.58
3:C:1575:LEU:HD13	3:C:1579:MET:HE3	1.86	0.58
3:B:1505:GLN:HG3	3:B:1508:ARG:HH21	1.67	0.58
3:D:4773:VAL:O	3:D:4777:ILE:HD12	2.04	0.58
3:B:1168:VAL:HG11	3:B:1176:GLU:HG2	1.86	0.58
3:B:4104:THR:O	3:B:4108:ILE:HG12	2.04	0.58
3:A:3053:ARG:HB3	3:A:3056:LEU:HB2	1.85	0.58
3:C:12:GLN:HG2	6:C:6345:HOH:O	2.04	0.58
3:C:1116:GLY:HA3	3:C:1132:TRP:HB3	1.85	0.58
3:D:4001:MET:HE2	3:D:4057:MET:HB3	1.85	0.58
2:G:5:ILE:HD11	2:G:63:GLY:HA2	1.85	0.58
2:G:57:ILE:HG13	2:G:60:PHE:HB2	1.86	0.58
3:A:3604:TYR:O	3:A:3608:GLN:HG2	2.03	0.57
3:D:1575:LEU:HD13	3:D:1579:MET:HE3	1.86	0.57
1:K:99:TYR:CB	6:K:231:HOH:O	2.52	0.57
3:C:823:LEU:HB2	3:C:1617:THR:HG21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2626:LEU:HD22	3:A:2640:PRO:HB3	1.86	0.57
3:C:2250:MET:HA	3:C:2250:MET:HE2	1.87	0.57
3:D:4721:LYS:HD3	3:D:4741:LEU:HB3	1.85	0.57
3:A:4104:THR:O	3:A:4108:ILE:HG12	2.04	0.57
3:C:399:GLN:O	3:C:403:MET:HG3	2.04	0.57
3:C:2813:LEU:HA	3:C:2816:MET:HG2	1.86	0.57
3:D:2336:ARG:NH2	6:D:5757:HOH:O	2.36	0.57
3:D:4104:THR:O	3:D:4108:ILE:HG12	2.05	0.57
3:C:4721:LYS:HD3	3:C:4741:LEU:HB3	1.87	0.57
3:D:3085:PRO:HG2	3:D:3088:VAL:HG23	1.87	0.57
3:B:3812:VAL:O	3:B:3816:MET:HG3	2.04	0.57
1:I:82:GLU:CD	1:I:82:GLU:H	2.13	0.57
3:A:1575:LEU:HD13	3:A:1579:MET:HE3	1.86	0.57
3:A:3948:LYS:NZ	3:A:4009:GLN:HG2	2.20	0.57
3:A:484:LEU:HB2	6:A:6300:HOH:O	2.04	0.57
3:A:1680:ARG:HD3	3:A:1797:ARG:HB2	1.86	0.57
3:A:3630:ARG:C	3:A:3630:ARG:HD3	2.30	0.57
3:C:3604:TYR:O	3:C:3608:GLN:HG2	2.05	0.57
3:B:2614:ILE:HG23	3:B:2618:MET:HE3	1.87	0.57
3:D:12:GLN:HG2	6:D:6365:HOH:O	2.05	0.57
3:D:3053:ARG:HB3	3:D:3056:LEU:HB2	1.86	0.57
3:B:3093:ARG:O	3:B:3097:GLU:HG2	2.05	0.57
3:A:2208:MET:HE3	3:A:2256:TYR:CE2	2.40	0.56
3:C:3093:ARG:O	3:C:3097:GLU:HG2	2.05	0.56
3:C:4104:THR:O	3:C:4108:ILE:HG12	2.04	0.56
3:C:4773:VAL:O	3:C:4777:ILE:HD12	2.04	0.56
3:D:1680:ARG:HD3	3:D:1797:ARG:HB2	1.86	0.56
3:D:2813:LEU:HA	3:D:2816:MET:HG2	1.87	0.56
3:B:823:LEU:HB2	3:B:1617:THR:HG21	1.85	0.56
3:B:873:LYS:HD3	3:B:1049:TYR:HE2	1.69	0.56
3:A:3093:ARG:O	3:A:3097:GLU:HG2	2.05	0.56
3:C:3085:PRO:HG2	3:C:3088:VAL:HG23	1.86	0.56
3:D:823:LEU:HB2	3:D:1617:THR:HG21	1.85	0.56
3:B:975:VAL:CB	6:B:5732:HOH:O	2.47	0.56
2:H:50:ARG:HE	2:H:53:LYS:HG3	1.70	0.56
1:J:100:ILE:HD11	1:J:105:LEU:HD13	1.87	0.56
3:A:399:GLN:O	3:A:403:MET:HG3	2.05	0.56
3:A:1168:VAL:HG11	3:A:1176:GLU:HG3	1.87	0.56
3:D:2166:LEU:HD11	3:D:2206:THR:HG23	1.87	0.56
3:B:75:VAL:O	3:B:79:GLN:HG3	2.05	0.56
3:B:710:ASP:OD2	6:B:5722:HOH:O	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2970:SER:HA	3:B:2973:PHE:CE2	2.41	0.56
3:B:4773:VAL:O	3:B:4777:ILE:HD12	2.05	0.56
2:F:57:ILE:HG13	2:F:60:PHE:HB2	1.87	0.56
3:D:870:ILE:HD11	3:D:1051:TYR:CE1	2.41	0.56
3:A:3948:LYS:HZ1	3:A:4009:GLN:HG2	1.70	0.56
3:D:2208:MET:HG3	3:D:2250:MET:HE1	1.86	0.56
3:B:12:GLN:HG2	6:B:6368:HOH:O	2.06	0.56
3:B:1575:LEU:HD13	3:B:1579:MET:HE3	1.87	0.56
3:B:2166:LEU:HD11	3:B:2206:THR:HG23	1.86	0.56
3:A:1116:GLY:HA3	3:A:1132:TRP:HB3	1.86	0.56
3:D:3985:LEU:HD11	3:D:4026:MET:HE1	1.86	0.56
3:B:3362:ILE:HB	3:B:3437:MET:HE3	1.88	0.56
3:B:3604:TYR:O	3:B:3608:GLN:HG2	2.05	0.56
3:B:3630:ARG:C	3:B:3630:ARG:HD3	2.30	0.56
2:H:57:ILE:HG13	2:H:60:PHE:HB2	1.86	0.56
2:F:5:ILE:HD11	2:F:63:GLY:HA2	1.87	0.56
3:A:4721:LYS:HD3	3:A:4741:LEU:HB3	1.86	0.56
3:B:399:GLN:O	3:B:403:MET:HG3	2.06	0.56
3:A:2871:LEU:HD13	3:A:2874:MET:HE2	1.88	0.56
3:A:2970:SER:HA	3:A:2973:PHE:CE2	2.41	0.56
3:C:3362:ILE:HB	3:C:3437:MET:HE3	1.88	0.56
3:B:2626:LEU:HD22	3:B:2640:PRO:HB3	1.87	0.56
3:A:12:GLN:HG2	6:A:6370:HOH:O	2.06	0.56
3:C:2970:SER:HA	3:C:2973:PHE:CE2	2.41	0.56
3:D:2250:MET:HE2	3:D:2250:MET:HA	1.88	0.56
3:D:3093:ARG:O	3:D:3097:GLU:HG2	2.05	0.56
3:B:156:GLN:HA	3:B:156:GLN:HE21	1.71	0.56
3:A:156:GLN:HA	3:A:156:GLN:HE21	1.71	0.55
3:A:275:ARG:HG3	6:A:5896:HOH:O	2.06	0.55
3:B:201:ASN:OD1	6:B:5721:HOH:O	2.17	0.55
3:A:2813:LEU:HA	3:A:2816:MET:HG2	1.88	0.55
3:C:3630:ARG:HD3	3:C:3630:ARG:C	2.30	0.55
2:E:57:ILE:HG13	2:E:60:PHE:HB2	1.86	0.55
3:C:960:MET:HE1	3:C:967:PRO:HB3	1.89	0.55
3:D:3630:ARG:C	3:D:3630:ARG:HD3	2.30	0.55
3:D:4135:PRO:O	3:D:4139:ILE:HG23	2.07	0.55
3:A:3362:ILE:HB	3:A:3437:MET:HE3	1.89	0.55
3:C:275:ARG:HG3	6:C:5901:HOH:O	2.05	0.55
2:E:30:MET:HE3	2:E:34:GLY:HA2	1.89	0.55
3:A:939:VAL:HG13	3:A:1053:ILE:HG12	1.89	0.55
3:C:1492:CYS:SG	3:C:1494:MET:HG3	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3711:THR:HB	3:D:3713:LYS:HE2	1.89	0.55
3:B:275:ARG:HG3	6:B:5880:HOH:O	2.06	0.55
3:B:3553:LEU:HB2	3:B:3593:VAL:HG23	1.89	0.55
3:A:874:LEU:HD22	3:A:1046:LEU:HD21	1.89	0.55
3:B:2813:LEU:HA	3:B:2816:MET:HG2	1.89	0.55
3:C:1744:ALA:HB3	6:C:5973:HOH:O	2.07	0.55
3:C:1797:ARG:NH2	6:C:5757:HOH:O	2.39	0.55
3:D:2970:SER:HA	3:D:2973:PHE:CE2	2.41	0.55
3:B:2639:MET:HE3	3:B:2640:PRO:HD3	1.89	0.55
3:A:955:LEU:HB3	3:A:967:PRO:HB2	1.89	0.55
3:A:3312:LEU:HD22	3:A:3348:ARG:HG3	1.89	0.55
3:A:4135:PRO:O	3:A:4139:ILE:HG12	2.07	0.55
3:C:2166:LEU:HD11	3:C:2206:THR:HG23	1.88	0.55
3:C:2626:LEU:HD22	3:C:2640:PRO:HB3	1.89	0.55
3:D:156:GLN:HA	3:D:156:GLN:HE21	1.71	0.55
3:C:622:THR:HG23	3:C:626:LEU:HD22	1.89	0.55
3:D:13:PHE:HE2	3:D:164:ARG:HD2	1.71	0.55
3:D:275:ARG:HG3	6:D:5900:HOH:O	2.05	0.55
3:D:399:GLN:O	3:D:403:MET:HG3	2.06	0.55
3:D:4003:LEU:HD21	3:D:4012:LEU:HD23	1.89	0.55
3:C:3546:ASP:HB3	3:C:3550:ARG:HH21	1.72	0.55
3:B:622:THR:HG23	3:B:626:LEU:HD22	1.89	0.55
3:B:2545:GLU:HG3	6:B:6248:HOH:O	2.07	0.55
3:D:3312:LEU:HD22	3:D:3348:ARG:HG3	1.89	0.54
3:B:1116:GLY:HA3	3:B:1132:TRP:HB3	1.87	0.54
3:C:4052:SER:HA	3:C:4163:PHE:HZ	1.73	0.54
3:D:622:THR:HG23	3:D:626:LEU:HD22	1.89	0.54
3:D:1797:ARG:NH2	6:D:5774:HOH:O	2.40	0.54
3:B:4135:PRO:O	3:B:4139:ILE:HG23	2.07	0.54
3:C:156:GLN:HE21	3:C:156:GLN:HA	1.71	0.54
3:D:484:LEU:HB3	6:D:6290:HOH:O	2.06	0.54
3:D:1116:GLY:HA3	3:D:1132:TRP:HB3	1.87	0.54
3:C:892:THR:HG22	3:C:893:TYR:H	1.73	0.54
2:F:30:MET:HE3	2:F:34:GLY:HA2	1.90	0.54
3:D:1744:ALA:HB3	6:D:5978:HOH:O	2.07	0.54
1:J:49:GLN:CB	6:J:230:HOH:O	2.54	0.54
3:A:622:THR:HG23	3:A:626:LEU:HD22	1.89	0.54
3:A:2166:LEU:HD11	3:A:2206:THR:HG23	1.88	0.54
3:C:4151:SER:HB3	3:C:4164:LEU:HD21	1.89	0.54
3:A:4001:MET:HE1	3:A:4061:PHE:HB2	1.89	0.54
3:D:4067:LYS:O	3:D:4071:ILE:HB	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4151:SER:HB3	3:D:4164:LEU:HD21	1.89	0.54
3:A:1448:VAL:HG22	3:A:1554:VAL:HG23	1.90	0.54
3:A:1744:ALA:HB3	6:A:5981:HOH:O	2.07	0.54
3:A:3266:MET:HG3	3:A:3270:ILE:HG13	1.90	0.54
3:A:3553:LEU:HB2	3:A:3593:VAL:HG23	1.90	0.54
3:C:13:PHE:HE2	3:C:164:ARG:HD2	1.73	0.54
3:B:3312:LEU:HD22	3:B:3348:ARG:HG3	1.89	0.54
3:A:870:ILE:HD12	3:A:1051:TYR:CE1	2.43	0.53
3:C:1448:VAL:HG22	3:C:1554:VAL:HG23	1.90	0.53
3:C:2228:MET:HE2	3:C:2232:CYS:SG	2.48	0.53
3:C:4934:GLY:HA2	3:B:4937:ILE:HG12	1.90	0.53
3:D:2545:GLU:HG3	6:D:6286:HOH:O	2.07	0.53
3:D:3362:ILE:HB	3:D:3437:MET:HE3	1.90	0.53
3:B:2250:MET:HE2	3:B:2250:MET:HA	1.91	0.53
3:A:331:VAL:HG23	6:A:6309:HOH:O	2.08	0.53
3:C:636:ASN:HB2	3:C:702:TRP:CZ3	2.44	0.53
3:B:1448:VAL:HG22	3:B:1554:VAL:HG23	1.90	0.53
3:C:2552:ARG:HG3	6:C:5980:HOH:O	2.08	0.53
3:C:4937:ILE:HG12	3:D:4934:GLY:HA2	1.91	0.53
3:D:3034:LYS:HD3	3:D:3034:LYS:N	2.24	0.53
3:B:1744:ALA:HB3	6:B:5975:HOH:O	2.07	0.53
3:A:2519:LEU:HD22	3:A:2578:MET:HE1	1.89	0.53
3:C:955:LEU:HB3	3:C:967:PRO:HB2	1.89	0.53
3:C:2967:MET:HE1	3:C:3046:LEU:HD13	1.91	0.53
3:C:3266:MET:HG3	3:C:3270:ILE:HG13	1.90	0.53
3:D:4583:SER:HB2	3:D:4631:PHE:HE2	1.72	0.53
1:K:-1:HIS:CD2	6:K:202:HOH:O	2.53	0.53
3:A:2639:MET:HE3	3:A:2640:PRO:HD3	1.90	0.53
3:A:4934:GLY:HA2	3:D:4937:ILE:HG12	1.90	0.53
3:A:4937:ILE:HG12	3:B:4934:GLY:HA2	1.90	0.53
3:C:3034:LYS:N	3:C:3034:LYS:HD3	2.24	0.53
3:D:636:ASN:HB2	3:D:702:TRP:CZ3	2.44	0.53
3:D:2167:ILE:HD11	6:D:6257:HOH:O	2.09	0.53
3:D:2626:LEU:HD22	3:D:2640:PRO:HB3	1.89	0.53
3:D:2788:HIS:ND1	3:D:2789:PRO:HD2	2.22	0.53
3:B:3066:ASN:O	3:B:3070:ILE:HD12	2.09	0.53
3:B:3266:MET:HG3	3:B:3270:ILE:HG13	1.90	0.53
3:A:13:PHE:HE1	3:A:164:ARG:HD2	1.74	0.53
3:A:2250:MET:HE2	3:A:2250:MET:HA	1.90	0.53
3:B:2519:LEU:HD22	3:B:2578:MET:HE1	1.91	0.53
3:B:2552:ARG:HG3	6:B:6000:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2788:HIS:ND1	3:B:2789:PRO:HD2	2.23	0.53
3:B:3625:SER:O	3:B:3629:ARG:HG3	2.09	0.53
1:K:100:ILE:HD11	1:K:105:LEU:HD13	1.91	0.53
3:A:2336:ARG:HG2	3:A:2432:LEU:HB2	1.90	0.53
3:D:3553:LEU:HB2	3:D:3593:VAL:HG23	1.90	0.53
3:A:892:THR:HG22	3:A:893:TYR:H	1.74	0.53
3:A:1212:ARG:NH2	6:A:5710:HOH:O	2.10	0.53
3:A:2552:ARG:HG3	6:A:5988:HOH:O	2.09	0.53
3:C:710:ASP:OD2	6:C:5712:HOH:O	2.19	0.53
3:C:2886:TRP:HH2	3:C:2904:LEU:HD12	1.74	0.53
3:D:892:THR:HG22	3:D:893:TYR:H	1.73	0.53
3:B:909:ASN:HA	3:B:965:TYR:HD1	1.73	0.53
3:B:2753:SER:HA	3:B:2756:ASN:HD21	1.74	0.53
3:B:2785:LEU:C	3:B:2786:LYS:HD3	2.34	0.53
3:B:4067:LYS:O	3:B:4071:ILE:HB	2.09	0.53
1:I:1:HIS:O	1:I:3:GLN:HG2	2.08	0.53
3:B:2228:MET:HE2	3:B:2232:CYS:SG	2.49	0.53
2:E:45:LYS:HD2	2:E:45:LYS:O	2.10	0.52
3:A:636:ASN:HB2	3:A:702:TRP:CZ3	2.44	0.52
3:A:2753:SER:HA	3:A:2756:ASN:HD21	1.74	0.52
3:A:909:ASN:HA	3:A:965:TYR:HD1	1.72	0.52
3:D:874:LEU:HD22	3:D:1046:LEU:HD21	1.91	0.52
3:D:1448:VAL:HG22	3:D:1554:VAL:HG23	1.90	0.52
3:D:2753:SER:HA	3:D:2756:ASN:HD21	1.74	0.52
3:D:2871:LEU:HD13	3:D:2874:MET:HE2	1.91	0.52
3:B:874:LEU:HD22	3:B:1046:LEU:HD21	1.90	0.52
3:B:892:THR:HG22	3:B:893:TYR:H	1.74	0.52
3:A:2167:ILE:HD11	6:A:6257:HOH:O	2.08	0.52
3:C:2545:GLU:HG3	6:C:6296:HOH:O	2.09	0.52
3:C:3312:LEU:HD22	3:C:3348:ARG:HG3	1.91	0.52
3:D:2552:ARG:HG3	6:D:5979:HOH:O	2.08	0.52
3:B:4093:PHE:O	3:B:4097:MET:HG2	2.09	0.52
3:A:4991:PHE:HE2	3:A:5010:VAL:HG11	1.75	0.52
3:C:2519:LEU:HD22	3:C:2578:MET:HE1	1.90	0.52
3:A:3993:LEU:HG	3:A:4023:MET:HE1	1.92	0.52
3:C:75:VAL:O	3:C:79:GLN:HG3	2.10	0.52
3:C:2753:SER:HA	3:C:2756:ASN:HD21	1.74	0.52
3:D:3625:SER:O	3:D:3629:ARG:HG3	2.09	0.52
1:J:1:HIS:CD2	6:J:202:HOH:O	2.58	0.52
3:A:2886:TRP:HH2	3:A:2904:LEU:HD12	1.75	0.52
3:A:4680:LYS:HD2	3:A:4686:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4773:VAL:O	3:A:4777:ILE:HD12	2.10	0.52
3:C:156:GLN:HA	3:C:156:GLN:NE2	2.25	0.52
3:C:3563:VAL:HA	3:C:3569:LEU:HD22	1.92	0.52
3:D:2519:LEU:HD22	3:D:2578:MET:HE1	1.91	0.52
3:B:4991:PHE:HE2	3:B:5010:VAL:HG11	1.75	0.52
3:C:2165:LEU:HD11	3:C:2177:LEU:HD23	1.92	0.52
3:B:2644:LEU:HD13	3:B:2678:LEU:HD21	1.91	0.52
1:L:82:GLU:H	1:L:82:GLU:CD	2.18	0.52
3:A:2545:GLU:HG3	6:A:6287:HOH:O	2.09	0.52
3:A:3085:PRO:HG2	3:A:3088:VAL:HG23	1.92	0.52
3:B:4090:LYS:HG2	3:B:4123:ILE:HD11	1.92	0.52
3:B:4151:SER:HB3	3:B:4164:LEU:HD21	1.91	0.52
2:F:45:LYS:HD2	2:F:45:LYS:O	2.10	0.52
1:K:82:GLU:CD	1:K:82:GLU:H	2.18	0.51
3:C:459:LEU:HD23	3:C:460:GLN:N	2.25	0.51
3:D:4948:GLU:HG2	6:D:6322:HOH:O	2.10	0.51
3:B:2167:ILE:HD11	6:B:6241:HOH:O	2.09	0.51
1:L:30:LYS:C	6:L:219:HOH:O	2.53	0.51
3:A:2644:LEU:HD13	3:A:2678:LEU:HD21	1.91	0.51
3:C:2644:LEU:HD13	3:C:2678:LEU:HD21	1.92	0.51
3:C:3553:LEU:HB2	3:C:3593:VAL:HG23	1.93	0.51
3:D:3563:VAL:HA	3:D:3569:LEU:HD22	1.91	0.51
3:B:636:ASN:HB2	3:B:702:TRP:CZ3	2.44	0.51
3:A:3883:ASP:OD2	6:A:5723:HOH:O	2.19	0.51
3:C:2742:THR:HB	3:C:2814:LYS:HD2	1.92	0.51
3:D:2208:MET:HG2	3:D:2236:LEU:HD11	1.91	0.51
3:D:2294:ASP:OD2	6:D:5722:HOH:O	2.19	0.51
3:D:3066:ASN:O	3:D:3070:ILE:HD12	2.10	0.51
3:B:894:GLY:HA3	3:B:903:LEU:HD13	1.93	0.51
1:J:92:PHE:CD1	1:J:104:GLU:HG2	2.46	0.51
3:A:4003:LEU:HD21	3:A:4012:LEU:HD23	1.93	0.51
3:D:2644:LEU:HD13	3:D:2678:LEU:HD21	1.91	0.51
3:B:4583:SER:HB2	3:B:4631:PHE:HE2	1.76	0.51
2:H:45:LYS:HD2	2:H:45:LYS:O	2.10	0.51
1:I:143:GLN:CB	6:I:207:HOH:O	2.58	0.51
3:C:874:LEU:HB3	3:C:925:SER:OG	2.10	0.51
3:C:2716:ASP:HB3	3:C:2719:TYR:HB2	1.92	0.51
3:C:2753:SER:HA	3:C:2756:ASN:ND2	2.26	0.51
3:C:3066:ASN:O	3:C:3070:ILE:HD12	2.10	0.51
3:D:75:VAL:O	3:D:79:GLN:HG3	2.09	0.51
3:D:5017:ARG:NH1	6:D:5772:HOH:O	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3989:VAL:HG13	3:B:4023:MET:HE3	1.93	0.51
1:J:37:ARG:HG3	6:J:220:HOH:O	1.88	0.51
3:A:4151:SER:HB3	3:A:4164:LEU:HD21	1.92	0.51
3:C:982:THR:HA	3:C:985:VAL:HG12	1.93	0.51
3:C:4160:LEU:O	3:C:4164:LEU:HD22	2.10	0.51
3:D:3416:VAL:HG11	3:D:3517:MET:HG2	1.93	0.51
3:B:1424:PRO:HA	3:B:1427:ILE:HG22	1.93	0.51
3:B:3085:PRO:HG2	3:B:3088:VAL:HG23	1.93	0.51
3:A:3132:THR:HA	3:A:3136:LEU:HB3	1.93	0.51
3:A:3563:VAL:HA	3:A:3569:LEU:HD22	1.93	0.51
3:D:982:THR:HA	3:D:985:VAL:HG12	1.93	0.51
3:D:2753:SER:HA	3:D:2756:ASN:ND2	2.26	0.51
3:B:2886:TRP:HH2	3:B:2904:LEU:HD12	1.75	0.51
3:C:1694:LEU:HB3	3:C:1715:LEU:HD12	1.93	0.51
3:C:3722:TYR:CE1	3:C:3778:MET:HE3	2.46	0.51
3:C:4069:LYS:HZ2	3:C:4133:GLN:HG2	1.76	0.51
3:C:1619:ARG:HH12	3:C:1622:GLU:HG2	1.75	0.51
3:D:894:GLY:HA3	3:D:903:LEU:HD13	1.93	0.51
3:D:2785:LEU:C	3:D:2786:LYS:HD3	2.36	0.51
3:A:392[A]:ARG:NH2	6:A:5708:HOH:O	2.08	0.51
3:A:1272:LEU:HD22	3:A:1289:LEU:HD11	1.93	0.51
3:A:2753:SER:HA	3:A:2756:ASN:ND2	2.26	0.51
3:A:3985:LEU:HD11	3:A:4026:MET:HE1	1.92	0.51
3:A:4090:LYS:HG2	3:A:4123:ILE:HD11	1.92	0.51
3:C:2167:ILE:HD11	6:C:6242:HOH:O	2.11	0.51
3:D:156:GLN:HA	3:D:156:GLN:NE2	2.25	0.51
3:B:1272:LEU:HD22	3:B:1289:LEU:HD11	1.93	0.51
3:D:909:ASN:HA	3:D:965:TYR:HD1	1.76	0.50
3:D:1694:LEU:HB3	3:D:1715:LEU:HD12	1.93	0.50
3:D:2639:MET:HE3	3:D:2640:PRO:HD3	1.93	0.50
3:D:4160:LEU:O	3:D:4164:LEU:HD22	2.10	0.50
3:B:156:GLN:HA	3:B:156:GLN:NE2	2.25	0.50
3:B:2753:SER:HA	3:B:2756:ASN:ND2	2.26	0.50
3:B:4003:LEU:HD21	3:B:4012:LEU:HD23	1.93	0.50
3:B:4160:LEU:O	3:B:4164:LEU:HD22	2.11	0.50
3:A:156:GLN:HA	3:A:156:GLN:NE2	2.25	0.50
3:A:4160:LEU:O	3:A:4164:LEU:HD22	2.11	0.50
3:C:3107:VAL:HG22	3:C:3175:LEU:HD11	1.94	0.50
3:C:4181:ILE:HG13	3:C:4193:ILE:HB	1.94	0.50
3:C:4991:PHE:HE2	3:C:5010:VAL:HG11	1.74	0.50
3:D:2886:TRP:HH2	3:D:2904:LEU:HD12	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4087:LEU:HB3	3:D:4122:MET:HE1	1.93	0.50
3:B:1694:LEU:HB3	3:B:1715:LEU:HD12	1.93	0.50
1:K:60:ASN:HB3	6:K:205:HOH:O	2.11	0.50
3:B:987:ARG:CD	6:B:5720:HOH:O	2.59	0.50
3:B:1854:PHE:HD1	3:B:1858:ASP:HB3	1.75	0.50
3:B:3996:PHE:CD2	3:B:4020:GLN:HG3	2.46	0.50
2:E:45:LYS:HD2	2:E:45:LYS:C	2.36	0.50
3:C:3416:VAL:HG11	3:C:3517:MET:HG2	1.93	0.50
3:D:797:HIS:CG	3:D:821:LEU:HD23	2.46	0.50
3:D:3132:THR:HA	3:D:3136:LEU:HB3	1.94	0.50
3:B:955:LEU:HB3	3:B:967:PRO:HB2	1.92	0.50
3:B:1179:PHE:HB2	3:B:1182:ILE:HD11	1.94	0.50
1:J:94:LYS:HD2	6:J:221:HOH:O	2.12	0.50
3:A:650:VAL:HA	3:A:658:GLN:NE2	2.27	0.50
3:A:894:GLY:HA3	3:A:903:LEU:HD13	1.93	0.50
3:A:4181:ILE:HG13	3:A:4193:ILE:HB	1.94	0.50
3:C:3862:ASP:HB3	6:C:6459:HOH:O	2.12	0.50
3:D:1179:PHE:HB2	3:D:1182:ILE:HD11	1.93	0.50
3:D:1272:LEU:HD22	3:D:1289:LEU:HD11	1.93	0.50
3:B:797:HIS:CG	3:B:821:LEU:HD23	2.46	0.50
3:B:2004:GLU:O	3:B:2008:MET:HG3	2.12	0.50
3:A:152:PRO:HB3	3:A:157:ARG:HB2	1.93	0.50
3:C:2004:GLU:O	3:C:2008:MET:HG3	2.12	0.50
3:C:3996:PHE:CD2	3:C:4020:GLN:HG3	2.47	0.50
3:B:4052:SER:O	3:B:4056:GLU:HG3	2.11	0.50
3:B:4181:ILE:HG13	3:B:4193:ILE:HB	1.94	0.50
3:B:2599:GLN:O	3:B:2603:ILE:HG13	2.12	0.50
3:B:3416:VAL:HG11	3:B:3517:MET:HG2	1.93	0.50
2:H:45:LYS:HD2	2:H:45:LYS:C	2.36	0.50
3:C:331:VAL:HG23	6:C:6372:HOH:O	2.11	0.50
3:C:459:LEU:HD21	3:C:463:GLU:OE1	2.12	0.50
3:C:1179:PHE:HB2	3:C:1182:ILE:HD11	1.94	0.50
3:C:3281:LEU:HD12	3:C:3315:LEU:HD22	1.93	0.50
3:D:2921:GLU:O	3:D:2925:GLU:HG2	2.12	0.50
3:D:3865:VAL:HG11	6:D:6129:HOH:O	2.11	0.50
3:B:2165:LEU:HD11	3:B:2177:LEU:HD23	1.93	0.50
3:A:797:HIS:CG	3:A:821:LEU:HD23	2.47	0.50
3:C:2241:ARG:NH2	6:C:5749:HOH:O	2.38	0.50
3:D:4090:LYS:HG2	3:D:4123:ILE:HD11	1.93	0.50
3:B:13:PHE:HE2	3:B:164:ARG:HD2	1.77	0.50
3:B:1575:LEU:O	3:B:1579:MET:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2599:GLN:O	3:A:2603:ILE:HG13	2.12	0.49
3:C:2312:MET:HE2	3:C:2316:LYS:HE3	1.93	0.49
3:C:2599:GLN:O	3:C:2603:ILE:HG13	2.12	0.49
3:C:3591:LYS:O	3:C:3595:ARG:HG2	2.12	0.49
3:D:650:VAL:HA	3:D:658:GLN:NE2	2.26	0.49
2:F:45:LYS:HD2	2:F:45:LYS:C	2.36	0.49
1:J:30:LYS:C	6:J:227:HOH:O	2.54	0.49
3:A:978:THR:HG22	3:A:980:ALA:H	1.77	0.49
3:A:3591:LYS:O	3:A:3595:ARG:HG2	2.12	0.49
3:D:4052:SER:O	3:D:4056:GLU:HG3	2.12	0.49
3:B:152:PRO:HB3	3:B:157:ARG:HB2	1.92	0.49
3:B:3352:GLU:CD	3:B:3352:GLU:H	2.20	0.49
3:B:4948:GLU:HG2	6:B:6311:HOH:O	2.11	0.49
1:L:143:GLN:CB	6:L:202:HOH:O	2.60	0.49
3:D:4634:GLU:CD	3:D:4639:MET:HB2	2.37	0.49
3:D:152:PRO:HB3	3:D:157:ARG:HB2	1.93	0.49
3:D:3281:LEU:HD12	3:D:3315:LEU:HD22	1.93	0.49
3:B:2214:VAL:HG21	3:B:2228:MET:SD	2.52	0.49
3:B:2312:MET:HE2	3:B:2316:LYS:HE3	1.94	0.49
3:B:3132:THR:HA	3:B:3136:LEU:HB3	1.93	0.49
3:B:4680:LYS:HD2	3:B:4686:LEU:HD22	1.93	0.49
3:A:3281:LEU:HD12	3:A:3315:LEU:HD22	1.93	0.49
3:C:1272:LEU:HD22	3:C:1289:LEU:HD11	1.93	0.49
3:C:3536:ALA:HB2	3:C:3553:LEU:HD11	1.94	0.49
3:C:3720:TYR:HA	3:C:3723:MET:HE3	1.95	0.49
3:C:3990:VAL:HG23	3:C:4047:MET:HG2	1.94	0.49
3:D:4181:ILE:HG13	3:D:4193:ILE:HB	1.94	0.49
3:B:3281:LEU:HD12	3:B:3315:LEU:HD22	1.93	0.49
3:A:3066:ASN:O	3:A:3070:ILE:HD12	2.12	0.49
3:A:3416:VAL:HG11	3:A:3517:MET:HG2	1.94	0.49
3:D:957:LYS:O	3:D:960:MET:HG2	2.13	0.49
3:D:3107:VAL:HG22	3:D:3175:LEU:HD11	1.94	0.49
1:K:130:ILE:HD13	6:K:238:HOH:O	2.12	0.49
3:D:1286:MET:HE1	3:D:1553:PHE:HB3	1.94	0.49
3:B:650:VAL:HA	3:B:658:GLN:NE2	2.27	0.49
3:B:2921:GLU:O	3:B:2925:GLU:HG2	2.12	0.49
1:L:13:LYS:HG2	3:D:2189:LYS:HB3	1.94	0.49
3:A:331:VAL:CG2	6:A:6309:HOH:O	2.60	0.49
3:A:2018:GLU:HG2	3:A:2028:ARG:NH1	2.28	0.49
3:A:2312:MET:HE2	3:A:2316:LYS:HE3	1.94	0.49
3:A:3318:ASN:ND2	6:A:5754:HOH:O	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4000:MET:HE1	3:A:4058:ILE:HA	1.95	0.49
3:A:4634:GLU:CD	3:A:4639:MET:HB2	2.37	0.49
3:C:331:VAL:CG2	6:C:6372:HOH:O	2.60	0.49
3:C:650:VAL:HA	3:C:658:GLN:NE2	2.27	0.49
3:C:2765:LYS:NZ	3:C:2860:PRO:HD2	2.28	0.49
3:C:3132:THR:HA	3:C:3136:LEU:HB3	1.94	0.49
3:C:4090:LYS:HG2	3:C:4123:ILE:HD11	1.94	0.49
3:D:408:ALA:HB2	3:D:483:MET:HE1	1.95	0.49
3:D:526:LEU:HD11	3:D:540:PHE:HZ	1.77	0.49
3:D:2599:GLN:O	3:D:2603:ILE:HG13	2.12	0.49
3:B:2018:GLU:HG2	3:B:2028:ARG:NH1	2.27	0.49
3:B:3536:ALA:HB2	3:B:3553:LEU:HD11	1.95	0.49
1:J:79:THR:CB	6:J:203:HOH:O	2.61	0.49
3:A:1089:TYR:HD2	3:A:1152:MET:HG3	1.78	0.49
3:A:1286:MET:HE1	3:A:1553:PHE:HB3	1.95	0.49
3:C:797:HIS:CG	3:C:821:LEU:HD23	2.47	0.49
3:D:684:VAL:HG22	3:D:781:VAL:HG12	1.95	0.49
3:D:3722:TYR:CE1	3:D:3778:MET:HE3	2.46	0.49
3:B:2967:MET:HE1	3:B:3046:LEU:HD13	1.94	0.49
3:A:3107:VAL:HG22	3:A:3175:LEU:HD11	1.95	0.49
3:C:684:VAL:HG22	3:C:781:VAL:HG12	1.95	0.49
3:C:1089:TYR:HD2	3:C:1152:MET:HG3	1.78	0.49
3:D:1089:TYR:HD2	3:D:1152:MET:HG3	1.78	0.49
3:B:3974:THR:O	3:B:3978:GLN:HG2	2.13	0.49
1:K:79:THR:CB	6:K:207:HOH:O	2.60	0.48
3:B:404:ILE:HG21	3:B:481:GLU:HG3	1.95	0.48
3:B:1089:TYR:HD2	3:B:1152:MET:HG3	1.78	0.48
3:B:4134:GLU:OE1	3:B:4135:PRO:HD3	2.13	0.48
3:A:1179:PHE:HB2	3:A:1182:ILE:HD11	1.95	0.48
3:A:3536:ALA:HB2	3:A:3553:LEU:HD11	1.96	0.48
3:C:1847:THR:O	3:C:1851:MET:HG3	2.12	0.48
3:C:2018:GLU:HG2	3:C:2028:ARG:NH1	2.27	0.48
3:C:3368:ARG:HG2	3:C:3401:LEU:HD13	1.95	0.48
3:C:3962:PHE:CZ	3:C:4023:MET:HG3	2.48	0.48
3:C:4634:GLU:CD	3:C:4639:MET:HB2	2.38	0.48
3:D:3989:VAL:HG13	3:D:4023:MET:HE3	1.94	0.48
3:B:3722:TYR:CE1	3:B:3778:MET:HE3	2.46	0.48
3:A:215:THR:HG22	3:A:273:HIS:HA	1.94	0.48
3:C:215:THR:HG22	3:C:273:HIS:HA	1.94	0.48
3:C:4047:MET:HB3	3:C:4047:MET:HE3	1.75	0.48
3:D:1977:TYR:CE1	3:D:1981:MET:HE3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3266:MET:HG3	3:D:3270:ILE:HG13	1.95	0.48
3:B:1286:MET:HE1	3:B:1553:PHE:HB3	1.95	0.48
3:B:1438:ARG:HB3	3:B:1563:GLN:HG2	1.94	0.48
3:B:4634:GLU:CD	3:B:4639:MET:HB2	2.38	0.48
1:K:130:ILE:CB	6:K:238:HOH:O	2.17	0.48
3:A:684:VAL:HG22	3:A:781:VAL:HG12	1.95	0.48
3:A:1694:LEU:HB3	3:A:1715:LEU:HD12	1.94	0.48
3:A:2369:ARG:HA	6:A:6145:HOH:O	2.13	0.48
3:A:2921:GLU:O	3:A:2925:GLU:HG2	2.13	0.48
3:A:3416:VAL:O	3:A:3420:ARG:HB2	2.13	0.48
3:A:3949:ARG:HB3	3:A:3949:ARG:HH11	1.78	0.48
3:A:4577:LEU:HD21	3:A:4806:ASN:HB3	1.96	0.48
3:C:2604:GLU:HB3	3:C:2639:MET:HG3	1.95	0.48
3:C:4003:LEU:HD21	3:C:4012:LEU:HD23	1.95	0.48
3:D:215:THR:HG22	3:D:273:HIS:HA	1.94	0.48
3:D:2312:MET:HE2	3:D:2316:LYS:HE3	1.95	0.48
3:B:215:THR:HG22	3:B:273:HIS:HA	1.94	0.48
3:B:684:VAL:HG22	3:B:781:VAL:HG12	1.95	0.48
3:B:978:THR:HG22	3:B:980:ALA:H	1.79	0.48
3:B:3416:VAL:O	3:B:3420:ARG:HB2	2.13	0.48
3:A:871:ARG:HH21	3:A:926:GLY:HA3	1.79	0.48
3:A:1438:ARG:HB3	3:A:1563:GLN:HG2	1.94	0.48
3:C:2608:MET:HE3	3:C:2608:MET:HB3	1.78	0.48
3:C:4627:MET:HB2	3:C:4628:VAL:H	1.53	0.48
3:B:2812:SER:HB2	3:B:2878:LEU:HD11	1.96	0.48
3:A:2330:ARG:HD3	6:A:5848:HOH:O	2.13	0.48
3:A:2332:LEU:O	3:A:2336:ARG:HG3	2.13	0.48
3:C:544:LEU:HD21	3:C:578:ILE:HD13	1.95	0.48
3:C:1854:PHE:HD1	3:C:1858:ASP:HB3	1.79	0.48
3:C:2214:VAL:HG21	3:C:2228:MET:SD	2.53	0.48
3:C:2526:PHE:O	3:C:2530:MET:HG3	2.14	0.48
3:D:978:THR:HG22	3:D:980:ALA:H	1.79	0.48
3:D:2018:GLU:HG2	3:D:2028:ARG:NH1	2.28	0.48
3:D:3996:PHE:CD2	3:D:4020:GLN:HG3	2.49	0.48
3:B:2871:LEU:HA	3:B:2874:MET:SD	2.53	0.48
3:A:2765:LYS:NZ	3:A:2860:PRO:HD2	2.28	0.48
3:C:404:ILE:HG21	3:C:481:GLU:HG3	1.96	0.48
3:C:642:THR:OG1	6:C:5713:HOH:O	2.20	0.48
3:C:3352:GLU:H	3:C:3352:GLU:CD	2.22	0.48
3:D:404:ILE:HG21	3:D:481:GLU:HG3	1.96	0.48
3:D:2522:LEU:O	3:D:2527:LEU:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4576:ILE:HG21	3:B:4643:LEU:HB2	1.96	0.48
1:I:105:LEU:O	1:I:109:MET:HG2	2.14	0.48
1:J:60:ASN:C	6:J:205:HOH:O	2.55	0.48
3:A:2214:VAL:HG21	3:A:2228:MET:SD	2.54	0.48
3:A:2522:LEU:O	3:A:2527:LEU:HB2	2.14	0.48
3:A:3352:GLU:H	3:A:3352:GLU:CD	2.22	0.48
3:D:1028:ASP:OD2	6:D:5723:HOH:O	2.20	0.48
3:D:2292:GLU:O	3:D:2296:GLU:HG3	2.14	0.48
3:B:2522:LEU:O	3:B:2527:LEU:HB2	2.14	0.48
3:A:404:ILE:HG21	3:A:481:GLU:HG3	1.96	0.48
3:C:972:LEU:HB2	3:C:1044:ARG:NH2	2.29	0.48
3:C:1575:LEU:O	3:C:1579:MET:HG3	2.14	0.48
3:C:4677:LEU:HD11	3:C:4687:TYR:HE2	1.78	0.48
3:C:5017:ARG:NH1	6:C:5766:HOH:O	2.43	0.48
3:D:544:LEU:HD21	3:D:578:ILE:HD13	1.95	0.48
3:D:2336:ARG:HE	3:D:2431:ASP:HB3	1.78	0.48
3:B:3666:ASP:O	3:B:3666:ASP:OD2	2.31	0.48
1:I:72:MET:HE2	1:I:72:MET:HA	1.96	0.48
3:A:544:LEU:HD21	3:A:578:ILE:HD13	1.95	0.48
3:A:901:LYS:HD3	3:A:901:LYS:HA	1.65	0.48
3:C:82:LEU:HD13	3:C:144:GLU:HG2	1.96	0.48
3:C:408:ALA:HB2	3:C:483:MET:HE1	1.96	0.48
3:C:2522:LEU:O	3:C:2527:LEU:HB2	2.14	0.48
3:D:82:LEU:HD13	3:D:144:GLU:HG2	1.96	0.48
3:D:3416:VAL:O	3:D:3420:ARG:HB2	2.13	0.48
3:B:1505:GLN:HA	3:B:1508:ARG:HH21	1.79	0.48
3:B:3563:VAL:HA	3:B:3569:LEU:HD22	1.96	0.48
3:A:82:LEU:HD13	3:A:144:GLU:HG2	1.95	0.47
3:A:1854:PHE:HD1	3:A:1858:ASP:HB3	1.79	0.47
3:D:2604:GLU:HB3	3:D:2639:MET:HG3	1.95	0.47
3:D:2812:SER:HB2	3:D:2878:LEU:HD11	1.94	0.47
2:G:15:THR:HG22	2:G:107:LEU:HD12	1.96	0.47
3:C:152:PRO:HB3	3:C:157:ARG:HB2	1.94	0.47
3:D:1424:PRO:HA	3:D:1427:ILE:HG22	1.96	0.47
3:D:4134:GLU:OE1	3:D:4135:PRO:HD3	2.13	0.47
3:B:2765:LYS:NZ	3:B:2860:PRO:HD2	2.29	0.47
3:A:1530:THR:HG22	3:A:1535:GLU:HA	1.96	0.47
3:A:4047:MET:HE3	3:A:4047:MET:HB3	1.74	0.47
3:C:2369:ARG:HA	6:C:6130:HOH:O	2.14	0.47
3:C:4577:LEU:HD21	3:C:4806:ASN:HB3	1.96	0.47
3:D:1438:ARG:HB3	3:D:1563:GLN:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2765:LYS:NZ	3:D:2860:PRO:HD2	2.29	0.47
3:D:3352:GLU:H	3:D:3352:GLU:CD	2.22	0.47
3:D:4677:LEU:HD11	3:D:4687:TYR:HE2	1.78	0.47
3:B:544:LEU:HD21	3:B:578:ILE:HD13	1.95	0.47
3:B:3107:VAL:HG22	3:B:3175:LEU:HD11	1.95	0.47
3:B:3318:ASN:ND2	6:B:5760:HOH:O	2.37	0.47
3:B:4087:LEU:HB3	3:B:4122:MET:HE1	1.97	0.47
3:A:3588:ASP:HB2	3:A:3590:GLU:OE2	2.15	0.47
3:A:3865:VAL:HG11	6:A:6018:HOH:O	2.13	0.47
3:A:4052:SER:O	3:A:4056:GLU:HG3	2.14	0.47
3:C:3416:VAL:O	3:C:3420:ARG:HB2	2.13	0.47
3:B:2584:HIS:O	3:B:2588:ARG:HG3	2.14	0.47
3:B:2785:LEU:O	3:B:2787:THR:HG23	2.14	0.47
3:B:4577:LEU:HD21	3:B:4806:ASN:HB3	1.96	0.47
2:H:43:ARG:HE	2:H:45:LYS:HE3	1.80	0.47
3:A:526:LEU:HD11	3:A:540:PHE:HZ	1.78	0.47
3:A:1424:PRO:HA	3:A:1427:ILE:HG22	1.96	0.47
3:A:1575:LEU:O	3:A:1579:MET:HG3	2.15	0.47
3:C:909:ASN:HA	3:C:965:TYR:HD1	1.79	0.47
3:C:2639:MET:HE3	3:C:2639:MET:HB3	1.81	0.47
3:C:4948:GLU:HG2	6:C:6343:HOH:O	2.13	0.47
3:B:2679:PHE:HB2	3:B:2706:ILE:HG21	1.97	0.47
3:A:1980:LEU:HD21	3:A:1994:ARG:HB3	1.94	0.47
3:A:2812:SER:HB2	3:A:2878:LEU:HD11	1.96	0.47
3:A:4677:LEU:HD11	3:A:4687:TYR:HE2	1.79	0.47
3:C:1438:ARG:HB3	3:C:1563:GLN:HG2	1.95	0.47
3:C:4999:ASP:HB3	3:C:5002:GLU:OE2	2.15	0.47
3:D:4577:LEU:HD21	3:D:4806:ASN:HB3	1.96	0.47
3:B:303:ASP:H	3:B:306:LYS:HE3	1.79	0.47
3:B:2876:GLU:HG3	3:B:2920:ARG:HH22	1.78	0.47
3:A:1000:ARG:HD3	3:A:1000:ARG:HA	1.70	0.47
3:A:3604:TYR:HD2	3:A:3608:GLN:HE21	1.62	0.47
3:A:3722:TYR:CE1	3:A:3778:MET:HE3	2.45	0.47
3:A:3974:THR:O	3:A:3978:GLN:HG2	2.14	0.47
3:C:1286:MET:HE1	3:C:1553:PHE:HB3	1.96	0.47
3:C:2004:GLU:HG3	3:C:2008:MET:HE2	1.95	0.47
3:C:2520:HIS:O	3:C:2524:VAL:HG22	2.15	0.47
3:C:2904:LEU:O	3:C:2904:LEU:HD13	2.14	0.47
3:C:3318:ASN:ND2	6:C:5748:HOH:O	2.37	0.47
3:C:3405:LEU:O	3:C:3409:TYR:HB2	2.15	0.47
3:C:3693:LYS:O	6:C:5714:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4044:MET:HE3	3:C:4044:MET:HB2	1.82	0.47
3:D:722:TRP:CZ2	3:D:727:ALA:HB2	2.50	0.47
3:D:993:HIS:CE1	3:D:1027:LEU:HD11	2.50	0.47
3:D:1505:GLN:HA	3:D:1508:ARG:HH21	1.79	0.47
3:D:1575:LEU:O	3:D:1579:MET:HG3	2.15	0.47
3:D:2004:GLU:O	3:D:2008:MET:HG3	2.15	0.47
3:D:2214:VAL:HG21	3:D:2228:MET:SD	2.54	0.47
3:D:2742:THR:HB	3:D:2814:LYS:HD2	1.96	0.47
3:D:2876:GLU:HG3	3:D:2920:ARG:HH22	1.79	0.47
3:D:4839:MET:HA	3:D:4839:MET:HE3	1.97	0.47
3:B:987:ARG:HD2	6:B:5720:HOH:O	2.15	0.47
3:B:2292:GLU:O	3:B:2296:GLU:HG3	2.14	0.47
3:B:2765:LYS:HD3	3:B:2765:LYS:HA	1.57	0.47
3:A:2182:ILE:O	3:A:2186:MET:HG3	2.14	0.47
3:D:3588:ASP:HB2	3:D:3590:GLU:OE1	2.14	0.47
3:B:2520:HIS:O	3:B:2524:VAL:HG22	2.15	0.47
1:I:30:LYS:C	6:I:226:HOH:O	2.57	0.47
3:A:2292:GLU:O	3:A:2296:GLU:HG3	2.15	0.47
3:A:2359:ARG:HD3	3:A:2359:ARG:HA	1.70	0.47
3:A:2742:THR:HB	3:A:2814:LYS:HD2	1.96	0.47
3:A:4576:ILE:HG21	3:A:4643:LEU:HB2	1.97	0.47
3:C:941:MET:HA	3:C:941:MET:HE3	1.97	0.47
3:D:1854:PHE:HD1	3:D:1858:ASP:HB3	1.79	0.47
3:D:4576:ILE:HG21	3:D:4643:LEU:HB2	1.97	0.47
3:B:993:HIS:CE1	3:B:1027:LEU:HD11	2.50	0.47
3:B:2742:THR:HB	3:B:2814:LYS:HD2	1.96	0.47
3:B:3573:MET:O	3:B:3577:ARG:HG2	2.14	0.47
2:E:43:ARG:HE	2:E:45:LYS:HE3	1.80	0.47
3:A:408:ALA:HB2	3:A:483:MET:HE1	1.96	0.47
3:A:863:LEU:HD21	3:A:929:LEU:HB3	1.97	0.47
3:C:2204:HIS:HD2	3:C:2250:MET:HE3	1.80	0.47
3:D:3405:LEU:O	3:D:3409:TYR:HB2	2.14	0.47
3:B:982:THR:HA	3:B:985:VAL:HG12	1.96	0.47
3:B:1170:MET:HE3	3:B:1174:GLY:HA2	1.97	0.47
2:G:50:ARG:HH22	2:G:53:LYS:HE3	1.79	0.47
3:A:19:GLU:HB3	3:A:205:ILE:HB	1.97	0.46
3:A:982:THR:HA	3:A:985:VAL:HG12	1.97	0.46
3:A:2584:HIS:O	3:A:2588:ARG:HG3	2.15	0.46
3:A:2679:PHE:HB2	3:A:2706:ILE:HG21	1.97	0.46
3:A:2876:GLU:HG3	3:A:2920:ARG:HH22	1.78	0.46
3:A:4839:MET:HA	3:A:4839:MET:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1424:PRO:HA	3:C:1427:ILE:HG22	1.96	0.46
3:D:201:ASN:OD1	6:D:5724:HOH:O	2.21	0.46
3:D:2520:HIS:O	3:D:2524:VAL:HG22	2.15	0.46
3:D:3631:ALA:HB1	3:D:3859:VAL:HB	1.97	0.46
3:D:4021:LYS:HB2	3:D:4139:ILE:HG22	1.97	0.46
1:J:36:MET:HG2	1:J:43:PRO:HG3	1.98	0.46
3:A:3768:SER:HA	3:A:3771:HIS:CD2	2.51	0.46
3:C:4576:ILE:HG21	3:C:4643:LEU:HB2	1.97	0.46
3:D:331:VAL:HG21	6:D:6394:HOH:O	2.14	0.46
3:D:1530:THR:HG22	3:D:1535:GLU:HA	1.97	0.46
3:B:3354:LEU:HB2	3:B:3415:TYR:HE2	1.81	0.46
3:A:745:SER:HB2	3:A:758:ARG:HB2	1.98	0.46
3:A:4627:MET:HB2	3:A:4628:VAL:H	1.53	0.46
3:C:722:TRP:CZ2	3:C:727:ALA:HB2	2.50	0.46
3:C:870:ILE:HD11	3:C:1051:TYR:CE1	2.50	0.46
3:C:2208:MET:HE1	3:C:2253:HIS:CG	2.50	0.46
3:C:3788:GLY:HA3	3:C:3834:ALA:HB3	1.97	0.46
3:D:937:CYS:SG	3:D:984:LEU:HD13	2.55	0.46
3:D:2785:LEU:O	3:D:2787:THR:HG23	2.15	0.46
3:D:3232:LEU:HD22	3:D:3239:MET:HE1	1.97	0.46
3:B:2782:ASP:HB3	3:B:2785:LEU:HD22	1.96	0.46
3:B:3865:VAL:HG11	6:B:6168:HOH:O	2.14	0.46
1:I:79:THR:CB	6:I:206:HOH:O	2.64	0.46
3:A:211:GLU:OE1	3:A:211:GLU:HA	2.16	0.46
3:A:648:ILE:HG23	3:A:814:ALA:HB3	1.98	0.46
3:A:1435:TYR:HB3	3:A:1575:LEU:HG	1.98	0.46
3:A:3590:GLU:CD	3:A:3590:GLU:H	2.24	0.46
3:A:4087:LEU:HB3	3:A:4122:MET:HE1	1.97	0.46
3:C:1170:MET:HE3	3:C:1174:GLY:HA2	1.97	0.46
3:C:1986:MET:HG2	3:C:1991:THR:HB	1.96	0.46
3:C:3768:SER:HA	3:C:3771:HIS:CD2	2.51	0.46
3:D:3709:ALA:HB2	3:D:3782:MET:HE2	1.96	0.46
3:D:3768:SER:HA	3:D:3771:HIS:CD2	2.51	0.46
3:B:82:LEU:HD13	3:B:144:GLU:HG2	1.96	0.46
3:B:275:ARG:HD3	6:B:5880:HOH:O	2.16	0.46
3:B:2304:GLY:O	3:B:2308:GLN:NE2	2.47	0.46
3:B:3078:ARG:HG2	3:B:3082:LYS:HE3	1.98	0.46
3:A:379:HIS:CE1	6:A:5873:HOH:O	2.68	0.46
3:A:2967:MET:HE1	3:A:3046:LEU:HD13	1.98	0.46
3:C:2765:LYS:HD3	3:C:2765:LYS:HA	1.58	0.46
3:C:2876:GLU:HG3	3:C:2920:ARG:HH22	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3354:LEU:HB2	3:C:3415:TYR:HE2	1.81	0.46
3:D:4060:LYS:O	3:D:4064:MET:HG2	2.16	0.46
3:B:26:ALA:HB2	3:B:182:LEU:HD21	1.97	0.46
3:B:1847:THR:O	3:B:1851:MET:HG3	2.16	0.46
3:A:722:TRP:CZ2	3:A:727:ALA:HB2	2.50	0.46
3:A:993:HIS:CE1	3:A:1027:LEU:HD11	2.50	0.46
3:A:4067:LYS:O	3:A:4071:ILE:HB	2.16	0.46
3:C:412:ASN:O	3:C:416:LYS:HE3	2.15	0.46
3:C:2304:GLY:O	3:C:2308:GLN:NE2	2.47	0.46
3:D:462:GLU:HG3	3:D:3710:LEU:HD13	1.97	0.46
3:D:3318:ASN:ND2	6:D:5763:HOH:O	2.38	0.46
3:B:211:GLU:HA	3:B:211:GLU:OE2	2.15	0.46
3:A:2520:HIS:O	3:A:2524:VAL:HG22	2.15	0.46
3:A:3996:PHE:HZ	3:A:4019:LEU:HG	1.81	0.46
3:C:19:GLU:HB3	3:C:205:ILE:HB	1.98	0.46
3:C:993:HIS:CE1	3:C:1027:LEU:HD11	2.50	0.46
3:C:2679:PHE:HB2	3:C:2706:ILE:HG21	1.97	0.46
3:C:2812:SER:HB2	3:C:2878:LEU:HD11	1.97	0.46
3:D:1435:TYR:HB3	3:D:1575:LEU:HG	1.98	0.46
3:D:2414:ASN:N	6:D:5804:HOH:O	2.49	0.46
3:B:2369:ARG:HA	6:B:6151:HOH:O	2.16	0.46
3:A:1170:MET:HE3	3:A:1174:GLY:HA2	1.97	0.46
3:A:2004:GLU:HG3	3:A:2008:MET:HE2	1.97	0.46
3:A:3354:LEU:HB2	3:A:3415:TYR:HE2	1.80	0.46
3:C:26:ALA:HB2	3:C:182:LEU:HD21	1.97	0.46
3:C:491:ILE:O	3:C:495:ASN:HB2	2.15	0.46
3:C:871:ARG:HH21	3:C:926:GLY:HA3	1.81	0.46
3:C:4052:SER:O	3:C:4056:GLU:HG3	2.15	0.46
3:D:1170:MET:HE3	3:D:1174:GLY:HA2	1.97	0.46
3:D:2679:PHE:HB2	3:D:2706:ILE:HG21	1.97	0.46
3:D:4813:LEU:O	3:D:4816:ILE:HG12	2.16	0.46
3:B:722:TRP:CZ2	3:B:727:ALA:HB2	2.50	0.46
3:A:491:ILE:O	3:A:495:ASN:HB2	2.15	0.46
3:A:1505:GLN:HA	3:A:1508:ARG:HH21	1.80	0.46
3:A:2604:GLU:HB3	3:A:2639:MET:HG3	1.97	0.46
3:C:1469:VAL:HG13	3:C:1492:CYS:HB3	1.98	0.46
3:C:2336:ARG:HG2	3:C:2432:LEU:HB2	1.97	0.46
3:C:3865:VAL:HG11	6:C:6188:HOH:O	2.15	0.46
3:D:648:ILE:HG23	3:D:814:ALA:HB3	1.98	0.46
3:D:901:LYS:HD3	3:D:901:LYS:HA	1.65	0.46
3:B:1980:LEU:HD21	3:B:1994:ARG:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2918:ARG:O	3:C:2921:GLU:HG3	2.16	0.46
3:D:3445:TRP:CD1	3:D:3510:ILE:HD12	2.51	0.46
3:B:491:ILE:O	3:B:495:ASN:HB2	2.15	0.46
3:B:1768:THR:HG21	6:B:6460:HOH:O	2.16	0.46
3:A:823:LEU:HD11	3:A:1626:TRP:HB3	1.97	0.45
3:C:978:THR:HG22	3:C:980:ALA:H	1.81	0.45
3:C:1505:GLN:HA	3:C:1508:ARG:HH21	1.81	0.45
3:C:2292:GLU:O	3:C:2296:GLU:HG3	2.16	0.45
3:C:2359:ARG:HD3	3:C:2359:ARG:HA	1.70	0.45
3:C:2871:LEU:HA	3:C:2874:MET:SD	2.56	0.45
3:C:3324:VAL:HA	3:C:3327:LEU:HG	1.98	0.45
3:C:3445:TRP:CD1	3:C:3510:ILE:HD12	2.51	0.45
3:C:3573:MET:O	3:C:3577:ARG:HG2	2.15	0.45
3:D:871:ARG:HH21	3:D:926:GLY:HA3	1.81	0.45
3:D:2918:ARG:O	3:D:2921:GLU:HG3	2.16	0.45
3:D:2967:MET:HE1	3:D:3046:LEU:HD13	1.97	0.45
3:B:1076:ARG:HB3	3:B:1191:VAL:HG23	1.98	0.45
3:B:3665:GLU:OE2	6:B:5724:HOH:O	2.21	0.45
3:B:4047:MET:HE3	3:B:4047:MET:HB3	1.73	0.45
2:F:43:ARG:HE	2:F:45:LYS:HE3	1.80	0.45
3:A:1993:ARG:NH1	3:A:1993:ARG:HB3	2.30	0.45
3:A:3989:VAL:HG13	3:A:4023:MET:CE	2.47	0.45
3:A:4813:LEU:O	3:A:4816:ILE:HG12	2.17	0.45
3:C:4087:LEU:HB3	3:C:4122:MET:HE1	1.98	0.45
3:D:26:ALA:HB2	3:D:182:LEU:HD21	1.98	0.45
3:D:275:ARG:HD3	6:D:5900:HOH:O	2.15	0.45
3:B:2182:ILE:O	3:B:2186:MET:HG3	2.16	0.45
3:A:4823:LEU:HD13	3:B:4839:MET:HB3	1.98	0.45
3:C:1986:MET:CG	3:C:1991:THR:HB	2.47	0.45
3:C:2538:THR:O	3:C:2542:SER:HB3	2.16	0.45
3:C:2782:ASP:HB3	3:C:2785:LEU:HD22	1.98	0.45
3:C:4067:LYS:O	3:C:4071:ILE:HB	2.16	0.45
3:D:3604:TYR:HD2	3:D:3608:GLN:HE21	1.63	0.45
3:B:2582:MET:HE2	3:B:2582:MET:HB3	1.82	0.45
3:B:3445:TRP:CD1	3:B:3510:ILE:HD12	2.52	0.45
3:B:3768:SER:HA	3:B:3771:HIS:CD2	2.51	0.45
3:C:745:SER:HB2	3:C:758:ARG:HB2	1.98	0.45
3:C:1087:ARG:HB3	3:C:1223:PHE:CD2	2.52	0.45
3:C:4062:PHE:HB3	3:C:4136:ALA:HB1	1.97	0.45
3:D:2765:LYS:HD3	3:D:2765:LYS:HA	1.58	0.45
3:D:3590:GLU:H	3:D:3590:GLU:CD	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4627:MET:HB2	3:D:4628:VAL:H	1.54	0.45
3:B:19:GLU:HB3	3:B:205:ILE:HB	1.98	0.45
3:B:665:GLU:HB2	3:B:792:LEU:HB2	1.98	0.45
3:B:4813:LEU:O	3:B:4816:ILE:HG12	2.16	0.45
3:A:462:GLU:HG3	3:A:3710:LEU:HD13	1.98	0.45
3:A:3003:LEU:HB2	3:A:3004:PRO:HD3	1.99	0.45
3:D:19:GLU:HB3	3:D:205:ILE:HB	1.97	0.45
3:D:3262:ARG:HG2	3:D:3262:ARG:HH11	1.82	0.45
3:D:3321:ARG:HD2	3:D:3321:ARG:HA	1.72	0.45
3:B:2918:ARG:O	3:B:2921:GLU:HG3	2.16	0.45
1:I:60:ASN:HB2	6:I:204:HOH:O	2.16	0.45
3:C:275:ARG:HD3	6:C:5901:HOH:O	2.16	0.45
3:C:1530:THR:HG22	3:C:1535:GLU:HA	1.98	0.45
3:C:2781:VAL:HG13	3:C:2788:HIS:CE1	2.51	0.45
3:C:4064:MET:N	3:C:4064:MET:SD	2.89	0.45
3:D:2228:MET:HE2	3:D:2232:CYS:SG	2.57	0.45
3:D:3078:ARG:HG2	3:D:3082:LYS:HE3	1.99	0.45
3:B:1435:TYR:HB3	3:B:1575:LEU:HG	1.99	0.45
3:A:244:LEU:HD22	3:A:375:LYS:HZ1	1.82	0.45
3:A:1076:ARG:HB3	3:A:1191:VAL:HG23	1.99	0.45
3:A:1436:SER:OG	3:A:1565:GLU:HB2	2.17	0.45
3:A:2024:PRO:HD2	3:A:2027:ILE:HD12	1.99	0.45
3:A:3405:LEU:O	3:A:3409:TYR:HB2	2.17	0.45
3:A:4005:GLN:HA	3:A:4114:CYS:HA	1.98	0.45
3:A:4687:TYR:HE1	3:A:4692:PRO:HG3	1.82	0.45
3:C:648:ILE:HG23	3:C:814:ALA:HB3	1.98	0.45
3:C:1205:GLY:HA3	3:C:1225:PRO:HB3	1.99	0.45
3:C:1849:LEU:HD22	3:C:1945:TYR:CE2	2.52	0.45
3:D:745:SER:HB2	3:D:758:ARG:HB2	1.98	0.45
3:D:3354:LEU:HB2	3:D:3415:TYR:HE2	1.81	0.45
3:D:3361:THR:HG21	3:D:3408:LEU:HD22	1.98	0.45
3:B:3003:LEU:HB2	3:B:3004:PRO:HD3	1.99	0.45
3:A:2228:MET:HE2	3:A:2232:CYS:SG	2.57	0.45
3:A:2918:ARG:O	3:A:2921:GLU:HG3	2.16	0.45
3:A:3539:ARG:O	3:A:3544:ASP:HB2	2.17	0.45
3:A:4204:GLN:HB3	3:A:4245:MET:HG2	1.99	0.45
3:A:4736:ARG:O	3:A:4739:GLU:HG3	2.17	0.45
3:C:823:LEU:HD11	3:C:1626:TRP:HB3	1.97	0.45
3:C:937:CYS:SG	3:C:984:LEU:HD13	2.57	0.45
3:C:3262:ARG:HG2	3:C:3262:ARG:HH11	1.82	0.45
3:C:4813:LEU:O	3:C:4816:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:491:ILE:O	3:D:495:ASN:HB2	2.15	0.45
3:B:648:ILE:HG23	3:B:814:ALA:HB3	1.98	0.45
3:B:1000:ARG:HD3	3:B:1000:ARG:HA	1.70	0.45
3:B:3262:ARG:HH11	3:B:3262:ARG:HG2	1.82	0.45
3:B:3510:ILE:HG23	6:B:5836:HOH:O	2.16	0.45
3:B:3591:LYS:O	3:B:3595:ARG:HG2	2.16	0.45
1:I:26:THR:HG21	1:I:62:THR:HB	1.99	0.45
3:A:3324:VAL:HA	3:A:3327:LEU:HG	1.99	0.45
3:C:1028:ASP:OD2	6:C:5715:HOH:O	2.20	0.45
3:C:3232:LEU:HD22	3:C:3239:MET:HE1	1.99	0.45
3:D:3996:PHE:HZ	3:D:4019:LEU:HG	1.82	0.45
3:B:1768:THR:CG2	6:B:6460:HOH:O	2.65	0.45
3:B:5017:ARG:NH1	6:B:5808:HOH:O	2.50	0.45
3:A:2004:GLU:O	3:A:2008:MET:HG3	2.16	0.45
3:A:3573:MET:O	3:A:3577:ARG:HG2	2.17	0.45
3:C:1435:TYR:HB3	3:C:1575:LEU:HG	1.98	0.45
3:C:1768:THR:CG2	6:C:6458:HOH:O	2.65	0.45
3:D:665:GLU:HB2	3:D:792:LEU:HB2	1.98	0.45
3:B:590:LEU:HD13	3:B:599:VAL:HB	1.99	0.45
3:B:3405:LEU:O	3:B:3409:TYR:HB2	2.17	0.45
1:J:91:VAL:HG21	3:B:1995:THR:HG21	1.98	0.44
3:A:266:ARG:HD2	3:A:268:SER:O	2.17	0.44
3:A:1847:THR:O	3:A:1851:MET:HG3	2.16	0.44
3:A:1965:TYR:CZ	3:A:2031:LEU:HB2	2.52	0.44
3:A:3590:GLU:HA	3:A:3593:VAL:HG12	1.99	0.44
3:A:4093:PHE:O	3:A:4097:MET:HG2	2.18	0.44
3:A:4823:LEU:HA	3:A:4823:LEU:HD12	1.81	0.44
3:C:1100:MET:HE3	3:C:1143:TRP:CZ2	2.52	0.44
3:C:1436:SER:OG	3:C:1565:GLU:HB2	2.17	0.44
3:C:2182:ILE:O	3:C:2186:MET:HG3	2.17	0.44
3:C:4116:GLU:HB3	3:C:4128:PHE:CZ	2.52	0.44
3:D:2211:MET:HE1	3:D:2236:LEU:HD12	1.99	0.44
3:D:4004:ALA:O	3:D:4005:GLN:HG3	2.18	0.44
3:D:4059:LEU:HA	3:D:4062:PHE:CE1	2.52	0.44
3:D:4063:ASP:OD1	3:D:4067:LYS:HD2	2.17	0.44
3:B:1436:SER:OG	3:B:1565:GLU:HB2	2.17	0.44
3:A:3445:TRP:CD1	3:A:3510:ILE:HD12	2.52	0.44
3:A:3788:GLY:HA3	3:A:3834:ALA:HB3	1.99	0.44
3:C:166:GLY:N	6:C:5742:HOH:O	2.33	0.44
3:C:2814:LYS:HB2	3:C:2814:LYS:HE3	1.63	0.44
3:C:3361:THR:HG21	3:C:3408:LEU:HD22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1674:CYS:HA	3:D:1678:ASN:HB3	2.00	0.44
3:D:1847:THR:O	3:D:1851:MET:HG3	2.18	0.44
3:D:3862:ASP:HB3	6:D:6465:HOH:O	2.17	0.44
3:D:4000:MET:HE2	3:D:4061:PHE:CD1	2.52	0.44
3:B:1087:ARG:HB3	3:B:1223:PHE:CD2	2.53	0.44
3:B:2604:GLU:HB3	3:B:2639:MET:HG3	1.97	0.44
3:B:3517:MET:HE3	3:B:3517:MET:HB3	1.92	0.44
3:B:4021:LYS:HB2	3:B:4139:ILE:HG22	1.99	0.44
1:L:49:GLN:CB	6:L:220:HOH:O	2.66	0.44
1:K:49:GLN:CB	6:K:226:HOH:O	2.65	0.44
2:E:8:ILE:HA	3:A:719:LEU:HD11	1.99	0.44
3:A:665:GLU:HB2	3:A:792:LEU:HB2	1.99	0.44
3:A:1087:ARG:HB3	3:A:1223:PHE:CD2	2.52	0.44
3:A:3591:LYS:HB3	3:A:3591:LYS:HE3	1.74	0.44
3:C:2376:LEU:O	3:C:2380:ILE:HG12	2.18	0.44
3:D:340:LYS:HB2	3:D:343:GLU:OE1	2.16	0.44
3:D:823:LEU:HD11	3:D:1626:TRP:HB3	1.98	0.44
3:D:1076:ARG:HB3	3:D:1191:VAL:HG23	1.98	0.44
3:D:1436:SER:OG	3:D:1565:GLU:HB2	2.17	0.44
3:D:3971:GLY:N	3:D:3972:PRO:HA	2.32	0.44
3:B:719:LEU:HD11	2:F:8:ILE:HA	1.99	0.44
3:B:1965:TYR:CZ	3:B:2031:LEU:HB2	2.52	0.44
3:B:4999:ASP:HB3	3:B:5002:GLU:OE1	2.16	0.44
3:A:1849:LEU:HD22	3:A:1945:TYR:CE2	2.52	0.44
3:A:1986:MET:HE2	3:A:1990:GLU:OE1	2.17	0.44
3:A:2304:GLY:O	3:A:2308:GLN:NE2	2.47	0.44
3:C:955:LEU:HD22	3:C:967:PRO:HB2	1.99	0.44
3:C:1071:ARG:H	3:C:1071:ARG:HG2	1.53	0.44
3:C:3329:ILE:CD1	6:C:6215:HOH:O	2.66	0.44
3:D:590:LEU:HD13	3:D:599:VAL:HB	1.99	0.44
3:D:823:LEU:HB2	3:D:1617:THR:CG2	2.48	0.44
3:D:1087:ARG:HB3	3:D:1223:PHE:CD2	2.53	0.44
3:D:4675:LYS:O	3:D:4679:ARG:HD3	2.17	0.44
3:B:1849:LEU:HD22	3:B:1945:TYR:CE2	2.53	0.44
3:B:3713:LYS:HB2	3:B:3713:LYS:HE3	1.58	0.44
2:G:45:LYS:HE3	2:G:45:LYS:HB3	1.60	0.44
3:A:157:ARG:CZ	3:A:164:ARG:HH21	2.30	0.44
3:A:275:ARG:HD3	6:A:5896:HOH:O	2.17	0.44
3:A:2208:MET:SD	3:A:2250:MET:HE1	2.58	0.44
3:A:4675:LYS:O	3:A:4679:ARG:HD3	2.17	0.44
3:C:3996:PHE:HZ	3:C:4019:LEU:HG	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4004:ALA:O	3:C:4005:GLN:HG3	2.18	0.44
3:D:719:LEU:HD11	2:H:8:ILE:HA	1.99	0.44
3:D:1965:TYR:CZ	3:D:2031:LEU:HB2	2.53	0.44
3:D:2004:GLU:HG3	3:D:2008:MET:HE2	1.98	0.44
3:D:2024:PRO:HD2	3:D:2027:ILE:HD12	1.99	0.44
3:D:2369:ARG:HA	6:D:6147:HOH:O	2.16	0.44
3:D:3990:VAL:HG23	3:D:4047:MET:HG2	1.99	0.44
3:B:3361:THR:HG21	3:B:3408:LEU:HD22	1.99	0.44
3:B:3971:GLY:N	3:B:3972:PRO:HA	2.32	0.44
3:B:4116:GLU:HB3	3:B:4128:PHE:CZ	2.53	0.44
3:A:823:LEU:HB2	3:A:1617:THR:CG2	2.48	0.44
3:A:1021:LEU:HA	3:A:1021:LEU:HD12	1.77	0.44
3:A:2012:PHE:CZ	3:A:2031:LEU:HD23	2.53	0.44
3:A:2904:LEU:O	3:A:2904:LEU:HD13	2.18	0.44
3:A:3262:ARG:HG2	3:A:3262:ARG:HH11	1.82	0.44
3:A:3277:LEU:HD23	3:A:3277:LEU:HA	1.82	0.44
3:A:3990:VAL:HG23	3:A:4047:MET:HG2	1.99	0.44
3:A:4116:GLU:HB3	3:A:4128:PHE:CZ	2.53	0.44
3:C:590:LEU:HD13	3:C:599:VAL:HB	1.99	0.44
3:C:937:CYS:SG	3:C:1055:PRO:HA	2.58	0.44
3:C:1668:ARG:NE	6:C:5788:HOH:O	2.48	0.44
3:C:2024:PRO:HD2	3:C:2027:ILE:HD12	1.99	0.44
3:C:3321:ARG:HD2	3:C:3321:ARG:HA	1.72	0.44
3:C:4687:TYR:HE1	3:C:4692:PRO:HG3	1.82	0.44
3:D:2790:MET:HA	3:D:2790:MET:HE3	2.00	0.44
3:B:823:LEU:HD11	3:B:1626:TRP:HB3	1.98	0.44
3:B:935:LEU:O	3:B:1056:PRO:HG3	2.18	0.44
3:A:1205:GLY:HA3	3:A:1225:PRO:HB3	2.00	0.44
3:C:823:LEU:HB2	3:C:1617:THR:CG2	2.47	0.44
3:C:3003:LEU:HB2	3:C:3004:PRO:HD3	1.99	0.44
3:C:3456:GLN:HG3	3:C:3503:TYR:CD2	2.53	0.44
3:C:3709:ALA:HB2	3:C:3782:MET:HE2	1.99	0.44
3:C:3971:GLY:N	3:C:3972:PRO:HA	2.32	0.44
3:D:2782:ASP:HB3	3:D:2785:LEU:HD22	2.00	0.44
3:D:4166:LEU:HD12	3:D:4166:LEU:HA	1.87	0.44
3:B:2376:LEU:O	3:B:2380:ILE:HG12	2.18	0.44
3:B:3996:PHE:HZ	3:B:4019:LEU:HG	1.82	0.44
3:B:4088:ILE:HG12	3:B:4089:SER:H	1.83	0.44
1:I:43:PRO:O	1:I:47:GLU:HB2	2.17	0.44
2:E:85:ALA:O	2:E:94:PRO:HB3	2.17	0.44
3:A:590:LEU:HD13	3:A:599:VAL:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1674:CYS:HA	3:A:1678:ASN:HB3	1.99	0.44
3:A:2376:LEU:O	3:A:2380:ILE:HG12	2.18	0.44
3:A:4725:LEU:HA	3:A:4737:ILE:HG21	2.00	0.44
3:C:244:LEU:HD22	3:C:375:LYS:HZ1	1.83	0.44
3:C:306:LYS:HB3	3:C:306:LYS:HE3	1.84	0.44
3:D:937:CYS:SG	3:D:1055:PRO:HA	2.57	0.44
3:D:3003:LEU:HB2	3:D:3004:PRO:HD3	1.99	0.44
3:D:3590:GLU:HA	3:D:3593:VAL:HG12	2.00	0.44
3:D:4093:PHE:O	3:D:4097:MET:HG2	2.18	0.44
3:B:2359:ARG:HD3	3:B:2359:ARG:HA	1.70	0.44
3:B:2584:HIS:HB3	6:B:6143:HOH:O	2.17	0.44
3:B:2608:MET:HE1	3:B:2642:LYS:HB3	2.00	0.44
3:B:3070:ILE:HG23	6:B:6210:HOH:O	2.18	0.44
3:B:3788:GLY:HA3	3:B:3834:ALA:HB3	1.99	0.44
2:G:85:ALA:O	2:G:94:PRO:HB3	2.17	0.44
1:I:6:GLU:HB2	6:I:218:HOH:O	2.17	0.44
3:A:129:ASP:HA	3:D:2370:GLY:O	2.18	0.44
3:A:657:THR:HG23	3:A:853:PRO:HD3	2.00	0.44
3:A:2199:ARG:HD3	3:A:2249:SER:HB3	2.00	0.44
3:C:881:LEU:O	3:C:885:THR:HG23	2.18	0.44
3:C:1021:LEU:HA	3:C:1021:LEU:HD12	1.76	0.44
3:C:1076:ARG:HB3	3:C:1191:VAL:HG23	1.99	0.44
3:D:1849:LEU:HD22	3:D:1945:TYR:CE2	2.53	0.44
3:D:2336:ARG:HG3	3:D:2432:LEU:HB2	1.99	0.44
3:D:2604:GLU:HG2	3:D:2639:MET:HE2	2.00	0.44
3:D:4047:MET:HE3	3:D:4047:MET:HB3	1.73	0.44
3:B:745:SER:HB2	3:B:758:ARG:HB2	2.00	0.44
3:B:937:CYS:SG	3:B:984:LEU:HD13	2.58	0.44
3:B:3324:VAL:HA	3:B:3327:LEU:HG	1.99	0.44
3:B:4005:GLN:HA	3:B:4114:CYS:HA	1.99	0.44
3:B:4675:LYS:O	3:B:4679:ARG:HD3	2.18	0.44
2:H:85:ALA:O	2:H:94:PRO:HB3	2.17	0.44
1:L:3:GLN:OE1	1:L:77:LYS:HG3	2.18	0.43
3:A:927:GLU:O	3:A:931:THR:HG22	2.18	0.43
3:A:2204:HIS:HD2	3:A:2250:MET:HE3	1.83	0.43
3:A:2904:LEU:HD21	3:A:2915:GLU:HG3	2.00	0.43
3:A:2912:THR:HG21	3:A:2914:LYS:HE3	2.00	0.43
3:C:665:GLU:HB2	3:C:792:LEU:HB2	1.98	0.43
3:C:4052:SER:HA	3:C:4163:PHE:CZ	2.53	0.43
3:D:3324:VAL:HA	3:D:3327:LEU:HG	1.98	0.43
3:D:3510:ILE:CG2	6:D:5835:HOH:O	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:972:LEU:HD12	3:B:1048:GLY:HA3	2.00	0.43
3:B:2912:THR:HG21	3:B:2914:LYS:HE3	2.00	0.43
1:I:14:GLU:HB3	6:I:232:HOH:O	2.17	0.43
3:A:3078:ARG:HG2	3:A:3082:LYS:HE3	1.99	0.43
3:A:3434:LEU:HA	3:A:3437:MET:HE2	2.00	0.43
3:C:2367:ALA:HB2	3:C:2379:ALA:HB2	2.00	0.43
3:C:2785:LEU:HG	3:C:2787:THR:HG23	2.00	0.43
3:C:2912:THR:HG21	3:C:2914:LYS:HE3	2.00	0.43
3:D:657:THR:HG23	3:D:853:PRO:HD3	2.00	0.43
3:D:1668:ARG:NE	6:D:5805:HOH:O	2.49	0.43
3:D:2608:MET:HE1	3:D:2642:LYS:HB3	1.99	0.43
3:D:2996:LYS:HD3	3:D:2996:LYS:HA	1.83	0.43
3:D:3510:ILE:HG23	6:D:5835:HOH:O	2.17	0.43
3:D:4096:ALA:HB3	3:D:4097:MET:HE2	2.00	0.43
3:B:886:ARG:NH1	3:B:904:HIS:HE1	2.16	0.43
3:B:4063:ASP:OD1	3:B:4067:LYS:HD2	2.18	0.43
3:B:4161:ARG:HD3	3:B:4161:ARG:HA	1.69	0.43
2:F:85:ALA:O	2:F:94:PRO:HB3	2.17	0.43
3:A:2351:ASN:HB3	3:A:2355:ARG:NH1	2.34	0.43
3:A:2582:MET:HE2	3:A:2582:MET:HB3	1.82	0.43
3:C:2012:PHE:CZ	3:C:2031:LEU:HD23	2.53	0.43
3:D:244:LEU:HD22	3:D:375:LYS:HZ1	1.84	0.43
3:D:1575:LEU:HD23	3:D:1575:LEU:HA	1.87	0.43
3:D:1854:PHE:CE1	3:D:1862:ILE:HD11	2.54	0.43
3:D:2578:MET:HE2	3:D:2578:MET:HB3	1.90	0.43
3:D:2912:THR:HG21	3:D:2914:LYS:HE3	2.00	0.43
3:D:3277:LEU:HD23	3:D:3277:LEU:HA	1.82	0.43
3:D:3434:LEU:HA	3:D:3437:MET:HE2	2.00	0.43
3:D:4713:SER:HB3	3:D:4714:ASN:H	1.69	0.43
3:B:823:LEU:HB2	3:B:1617:THR:CG2	2.48	0.43
3:B:969:PRO:O	3:B:970:LEU:HB3	2.17	0.43
3:B:2227:LYS:HB2	3:B:2227:LYS:HE2	1.85	0.43
3:A:2526:PHE:O	3:A:2530:MET:HG3	2.18	0.43
3:C:2637:ALA:C	3:C:2640:PRO:HD2	2.43	0.43
3:D:613:ALA:HB2	3:D:1676:LEU:HD12	2.00	0.43
3:D:872:GLU:HA	3:D:922:LEU:HD11	1.99	0.43
3:D:3535:LEU:HB3	3:D:3552:PHE:HE2	1.84	0.43
3:D:3788:GLY:HA3	3:D:3834:ALA:HB3	1.99	0.43
3:B:2996:LYS:HD3	3:B:2996:LYS:HA	1.82	0.43
3:B:3169:LEU:HD12	3:B:3194:LEU:HD11	2.01	0.43
3:B:4823:LEU:HD12	3:B:4823:LEU:HA	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:695:TYR:CD1	3:A:1240:LYS:HD2	2.53	0.43
3:A:1854:PHE:CE1	3:A:1862:ILE:HD11	2.53	0.43
3:A:2367:ALA:HB2	3:A:2379:ALA:HB2	2.00	0.43
3:C:1674:CYS:HA	3:C:1678:ASN:HB3	2.01	0.43
3:C:2589:LEU:O	3:C:2595:LEU:HD11	2.19	0.43
3:C:3974:THR:O	3:C:3978:GLN:HG2	2.19	0.43
3:D:3591:LYS:O	3:D:3595:ARG:HG2	2.17	0.43
3:D:4119:GLU:H	3:D:4119:GLU:HG3	1.65	0.43
3:D:4204:GLN:HB3	3:D:4245:MET:HG2	2.00	0.43
3:B:673:PRO:HG2	6:B:6424:HOH:O	2.18	0.43
3:B:2351:ASN:HB3	3:B:2355:ARG:NH1	2.33	0.43
3:B:4924:VAL:HA	3:B:4928:LEU:HD12	2.00	0.43
2:H:43:ARG:HE	2:H:45:LYS:CE	2.31	0.43
2:F:43:ARG:HE	2:F:45:LYS:CE	2.31	0.43
1:I:32:LEU:HA	1:I:35:VAL:HG12	2.00	0.43
2:E:43:ARG:HE	2:E:45:LYS:CE	2.31	0.43
3:A:25:SER:HB3	3:A:32:GLN:NE2	2.30	0.43
3:A:2485:LEU:HD23	3:A:2485:LEU:HA	1.85	0.43
3:A:2608:MET:HE1	3:A:2642:LYS:HB3	2.01	0.43
3:A:3321:ARG:HD2	3:A:3321:ARG:HA	1.72	0.43
3:A:3971:GLY:N	3:A:3972:PRO:HA	2.33	0.43
3:C:657:THR:HG23	3:C:853:PRO:HD3	2.01	0.43
3:C:927:GLU:O	3:C:931:THR:HG22	2.18	0.43
3:D:2376:LEU:O	3:D:2380:ILE:HG12	2.18	0.43
3:D:2904:LEU:O	3:D:2904:LEU:HD13	2.18	0.43
3:D:4116:GLU:HB3	3:D:4128:PHE:CZ	2.54	0.43
3:D:4817:ALA:O	3:D:4824:ARG:HG3	2.19	0.43
3:B:1674:CYS:HA	3:B:1678:ASN:HB3	2.01	0.43
3:B:2012:PHE:CZ	3:B:2031:LEU:HD23	2.53	0.43
3:B:2248:ARG:HH11	3:B:2248:ARG:HG3	1.84	0.43
3:B:4736:ARG:O	3:B:4739:GLU:HG3	2.19	0.43
3:A:1492:CYS:SG	3:A:1494:MET:HG3	2.59	0.43
3:A:2785:LEU:O	3:A:2787:THR:HG23	2.18	0.43
3:A:3575:LEU:HD23	3:A:3575:LEU:HA	1.90	0.43
3:A:4044:MET:HE3	3:A:4044:MET:HB2	1.87	0.43
3:C:1812:LEU:HG	3:C:1854:PHE:HE1	1.84	0.43
3:C:2307:LEU:HD23	3:C:2307:LEU:HA	1.83	0.43
3:C:2698:MET:HB3	3:C:2698:MET:HE3	1.72	0.43
3:C:3169:LEU:HD12	3:C:3194:LEU:HD11	2.00	0.43
3:D:874:LEU:HB3	3:D:925:SER:OG	2.18	0.43
3:D:1835:GLU:HG3	3:D:1934:SER:OG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1986:MET:HE2	3:D:1990:GLU:OE1	2.18	0.43
3:D:2012:PHE:CZ	3:D:2031:LEU:HD23	2.53	0.43
3:B:977:LEU:HD23	3:B:977:LEU:HA	1.88	0.43
3:B:1653:LEU:HD23	3:B:1707:LEU:HD11	2.01	0.43
3:B:4687:TYR:HE1	3:B:4692:PRO:HG3	1.84	0.43
3:B:4989:MET:HE3	3:B:4989:MET:HB3	1.86	0.43
1:L:79:THR:N	6:L:208:HOH:O	2.52	0.43
3:A:15:ARG:HG3	3:A:15:ARG:NH1	2.34	0.43
3:A:1128:ARG:NH1	3:A:1128:ARG:HB2	2.34	0.43
3:A:1575:LEU:HD23	3:A:1575:LEU:HA	1.88	0.43
3:A:2578:MET:HE2	3:A:2578:MET:HB3	1.90	0.43
3:A:3510:ILE:HG23	6:A:5832:HOH:O	2.19	0.43
3:A:3948:LYS:HG2	3:A:4012:LEU:HD22	2.01	0.43
3:C:3434:LEU:HA	3:C:3437:MET:HE2	2.00	0.43
3:D:592:LYS:HE2	6:D:6239:HOH:O	2.19	0.43
3:B:1668:ARG:NE	6:B:5805:HOH:O	2.49	0.43
3:B:2490:MET:HE3	3:B:2490:MET:HB3	1.88	0.43
3:B:4865:LYS:HA	3:B:4865:LYS:HD2	1.90	0.43
1:J:69:LEU:HD12	1:J:69:LEU:HA	1.89	0.43
3:C:638:ILE:HD11	3:C:1636:MET:HE2	2.00	0.43
3:C:1965:TYR:CZ	3:C:2031:LEU:HB2	2.53	0.43
3:C:2351:ASN:HB3	3:C:2355:ARG:NH1	2.34	0.43
3:D:1256:GLU:HB2	3:D:1275:ARG:CZ	2.49	0.43
3:D:2638:LYS:NZ	3:D:2698:MET:HG3	2.34	0.43
3:B:657:THR:HG23	3:B:853:PRO:HD3	2.00	0.43
3:B:863:LEU:HD21	3:B:929:LEU:HB3	2.00	0.43
1:J:14:GLU:HB3	6:J:235:HOH:O	2.19	0.43
3:A:886:ARG:NH1	3:A:904:HIS:HE1	2.17	0.43
3:A:1986:MET:CG	3:A:1991:THR:HB	2.47	0.43
3:A:3361:THR:HG21	3:A:3408:LEU:HD22	1.99	0.43
3:A:3384:LYS:H	3:A:3387:ALA:CB	2.31	0.43
3:C:349:GLN:HB2	3:C:356:TRP:CZ3	2.54	0.43
3:C:695:TYR:CD2	3:C:1240:LYS:HD2	2.54	0.43
3:C:969:PRO:O	3:C:970:LEU:HB3	2.18	0.43
3:C:1128:ARG:NH1	3:C:1128:ARG:HB2	2.34	0.43
3:C:4204:GLN:HB3	3:C:4245:MET:HG2	2.00	0.43
3:C:4209:GLN:HG2	3:C:4210:VAL:N	2.33	0.43
3:D:1094:ALA:HB1	3:D:1100:MET:HE1	2.01	0.43
3:D:2904:LEU:HD21	3:D:2915:GLU:HG3	2.00	0.43
3:D:3335:MET:HB3	3:D:3407:ALA:HB2	2.01	0.43
3:D:3536:ALA:HB2	3:D:3553:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:345:LEU:HD23	3:B:345:LEU:HA	1.85	0.43
3:B:3434:LEU:HA	3:B:3437:MET:HE2	2.00	0.43
3:B:3638:MET:HE1	3:B:3862:ASP:HA	2.00	0.43
3:B:4060:LYS:O	3:B:4064:MET:HG2	2.19	0.43
1:J:32:LEU:O	1:J:35:VAL:HG12	2.18	0.42
1:K:13:LYS:HG2	3:C:2189:LYS:HB3	2.01	0.42
1:K:14:GLU:HB3	6:K:232:HOH:O	2.19	0.42
2:E:107:LEU:HD23	2:E:107:LEU:HA	1.88	0.42
3:A:3510:ILE:CG2	6:A:5832:HOH:O	2.67	0.42
3:A:4713:SER:HB3	3:A:4714:ASN:H	1.68	0.42
3:C:653:ALA:HB3	3:C:656:SER:HB2	2.01	0.42
3:C:1768:THR:HG21	6:C:6458:HOH:O	2.17	0.42
3:C:3446:SER:HA	3:C:3452:LYS:HE3	2.01	0.42
3:C:3568:SER:HA	3:C:3571:TRP:NE1	2.34	0.42
3:C:4161:ARG:HA	3:C:4161:ARG:HD3	1.73	0.42
3:C:4675:LYS:O	3:C:4679:ARG:HD3	2.18	0.42
3:D:349:GLN:HB2	3:D:356:TRP:CZ3	2.54	0.42
3:D:818:ARG:HG2	3:D:1028:ASP:HA	2.01	0.42
3:D:955:LEU:HD23	3:D:956:PRO:O	2.19	0.42
3:D:2241:ARG:NH2	6:D:5764:HOH:O	2.39	0.42
3:D:2584:HIS:HB3	6:D:6132:HOH:O	2.19	0.42
3:B:2904:LEU:HD13	3:B:2904:LEU:O	2.18	0.42
3:B:3277:LEU:HD23	3:B:3277:LEU:HA	1.83	0.42
1:L:115:LYS:HA	1:L:115:LYS:HD3	1.86	0.42
1:J:43:PRO:O	1:J:47:GLU:HB2	2.20	0.42
3:A:955:LEU:HD23	3:A:956:PRO:O	2.18	0.42
3:A:2973:PHE:CD1	3:A:2973:PHE:C	2.98	0.42
3:A:3625:SER:O	3:A:3629:ARG:HG3	2.19	0.42
3:A:4242:ILE:HG23	3:A:4993:MET:HG3	2.01	0.42
3:A:4989:MET:HE3	3:A:4989:MET:HB3	1.86	0.42
3:C:1835:GLU:HG3	3:C:1934:SER:OG	2.19	0.42
3:C:2332:LEU:O	3:C:2336:ARG:HG3	2.19	0.42
3:C:2485:LEU:HA	3:C:2485:LEU:HD23	1.87	0.42
3:C:2584:HIS:HB3	6:C:6127:HOH:O	2.18	0.42
3:C:3638:MET:HE1	3:C:3862:ASP:HA	2.01	0.42
3:C:4736:ARG:O	3:C:4739:GLU:HG3	2.19	0.42
3:D:15:ARG:NH1	3:D:15:ARG:HG3	2.33	0.42
3:D:695:TYR:CD2	3:D:1240:LYS:HD2	2.54	0.42
3:D:1812:LEU:HG	3:D:1854:PHE:HE1	1.85	0.42
3:D:1958:LEU:HD23	3:D:2138:LEU:HD21	2.02	0.42
3:D:2304:GLY:O	3:D:2308:GLN:NE2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:331:VAL:HG21	6:B:6437:HOH:O	2.12	0.42
3:B:932:LEU:O	3:B:937:CYS:HB2	2.20	0.42
3:B:2904:LEU:HD21	3:B:2915:GLU:HG3	2.00	0.42
3:B:3631:ALA:HB1	3:B:3859:VAL:HB	2.01	0.42
3:B:4004:ALA:O	3:B:4005:GLN:HG3	2.19	0.42
3:A:1423:ASP:HB2	3:A:1426:ILE:HD12	2.02	0.42
3:A:3568:SER:HA	3:A:3571:TRP:NE1	2.34	0.42
3:C:673:PRO:HG2	6:C:6440:HOH:O	2.18	0.42
3:C:1653:LEU:HD23	3:C:1707:LEU:HD11	2.01	0.42
3:C:2973:PHE:CD1	3:C:2973:PHE:C	2.98	0.42
3:D:886:ARG:NH1	3:D:904:HIS:HE1	2.17	0.42
3:D:969:PRO:O	3:D:970:LEU:HB3	2.17	0.42
3:D:1993:ARG:HB3	3:D:1993:ARG:NH1	2.34	0.42
3:B:803:LEU:HD23	3:B:803:LEU:HA	1.90	0.42
3:B:4087:LEU:HB3	3:B:4122:MET:CE	2.49	0.42
1:K:32:LEU:HA	1:K:35:VAL:HG12	2.01	0.42
3:A:818:ARG:HG2	3:A:1028:ASP:HA	2.02	0.42
3:A:4661:TYR:OH	3:A:4788:SER:HB2	2.20	0.42
3:C:127:MET:HE3	3:C:127:MET:HB3	1.93	0.42
3:C:129:ASP:HA	3:B:2370:GLY:O	2.18	0.42
3:C:719:LEU:HD11	2:G:8:ILE:HA	2.00	0.42
3:C:872:GLU:HA	3:C:922:LEU:HD11	2.00	0.42
3:C:2001:PRO:O	3:C:2005:GLN:HG3	2.20	0.42
3:C:2766:TRP:CH2	3:C:2790:MET:HE3	2.54	0.42
3:D:955:LEU:HB3	3:D:967:PRO:HB2	2.01	0.42
3:D:3974:THR:O	3:D:3978:GLN:HG2	2.19	0.42
3:B:144:GLU:HB2	3:B:175:SER:HB3	2.01	0.42
3:B:695:TYR:CD1	3:B:1240:LYS:HD2	2.54	0.42
3:B:2024:PRO:HD2	3:B:2027:ILE:HD12	1.99	0.42
3:A:75:VAL:O	3:A:79:GLN:HG3	2.20	0.42
3:A:592:LYS:HE2	6:A:6272:HOH:O	2.20	0.42
3:A:1812:LEU:HG	3:A:1854:PHE:HE1	1.84	0.42
3:A:2208:MET:HE3	3:A:2256:TYR:HE2	1.82	0.42
3:A:2942:LYS:HG2	3:A:2943:ASP:N	2.34	0.42
3:C:901:LYS:HA	3:C:901:LYS:HD3	1.70	0.42
3:C:2959:PHE:HZ	3:C:3005:LEU:HG	1.83	0.42
3:C:4839:MET:HB3	3:B:4823:LEU:HD13	2.01	0.42
3:D:935:LEU:O	3:D:1056:PRO:HG3	2.19	0.42
3:D:2367:ALA:HB2	3:D:2379:ALA:HB2	2.01	0.42
3:D:2870:GLU:OE1	3:D:2944:MET:HG2	2.20	0.42
3:D:2942:LYS:HG2	3:D:2943:ASP:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2973:PHE:C	3:D:2973:PHE:CD1	2.98	0.42
3:B:555:GLU:HG2	3:B:556:ALA:N	2.34	0.42
3:B:955:LEU:HD23	3:B:956:PRO:O	2.19	0.42
3:B:1205:GLY:HA3	3:B:1225:PRO:HB3	2.01	0.42
3:B:1812:LEU:HG	3:B:1854:PHE:HE1	1.84	0.42
3:B:3326:ASN:O	3:B:3329:ILE:HG12	2.19	0.42
3:A:196:MET:CE	6:A:6231:HOH:O	2.60	0.42
3:A:1653:LEU:HD23	3:A:1707:LEU:HD11	2.01	0.42
3:A:2370:GLY:O	3:B:129:ASP:HA	2.19	0.42
3:A:2633:LEU:HD22	3:A:2695:LEU:HD11	2.00	0.42
3:A:4096:ALA:HB3	3:A:4097:MET:HE2	2.02	0.42
3:C:2211:MET:HE1	3:C:2236:LEU:HD12	2.02	0.42
3:C:2414:ASN:N	6:C:5812:HOH:O	2.52	0.42
3:C:2949:SER:HB3	3:C:2952:GLU:OE1	2.20	0.42
3:D:1205:GLY:HA3	3:D:1225:PRO:HB3	2.00	0.42
3:D:2364:PHE:HB3	3:D:2368:LEU:HB2	2.02	0.42
3:D:3591:LYS:HE3	3:D:3591:LYS:HB3	1.74	0.42
3:B:872:GLU:HA	3:B:922:LEU:HD21	2.01	0.42
3:B:3531:ASP:O	3:B:3535:LEU:HG	2.20	0.42
3:B:3990:VAL:HG23	3:B:4047:MET:HG2	2.02	0.42
3:B:4204:GLN:HB3	3:B:4245:MET:HG2	2.01	0.42
3:B:4713:SER:HB3	3:B:4714:ASN:H	1.69	0.42
3:A:144:GLU:HB2	3:A:175:SER:HB3	2.02	0.42
3:A:633:LEU:HD11	3:A:1659:LEU:HD22	2.01	0.42
3:A:935:LEU:O	3:A:1056:PRO:HG3	2.20	0.42
3:A:977:LEU:HD23	3:A:977:LEU:HA	1.88	0.42
3:A:4004:ALA:O	3:A:4005:GLN:HG3	2.20	0.42
3:C:613:ALA:HB2	3:C:1676:LEU:HD12	2.02	0.42
3:C:953:THR:HG21	3:C:971:ASP:HB3	2.01	0.42
3:C:1447:CYS:HB3	3:C:1555:LEU:HB3	2.02	0.42
3:C:3326:ASN:O	3:C:3329:ILE:HG12	2.19	0.42
3:C:4865:LYS:HA	3:C:4865:LYS:HD2	1.91	0.42
3:D:503:PHE:HD2	3:D:512:ALA:HA	1.84	0.42
3:D:1128:ARG:NH1	3:D:1128:ARG:HB2	2.34	0.42
3:D:2199:ARG:HD3	3:D:2249:SER:HB3	2.02	0.42
3:B:244:LEU:HD22	3:B:375:LYS:HZ1	1.85	0.42
3:B:816:LEU:HD21	3:B:851:PHE:HE2	1.85	0.42
3:B:2367:ALA:HB2	3:B:2379:ALA:HB2	2.01	0.42
3:B:2589:LEU:O	3:B:2595:LEU:HD11	2.20	0.42
3:B:2942:LYS:HG2	3:B:2943:ASP:N	2.34	0.42
1:K:43:PRO:O	1:K:47:GLU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:94:LYS:CG	6:K:211:HOH:O	2.37	0.42
3:A:1094:ALA:HB1	3:A:1100:MET:HE1	2.01	0.42
3:A:1152:MET:HB3	3:A:1223:PHE:CE2	2.54	0.42
3:A:1958:LEU:HD23	3:A:2138:LEU:HD21	2.01	0.42
3:A:1977:TYR:CZ	3:A:1981:MET:HE2	2.55	0.42
3:A:3134:VAL:O	6:A:5725:HOH:O	2.22	0.42
3:A:4067:LYS:HB3	3:A:4067:LYS:HE3	1.92	0.42
3:C:592:LYS:HE2	6:C:6236:HOH:O	2.19	0.42
3:C:1152:MET:HB3	3:C:1223:PHE:CE2	2.54	0.42
3:C:1422:ASP:OD2	3:C:1427:ILE:HD13	2.20	0.42
3:C:3335:MET:HB3	3:C:3407:ALA:HB2	2.02	0.42
3:C:4067:LYS:HB3	3:C:4067:LYS:HE3	1.92	0.42
3:C:4823:LEU:HD13	3:D:4839:MET:HB3	2.01	0.42
3:D:1152:MET:HB3	3:D:1223:PHE:CE2	2.54	0.42
3:D:3326:ASN:O	3:D:3329:ILE:HG12	2.19	0.42
3:D:3531:ASP:O	3:D:3535:LEU:HG	2.20	0.42
3:D:3916:ILE:H	3:D:3916:ILE:HG12	1.65	0.42
3:D:3989:VAL:HG13	3:D:4023:MET:CE	2.49	0.42
3:D:4989:MET:HE3	3:D:4989:MET:HB3	1.86	0.42
3:B:642:THR:OG1	6:B:5725:HOH:O	2.21	0.42
3:B:871:ARG:HH21	3:B:926:GLY:HA3	1.85	0.42
3:B:1128:ARG:NH1	3:B:1128:ARG:HB2	2.34	0.42
3:B:1530:THR:HG22	3:B:1535:GLU:HA	2.02	0.42
3:B:2948:THR:O	3:B:2953:LYS:HE2	2.19	0.42
3:B:3034:LYS:HD3	3:B:3034:LYS:N	2.35	0.42
3:B:4817:ALA:O	3:B:4824:ARG:HG3	2.20	0.42
1:J:90:ARG:NH2	3:B:1981:MET:HG3	2.35	0.42
3:A:673:PRO:HG2	6:A:6422:HOH:O	2.19	0.42
3:A:2227:LYS:HB2	3:A:2227:LYS:HE2	1.84	0.42
3:A:2364:PHE:HB3	3:A:2368:LEU:HB2	2.02	0.42
3:A:3335:MET:HB3	3:A:3407:ALA:HB2	2.02	0.42
3:A:3341:PHE:O	3:A:3344:PRO:HD2	2.20	0.42
3:A:3437:MET:HE2	3:A:3437:MET:HB2	1.86	0.42
3:A:3456:GLN:HG3	3:A:3503:TYR:CD2	2.54	0.42
3:A:3631:ALA:HB1	3:A:3859:VAL:HB	2.02	0.42
3:A:4673:ARG:CZ	3:A:4698:LYS:HG3	2.50	0.42
3:C:403:MET:HE2	3:C:403:MET:HB3	1.92	0.42
3:C:503:PHE:HD2	3:C:512:ALA:HA	1.84	0.42
3:C:1970:GLN:HG2	3:C:3642:TYR:HA	2.02	0.42
3:C:2010:LEU:HD21	3:C:3653:PHE:CE1	2.55	0.42
3:C:3531:ASP:O	3:C:3535:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3625:SER:O	3:C:3629:ARG:HG3	2.20	0.42
3:C:4096:ALA:HB3	3:C:4097:MET:HE2	2.02	0.42
3:D:922:LEU:HD12	3:D:922:LEU:HA	1.77	0.42
3:D:1071:ARG:H	3:D:1071:ARG:HG2	1.53	0.42
3:D:1212:ARG:NH2	6:D:5721:HOH:O	2.19	0.42
3:D:1653:LEU:HD23	3:D:1707:LEU:HD11	2.01	0.42
3:D:2690:LYS:HG3	3:D:2691:TYR:N	2.34	0.42
3:D:3169:LEU:HB2	3:D:3197:LEU:HD22	2.02	0.42
3:D:3659:ALA:HA	3:D:3663:LEU:HD12	2.01	0.42
3:D:4736:ARG:O	3:D:4739:GLU:HG3	2.19	0.42
3:B:349:GLN:HB2	3:B:356:TRP:CZ3	2.54	0.42
3:B:818:ARG:HG2	3:B:1028:ASP:HA	2.02	0.42
3:B:1854:PHE:CE1	3:B:1862:ILE:HD11	2.54	0.42
3:B:2001:PRO:O	3:B:2005:GLN:HG3	2.20	0.42
3:B:2211:MET:HE1	3:B:2236:LEU:HD12	2.02	0.42
3:B:3321:ARG:HD2	3:B:3321:ARG:HA	1.72	0.42
3:B:3437:MET:HE2	3:B:3437:MET:HB2	1.86	0.42
1:L:137:ASN:CB	6:L:231:HOH:O	2.68	0.42
3:A:3329:ILE:CD1	6:A:6229:HOH:O	2.68	0.42
3:A:4846:VAL:HG21	3:D:4816:ILE:HD13	2.01	0.42
3:A:4924:VAL:HA	3:A:4928:LEU:HD12	2.01	0.42
3:C:818:ARG:HG2	3:C:1028:ASP:HA	2.02	0.42
3:C:1854:PHE:CE1	3:C:1862:ILE:HD11	2.54	0.42
3:C:1963:GLU:HA	3:C:3650:CYS:SG	2.60	0.42
3:C:2991:HIS:O	3:C:2995:ILE:HG13	2.20	0.42
3:C:3277:LEU:HD23	3:C:3277:LEU:HA	1.83	0.42
3:D:609:CYS:HB3	6:D:6285:HOH:O	2.19	0.42
3:D:4661:TYR:OH	3:D:4788:SER:HB2	2.19	0.42
3:D:4687:TYR:HE1	3:D:4692:PRO:HG3	1.84	0.42
3:B:881:LEU:O	3:B:885:THR:HG23	2.20	0.42
3:B:901:LYS:HD3	3:B:901:LYS:HA	1.66	0.42
3:B:2336:ARG:HG2	3:B:2432:LEU:HB2	2.01	0.42
3:B:3341:PHE:O	3:B:3344:PRO:HD2	2.20	0.42
3:B:4000:MET:HE2	3:B:4061:PHE:CD1	2.55	0.42
3:B:4661:TYR:OH	3:B:4788:SER:HB2	2.19	0.42
1:I:91:VAL:HG21	3:A:1995:THR:HG21	2.02	0.41
3:A:555:GLU:HG2	3:A:556:ALA:N	2.34	0.41
3:A:2589:LEU:O	3:A:2595:LEU:HD11	2.20	0.41
3:A:3914:ASN:CG	3:A:3917:ILE:HG12	2.45	0.41
3:A:5017:ARG:NH1	6:A:5792:HOH:O	2.46	0.41
3:C:196:MET:CE	6:C:6211:HOH:O	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:460:GLN:OE1	3:C:460:GLN:HA	2.20	0.41
3:C:751:SER:HB3	6:C:6447:HOH:O	2.20	0.41
3:C:1000:ARG:HA	3:C:1000:ARG:HD3	1.66	0.41
3:C:1466:LEU:HD23	3:C:1466:LEU:HA	1.91	0.41
3:C:3510:ILE:HG23	6:C:5822:HOH:O	2.18	0.41
3:C:3914:ASN:CG	3:C:3917:ILE:HG12	2.45	0.41
3:C:4661:TYR:OH	3:C:4788:SER:HB2	2.20	0.41
3:D:957:LYS:HE2	3:D:957:LYS:HB2	1.95	0.41
3:D:1970:GLN:HG2	3:D:3642:TYR:HA	2.02	0.41
3:D:3914:ASN:CG	3:D:3917:ILE:HG12	2.45	0.41
3:B:157:ARG:CZ	3:B:164:ARG:HH21	2.32	0.41
3:B:653:ALA:HB3	3:B:656:SER:HB2	2.02	0.41
3:B:1447:CYS:HB3	3:B:1555:LEU:HB3	2.02	0.41
3:B:2161:GLN:NE2	6:B:5827:HOH:O	2.53	0.41
3:B:3329:ILE:CD1	6:B:6229:HOH:O	2.68	0.41
1:I:94:LYS:CD	6:I:221:HOH:O	2.63	0.41
2:E:58:LYS:HD3	2:E:81:VAL:HG12	2.02	0.41
3:A:460:GLN:OE1	3:A:460:GLN:HA	2.20	0.41
3:A:2765:LYS:HZ3	3:A:2860:PRO:HD2	1.85	0.41
3:A:3412:LEU:HD11	3:A:3434:LEU:HD21	2.03	0.41
3:C:1958:LEU:HD23	3:C:2138:LEU:HD21	2.02	0.41
3:C:4817:ALA:O	3:C:4824:ARG:HG3	2.20	0.41
3:D:555:GLU:HG2	3:D:556:ALA:N	2.34	0.41
3:D:955:LEU:HD22	3:D:967:PRO:HB2	2.01	0.41
3:D:1243:PRO:HA	3:D:1601:MET:O	2.20	0.41
3:D:1963:GLU:HA	3:D:3650:CYS:SG	2.60	0.41
3:D:2010:LEU:HD21	3:D:3653:PHE:CE1	2.56	0.41
3:D:2959:PHE:HZ	3:D:3005:LEU:HG	1.84	0.41
3:D:3573:MET:O	3:D:3577:ARG:HG2	2.20	0.41
3:D:4686:LEU:HD12	3:D:4686:LEU:HA	1.85	0.41
3:B:751:SER:HB3	6:B:6454:HOH:O	2.20	0.41
3:B:1256:GLU:HB2	3:B:1275:ARG:CZ	2.49	0.41
3:B:1970:GLN:HG2	3:B:3642:TYR:HA	2.02	0.41
3:B:2973:PHE:CD1	3:B:2973:PHE:C	2.97	0.41
3:B:2991:HIS:O	3:B:2995:ILE:HG13	2.20	0.41
1:K:130:ILE:CD1	6:K:238:HOH:O	2.68	0.41
3:A:872:GLU:HA	3:A:922:LEU:HD21	2.01	0.41
3:A:1668:ARG:NE	6:A:5804:HOH:O	2.48	0.41
3:A:3169:LEU:HB2	3:A:3197:LEU:HD22	2.02	0.41
3:A:3326:ASN:O	3:A:3329:ILE:HG12	2.19	0.41
3:A:3365:LEU:HD13	3:A:3405:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3446:SER:HA	3:A:3452:LYS:HE3	2.01	0.41
3:A:3875:MET:HE3	3:A:3875:MET:HB3	1.82	0.41
3:C:107:ILE:HD13	3:C:202:MET:HE1	2.02	0.41
3:C:144:GLU:HB2	3:C:175:SER:HB3	2.01	0.41
3:C:555:GLU:HG2	3:C:556:ALA:N	2.34	0.41
3:C:2227:LYS:HB2	3:C:2227:LYS:HE2	1.82	0.41
3:C:2745:VAL:HG11	3:C:2818:ALA:HB2	2.02	0.41
3:C:3341:PHE:O	3:C:3344:PRO:HD2	2.20	0.41
3:C:3384:LYS:H	3:C:3387:ALA:CB	2.31	0.41
3:C:3510:ILE:CG2	6:C:5822:HOH:O	2.67	0.41
3:C:3589:PRO:O	3:C:3593:VAL:HG12	2.19	0.41
3:D:2582:MET:HE2	3:D:2582:MET:HB3	1.82	0.41
3:D:3575:LEU:HD23	3:D:3575:LEU:HA	1.89	0.41
3:D:4924:VAL:HA	3:D:4928:LEU:HD12	2.02	0.41
3:B:983:THR:O	3:B:987:ARG:HG3	2.20	0.41
3:B:1152:MET:HB3	3:B:1223:PHE:CE2	2.54	0.41
3:B:1835:GLU:HG3	3:B:1934:SER:OG	2.19	0.41
3:B:1977:TYR:CZ	3:B:1981:MET:HE2	2.55	0.41
3:B:2364:PHE:HB3	3:B:2368:LEU:HB2	2.02	0.41
3:B:3535:LEU:HB3	3:B:3552:PHE:HE2	1.84	0.41
3:B:3989:VAL:HG13	3:B:4023:MET:CE	2.49	0.41
3:B:4673:ARG:CZ	3:B:4698:LYS:HG3	2.50	0.41
3:B:4677:LEU:HD11	3:B:4687:TYR:HE2	1.85	0.41
1:I:13:LYS:HG2	3:A:2189:LYS:HB3	2.02	0.41
3:A:1093:GLU:HB3	3:A:1201:HIS:HB3	2.02	0.41
3:A:3354:LEU:HB2	3:A:3415:TYR:CE2	2.56	0.41
3:C:935:LEU:O	3:C:1056:PRO:HG3	2.21	0.41
3:C:1093:GLU:HB3	3:C:1201:HIS:HB3	2.02	0.41
3:C:1851:MET:HE2	3:C:1851:MET:HB3	1.92	0.41
3:C:3875:MET:HE3	3:C:3875:MET:HB3	1.84	0.41
3:C:4093:PHE:CD1	3:C:4097:MET:HE3	2.54	0.41
3:D:751:SER:HB3	6:D:6445:HOH:O	2.20	0.41
3:D:1779:PRO:HA	3:D:1780:PRO:HD3	1.96	0.41
3:D:2001:PRO:O	3:D:2005:GLN:HG3	2.20	0.41
3:D:4209:GLN:HG2	3:D:4210:VAL:N	2.35	0.41
3:B:633:LEU:HD11	3:B:1659:LEU:HD22	2.02	0.41
3:B:2010:LEU:HD21	3:B:3653:PHE:CE1	2.55	0.41
3:A:751:SER:HB3	6:A:6448:HOH:O	2.20	0.41
3:A:1243:PRO:HA	3:A:1601:MET:O	2.21	0.41
3:A:1835:GLU:HG3	3:A:1934:SER:OG	2.21	0.41
3:A:2430:ILE:HG21	3:A:2502:MET:SD	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3531:ASP:O	3:A:3535:LEU:HG	2.20	0.41
3:C:2161:GLN:NE2	6:C:5818:HOH:O	2.53	0.41
3:C:2816:MET:HE3	3:C:2816:MET:HB2	1.83	0.41
3:C:2921:GLU:O	3:C:2925:GLU:HG2	2.20	0.41
3:C:3412:LEU:HD11	3:C:3434:LEU:HD21	2.03	0.41
3:C:3535:LEU:HB3	3:C:3552:PHE:HE2	1.84	0.41
3:D:2296:GLU:HG2	3:D:2356:LEU:HD21	2.02	0.41
3:D:2867:LEU:HB3	3:D:2871:LEU:HB3	2.02	0.41
3:D:2991:HIS:O	3:D:2995:ILE:HG13	2.20	0.41
3:D:3329:ILE:CD1	6:D:6210:HOH:O	2.68	0.41
3:D:3412:LEU:HD11	3:D:3434:LEU:HD21	2.02	0.41
3:B:696:PRO:HB3	6:B:6253:HOH:O	2.20	0.41
3:B:1963:GLU:HA	3:B:3650:CYS:SG	2.60	0.41
3:B:2430:ILE:HG21	3:B:2502:MET:SD	2.61	0.41
3:A:310:LYS:HB3	3:A:310:LYS:HE2	1.76	0.41
3:A:349:GLN:HB2	3:A:356:TRP:CZ3	2.54	0.41
3:A:1963:GLU:HA	3:A:3650:CYS:SG	2.61	0.41
3:A:2010:LEU:HD21	3:A:3653:PHE:CE1	2.55	0.41
3:A:2788:HIS:ND1	3:A:2789:PRO:HD2	2.35	0.41
3:A:2959:PHE:HZ	3:A:3005:LEU:HG	1.84	0.41
3:A:3364:ARG:HE	3:A:3364:ARG:HB3	1.73	0.41
3:A:3996:PHE:CD2	3:A:4020:GLN:HG3	2.56	0.41
3:C:15:ARG:NH1	3:C:15:ARG:HG3	2.34	0.41
3:C:633:LEU:HD11	3:C:1659:LEU:HD22	2.02	0.41
3:C:826:ILE:HG22	3:C:827:LYS:HG2	2.03	0.41
3:C:2942:LYS:HG2	3:C:2943:ASP:N	2.35	0.41
3:C:4001:MET:N	3:C:4001:MET:SD	2.93	0.41
3:C:4093:PHE:O	3:C:4097:MET:HG2	2.20	0.41
3:D:486:LEU:HD12	3:D:486:LEU:HA	1.91	0.41
3:D:881:LEU:O	3:D:885:THR:HG23	2.20	0.41
3:D:3354:LEU:HB2	3:D:3415:TYR:CE2	2.56	0.41
3:D:3446:SER:HA	3:D:3452:LYS:HE3	2.01	0.41
3:D:3517:MET:HE3	3:D:3517:MET:HB3	1.92	0.41
3:D:4725:LEU:HA	3:D:4737:ILE:HG21	2.02	0.41
3:B:19:GLU:HG2	3:B:66:CYS:HB3	2.03	0.41
3:B:884:LEU:O	3:B:888:GLU:HG2	2.21	0.41
3:B:2637:ALA:C	3:B:2640:PRO:HD2	2.45	0.41
3:B:3335:MET:HB3	3:B:3407:ALA:HB2	2.02	0.41
3:B:3384:LYS:H	3:B:3387:ALA:CB	2.31	0.41
3:B:3780:LEU:HD11	3:B:3816:MET:HB3	2.02	0.41
3:B:3875:MET:HE3	3:B:3875:MET:HB3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4209:GLN:HG2	3:B:4210:VAL:N	2.34	0.41
3:A:650:VAL:HA	3:A:658:GLN:HE22	1.86	0.41
3:A:1478:ASP:HB3	3:A:1484:HIS:CE1	2.55	0.41
3:C:1243:PRO:HA	3:C:1601:MET:O	2.21	0.41
3:C:2707:ALA:HB1	3:C:3009:TYR:HD1	1.86	0.41
3:C:3517:MET:HE3	3:C:3517:MET:HB3	1.96	0.41
3:D:650:VAL:HA	3:D:658:GLN:HE22	1.85	0.41
3:D:1051:TYR:CD1	3:D:1051:TYR:N	2.88	0.41
3:B:15:ARG:NH1	3:B:15:ARG:HG3	2.34	0.41
3:B:506:TYR:HE1	6:B:5719:HOH:O	2.03	0.41
3:B:613:ALA:HB2	3:B:1676:LEU:HD12	2.01	0.41
3:B:1094:ALA:HB1	3:B:1100:MET:HE1	2.01	0.41
3:B:1958:LEU:HD23	3:B:2138:LEU:HD21	2.02	0.41
3:B:3527:PRO:HD2	3:B:3573:MET:SD	2.60	0.41
2:G:107:LEU:HA	2:G:107:LEU:HD23	1.88	0.41
3:A:26:ALA:HB2	3:A:182:LEU:HD21	2.02	0.41
3:A:874:LEU:HB3	3:A:925:SER:OG	2.21	0.41
3:A:2186:MET:HE1	3:A:2238:TYR:CD2	2.56	0.41
3:A:2862:LEU:HD12	3:A:2928:LYS:HE3	2.03	0.41
3:A:4209:GLN:HG2	3:A:4210:VAL:N	2.36	0.41
3:C:955:LEU:HD23	3:C:956:PRO:O	2.21	0.41
3:C:1094:ALA:HB1	3:C:1100:MET:HE1	2.02	0.41
3:C:2370:GLY:O	3:D:129:ASP:HA	2.20	0.41
3:C:2495:VAL:HG22	3:C:2498:HIS:CE1	2.56	0.41
3:C:2584:HIS:O	3:C:2588:ARG:HG3	2.21	0.41
3:C:2700:MET:HE3	3:C:2700:MET:HB3	1.96	0.41
3:D:2165:LEU:HD11	3:D:2177:LEU:HD23	2.03	0.41
3:D:2589:LEU:O	3:D:2595:LEU:HD11	2.20	0.41
3:D:3365:LEU:HD13	3:D:3405:LEU:HD12	2.03	0.41
3:D:3384:LYS:H	3:D:3387:ALA:CB	2.33	0.41
3:D:3939:GLY:N	6:D:5797:HOH:O	2.48	0.41
3:B:592:LYS:HE2	6:B:6260:HOH:O	2.20	0.41
3:B:1743:ARG:HG3	6:B:6082:HOH:O	2.21	0.41
3:B:3194:LEU:HD12	3:B:3194:LEU:HA	1.88	0.41
1:J:13:LYS:HG2	3:B:2189:LYS:HB3	2.02	0.41
3:A:22:LEU:HD23	3:A:22:LEU:HA	1.96	0.41
3:A:266:ARG:NH2	6:A:5704:HOH:O	2.52	0.41
3:A:3250:MET:HE3	3:A:3250:MET:HB3	1.99	0.41
3:A:3638:MET:HE1	3:A:3862:ASP:HA	2.03	0.41
3:A:4675:LYS:HG3	3:A:4679:ARG:NH1	2.36	0.41
3:C:874:LEU:HD12	3:C:874:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2330:ARG:H	3:C:2330:ARG:HG2	1.69	0.41
3:C:2364:PHE:HB3	3:C:2368:LEU:HB2	2.02	0.41
3:C:2672:LEU:HD23	3:C:2672:LEU:HA	1.93	0.41
3:C:3169:LEU:HB2	3:C:3197:LEU:HD22	2.03	0.41
3:C:3194:LEU:HD12	3:C:3194:LEU:HA	1.88	0.41
3:C:3334:TRP:CD1	3:C:3334:TRP:H	2.39	0.41
3:C:3631:ALA:HB1	3:C:3859:VAL:HB	2.02	0.41
3:D:340:LYS:HE3	3:D:340:LYS:HB3	2.00	0.41
3:D:696:PRO:HB3	6:D:6258:HOH:O	2.20	0.41
3:D:2131:LEU:HD12	3:D:2131:LEU:HA	1.97	0.41
3:D:3341:PHE:O	3:D:3344:PRO:HD2	2.21	0.41
3:D:3456:GLN:HG3	3:D:3503:TYR:CD2	2.55	0.41
3:D:3638:MET:HE1	3:D:3862:ASP:HA	2.02	0.41
3:D:4242:ILE:HG23	3:D:4993:MET:HG3	2.02	0.41
3:B:403:MET:HE2	3:B:403:MET:HB3	1.93	0.41
3:B:468:LEU:O	3:B:472:ARG:HG2	2.20	0.41
3:B:650:VAL:HA	3:B:658:GLN:HE22	1.86	0.41
3:B:826:ILE:HG22	3:B:827:LYS:HG2	2.03	0.41
3:B:955:LEU:HD22	3:B:967:PRO:HB2	2.02	0.41
3:B:1021:LEU:HA	3:B:1021:LEU:HD12	1.77	0.41
3:B:1093:GLU:HB3	3:B:1201:HIS:HB3	2.02	0.41
3:B:1126:GLY:HA3	3:B:1143:TRP:CD2	2.56	0.41
3:B:2007:ASN:OD1	3:B:3656:SER:HB2	2.21	0.41
3:B:2199:ARG:HD3	3:B:2249:SER:HB3	2.03	0.41
3:B:2414:ASN:N	6:B:5828:HOH:O	2.54	0.41
3:B:3575:LEU:HD23	3:B:3575:LEU:HA	1.91	0.41
3:B:3663:LEU:HD12	3:B:3663:LEU:HA	1.90	0.41
3:B:3914:ASN:CG	3:B:3917:ILE:HG12	2.45	0.41
3:B:4059:LEU:HA	3:B:4062:PHE:CE1	2.56	0.41
3:A:1126:GLY:HA3	3:A:1143:TRP:CD2	2.56	0.41
3:A:2991:HIS:O	3:A:2995:ILE:HG13	2.20	0.41
3:A:3034:LYS:HD3	3:A:3034:LYS:N	2.35	0.41
3:A:4093:PHE:CD1	3:A:4097:MET:HE3	2.55	0.41
3:C:1126:GLY:HA3	3:C:1143:TRP:CD2	2.56	0.41
3:C:2101:MET:HE2	3:C:2102:VAL:HG23	2.03	0.41
3:D:633:LEU:HD11	3:D:1659:LEU:HD22	2.02	0.41
3:D:1126:GLY:HA3	3:D:1143:TRP:CD2	2.56	0.41
3:D:2707:ALA:HB1	3:D:3009:TYR:HD1	1.86	0.41
3:B:966:LYS:H	3:B:966:LYS:HG3	1.67	0.41
3:B:2959:PHE:HZ	3:B:3005:LEU:HG	1.84	0.41
2:H:107:LEU:HA	2:H:107:LEU:HD23	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:150:MET:HE3	3:A:150:MET:HB2	1.85	0.40
3:A:468:LEU:O	3:A:472:ARG:HG2	2.21	0.40
3:A:937:CYS:SG	3:A:984:LEU:HD13	2.61	0.40
3:A:1469:VAL:HG13	3:A:1492:CYS:HB3	2.03	0.40
3:A:2138:LEU:HD23	3:A:2138:LEU:HA	1.95	0.40
3:A:2495:VAL:HG22	3:A:2498:HIS:CE1	2.57	0.40
3:A:2752:ASP:O	3:A:2755:ILE:HG12	2.21	0.40
3:A:3939:GLY:N	6:A:5810:HOH:O	2.50	0.40
3:C:3354:LEU:HB2	3:C:3415:TYR:CE2	2.56	0.40
3:C:3591:LYS:HE3	3:C:3591:LYS:HB3	1.73	0.40
3:C:4242:ILE:HG23	3:C:4993:MET:HG3	2.03	0.40
3:D:927:GLU:O	3:D:931:THR:HG22	2.21	0.40
3:D:932:LEU:HD21	3:D:984:LEU:HD21	2.02	0.40
3:D:3169:LEU:HD12	3:D:3194:LEU:HD11	2.04	0.40
3:D:3274:LEU:HD23	3:D:3274:LEU:HA	1.92	0.40
3:D:3334:TRP:CD1	3:D:3334:TRP:H	2.39	0.40
3:D:4093:PHE:CD1	3:D:4097:MET:HE3	2.56	0.40
3:B:927:GLU:O	3:B:931:THR:HG22	2.21	0.40
3:B:2101:MET:HE2	3:B:2102:VAL:HG23	2.03	0.40
3:B:2739:PRO:HD3	3:B:2888:ARG:HG2	2.03	0.40
3:B:3169:LEU:HB2	3:B:3197:LEU:HD22	2.03	0.40
3:B:4021:LYS:HE3	3:B:4138:ASP:OD1	2.21	0.40
3:A:613:ALA:HB2	3:A:1676:LEU:HD12	2.02	0.40
3:A:886:ARG:NH1	3:A:904:HIS:CE1	2.89	0.40
3:A:937:CYS:SG	3:A:1055:PRO:HA	2.61	0.40
3:A:2241:ARG:NH2	6:A:5766:HOH:O	2.40	0.40
3:A:2638:LYS:NZ	3:A:2698:MET:HB2	2.37	0.40
3:C:2752:ASP:O	3:C:2755:ILE:HG12	2.21	0.40
3:C:3301:PRO:HA	3:C:3302:PRO:HD3	1.95	0.40
3:C:4673:ARG:CZ	3:C:4698:LYS:HG3	2.51	0.40
3:D:144:GLU:HB2	3:D:175:SER:HB3	2.02	0.40
3:D:2584:HIS:O	3:D:2588:ARG:HG3	2.21	0.40
3:D:3250:MET:HE3	3:D:3250:MET:HB3	1.99	0.40
3:B:664:PHE:CE1	3:B:746:CYS:HB2	2.56	0.40
3:B:2752:ASP:O	3:B:2755:ILE:HG12	2.21	0.40
3:B:3354:LEU:HB2	3:B:3415:TYR:CE2	2.56	0.40
3:B:3446:SER:HA	3:B:3452:LYS:HE3	2.03	0.40
3:B:4053:SER:O	3:B:4057:MET:HG3	2.22	0.40
3:B:4627:MET:HB2	3:B:4628:VAL:H	1.66	0.40
1:L:36:MET:HG2	1:L:43:PRO:HG3	2.03	0.40
1:I:3:GLN:OE1	1:I:77:LYS:HG3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:60:ASN:CA	6:J:205:HOH:O	2.57	0.40
1:K:92:PHE:CD1	1:K:104:GLU:HG2	2.57	0.40
3:A:2101:MET:HE2	3:A:2102:VAL:HG23	2.03	0.40
3:A:2165:LEU:HD11	3:A:2177:LEU:HD23	2.03	0.40
3:A:2208:MET:HE1	3:A:2253:HIS:CG	2.56	0.40
3:A:2973:PHE:CD1	3:A:2995:ILE:HG12	2.57	0.40
3:A:3334:TRP:CD1	3:A:3334:TRP:H	2.39	0.40
3:A:3526:ALA:H	3:A:3595:ARG:NH1	2.19	0.40
3:C:19:GLU:HG2	3:C:66:CYS:HB3	2.03	0.40
3:C:468:LEU:O	3:C:472:ARG:HG2	2.21	0.40
3:C:817:PRO:HG2	3:C:1022:VAL:HG21	2.03	0.40
3:C:972:LEU:HD12	3:C:1048:GLY:HA3	2.02	0.40
3:C:2996:LYS:HD3	3:C:2996:LYS:HA	1.83	0.40
3:C:4005:GLN:HB3	3:C:4114:CYS:HA	2.03	0.40
3:D:166:GLY:CA	6:D:5754:HOH:O	2.69	0.40
3:D:2101:MET:HE2	3:D:2102:VAL:HG23	2.03	0.40
3:D:4640:GLU:HB3	3:D:4641:PRO:HD3	2.03	0.40
3:B:976:ARG:H	3:B:976:ARG:HG2	1.63	0.40
3:B:2333:ASP:HA	3:B:2336:ARG:HG3	2.04	0.40
3:B:2623:LEU:HD23	3:B:2623:LEU:HA	1.88	0.40
3:B:3263:TYR:HD1	3:B:3270:ILE:HD12	1.86	0.40
3:B:3412:LEU:HD11	3:B:3434:LEU:HD21	2.03	0.40
3:B:3510:ILE:CG2	6:B:5836:HOH:O	2.67	0.40
3:B:3568:SER:HA	3:B:3571:TRP:NE1	2.36	0.40
3:B:3589:PRO:O	3:B:3593:VAL:HG12	2.20	0.40
3:B:3590:GLU:HA	3:B:3593:VAL:HG12	2.04	0.40
3:B:4564:PHE:CD1	3:B:4564:PHE:C	2.99	0.40
1:K:30:LYS:C	6:K:227:HOH:O	2.64	0.40
3:A:817:PRO:HG2	3:A:1022:VAL:HG21	2.03	0.40
3:A:2347:GLU:H	3:A:2347:GLU:HG2	1.65	0.40
3:C:922:LEU:HA	3:C:922:LEU:HD12	1.76	0.40
3:C:977:LEU:HD23	3:C:977:LEU:HA	1.89	0.40
3:C:2430:ILE:HG21	3:C:2502:MET:SD	2.61	0.40
3:C:2803:GLU:HA	3:C:2806:ARG:NH1	2.37	0.40
3:C:4166:LEU:HD12	3:C:4166:LEU:HA	1.87	0.40
3:D:1812:LEU:HD23	3:D:1812:LEU:HA	1.95	0.40
3:D:2430:ILE:HG21	3:D:2502:MET:SD	2.61	0.40
3:D:2638:LYS:HZ1	3:D:2698:MET:HG3	1.86	0.40
3:D:2942:LYS:HG2	3:D:2943:ASP:H	1.86	0.40
3:D:4675:LYS:HG3	3:D:4679:ARG:NH1	2.36	0.40
3:B:817:PRO:HG2	3:B:1022:VAL:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1868:PRO:O	3:B:1872:THR:HB	2.22	0.40
3:B:2707:ALA:HB1	3:B:3009:TYR:HD1	1.86	0.40
3:B:2908:TYR:CE2	3:B:2916:LYS:HD3	2.57	0.40
3:B:3842:LEU:HD23	3:B:3875:MET:HG3	2.04	0.40
3:B:4725:LEU:HA	3:B:4737:ILE:HG21	2.03	0.40
3:A:484:LEU:CB	6:A:6300:HOH:O	2.66	0.40
3:A:696:PRO:HB3	6:A:6258:HOH:O	2.21	0.40
3:A:816:LEU:HD21	3:A:851:PHE:HE2	1.86	0.40
3:A:881:LEU:O	3:A:885:THR:HG23	2.21	0.40
3:A:2948:THR:O	3:A:2953:LYS:HE2	2.21	0.40
3:C:650:VAL:HA	3:C:658:GLN:HE22	1.86	0.40
3:C:805:PRO:HG2	3:C:808:TYR:CD1	2.57	0.40
3:C:1256:GLU:HB2	3:C:1275:ARG:CZ	2.52	0.40
3:C:1868:PRO:O	3:C:1872:THR:HB	2.22	0.40
3:C:4675:LYS:HG3	3:C:4679:ARG:NH1	2.36	0.40
3:D:13:PHE:CE2	3:D:164:ARG:HD2	2.54	0.40
3:D:664:PHE:CE1	3:D:746:CYS:HB2	2.56	0.40
3:D:844:ARG:HD2	3:D:1196:PRO:HB2	2.04	0.40
3:D:972:LEU:HD12	3:D:1048:GLY:HA3	2.02	0.40
3:D:977:LEU:HD23	3:D:977:LEU:HA	1.88	0.40
3:D:1868:PRO:O	3:D:1872:THR:HB	2.21	0.40
3:D:2637:ALA:C	3:D:2640:PRO:HD2	2.47	0.40
3:D:2752:ASP:O	3:D:2755:ILE:HG12	2.21	0.40
3:D:2973:PHE:CD1	3:D:2995:ILE:HG12	2.56	0.40
3:D:4180:ARG:HG2	6:D:6326:HOH:O	2.21	0.40
3:B:503:PHE:HD2	3:B:512:ALA:HA	1.86	0.40
3:B:886:ARG:NH1	3:B:904:HIS:CE1	2.89	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 PDB entries followed by that with respect to all EM entries.

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	I	146/148 (99%)	143 (98%)	3 (2%)	0	100	100
1	J	146/148 (99%)	144 (99%)	2 (1%)	0	100	100
1	K	146/148 (99%)	144 (99%)	2 (1%)	0	100	100
1	L	146/148 (99%)	144 (99%)	2 (1%)	0	100	100
2	E	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
2	F	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
2	G	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
2	H	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
3	A	4198/5037 (83%)	4125 (98%)	72 (2%)	1 (0%)	100	100
3	B	4198/5037 (83%)	4124 (98%)	73 (2%)	1 (0%)	100	100
3	C	4198/5037 (83%)	4122 (98%)	75 (2%)	1 (0%)	100	100
3	D	4198/5037 (83%)	4128 (98%)	69 (2%)	1 (0%)	100	100
All	All	17796/21168 (84%)	17483 (98%)	309 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	970	LEU
3	D	970	LEU
3	B	970	LEU
3	C	969	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 PDB entries followed by that with respect to all EM entries.

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	I	82/127 (65%)	80 (98%)	2 (2%)	43	68
1	J	82/127 (65%)	81 (99%)	1 (1%)	63	82
1	K	82/127 (65%)	81 (99%)	1 (1%)	63	82
1	L	82/127 (65%)	80 (98%)	2 (2%)	43	68
2	E	88/88 (100%)	86 (98%)	2 (2%)	44	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	88/88 (100%)	85 (97%)	3 (3%)	32	58
2	G	88/88 (100%)	84 (96%)	4 (4%)	24	47
2	H	88/88 (100%)	83 (94%)	5 (6%)	18	38
3	A	3696/4276 (86%)	3630 (98%)	66 (2%)	51	74
3	B	3696/4276 (86%)	3633 (98%)	63 (2%)	53	76
3	C	3696/4276 (86%)	3629 (98%)	67 (2%)	51	74
3	D	3696/4276 (86%)	3628 (98%)	68 (2%)	51	74
All	All	15464/17964 (86%)	15180 (98%)	284 (2%)	51	74

All (284) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	29	THR
1	L	63	ILE
1	I	63	ILE
1	I	101	SER
1	J	63	ILE
1	K	101	SER
2	E	26	HIS
2	E	78	THR
3	A	73	LEU
3	A	227	MET
3	A	458	GLU
3	A	484	LEU
3	A	577	ILE
3	A	667	MET
3	A	892	THR
3	A	896	VAL
3	A	904	HIS
3	A	929	LEU
3	A	970	LEU
3	A	1071	ARG
3	A	1084	GLN
3	A	1183	GLU
3	A	1300	HIS
3	A	1934	SER
3	A	1980	LEU
3	A	2308	GLN
3	A	2597	LYS
3	A	2738	ARG

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Mol	Chain	Res	Type
3	A	2806	ARG
3	A	2813	LEU
3	A	2862	LEU
3	A	2870	GLU
3	A	2871	LEU
3	A	2874	MET
3	A	2888	ARG
3	A	2894	LEU
3	A	2922	LYS
3	A	2932	MET
3	A	2985	ARG
3	A	2986	VAL
3	A	3108	GLU
3	A	3158	LEU
3	A	3201	MET
3	A	3239	MET
3	A	3258	GLU
3	A	3333	THR
3	A	3394	VAL
3	A	3405	LEU
3	A	3409	TYR
3	A	3437	MET
3	A	3449	HIS
3	A	3528	THR
3	A	3590	GLU
3	A	3668	SER
3	A	3720	TYR
3	A	3762	ARG
3	A	3899	PHE
3	A	4000	MET
3	A	4001	MET
3	A	4060	LYS
3	A	4121	GLU
3	A	4137	ARG
3	A	4139	ILE
3	A	4164	LEU
3	A	4166	LEU
3	A	4200	THR
3	A	4224	GLU
3	A	4583	SER
3	A	4627	MET
3	A	4689	THR

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Mol	Chain	Res	Type
3	A	4720	VAL
3	A	4823	LEU
3	A	4948	GLU
3	A	4966	ASP
3	C	35	LEU
3	C	73	LEU
3	C	227	MET
3	C	577	ILE
3	C	667	MET
3	C	892	THR
3	C	896	VAL
3	C	922	LEU
3	C	1010	VAL
3	C	1046	LEU
3	C	1071	ARG
3	C	1084	GLN
3	C	1183	GLU
3	C	1212	ARG
3	C	1299	GLN
3	C	1300	HIS
3	C	1768	THR
3	C	1931	LEU
3	C	1980	LEU
3	C	2006	ILE
3	C	2308	GLN
3	C	2312	MET
3	C	2738	ARG
3	C	2806	ARG
3	C	2871	LEU
3	C	2874	MET
3	C	2888	ARG
3	C	2922	LYS
3	C	2924	GLN
3	C	2932	MET
3	C	2944	MET
3	C	2985	ARG
3	C	2986	VAL
3	C	3108	GLU
3	C	3201	MET
3	C	3239	MET
3	C	3333	THR
3	C	3394	VAL

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Mol	Chain	Res	Type
3	C	3399	SER
3	C	3405	LEU
3	C	3409	TYR
3	C	3437	MET
3	C	3449	HIS
3	C	3528	THR
3	C	3668	SER
3	C	3758	MET
3	C	3762	ARG
3	C	3899	PHE
3	C	3910	THR
3	C	3980	LEU
3	C	4000	MET
3	C	4001	MET
3	C	4002	LYS
3	C	4016	LEU
3	C	4064	MET
3	C	4067	LYS
3	C	4137	ARG
3	C	4164	LEU
3	C	4166	LEU
3	C	4200	THR
3	C	4224	GLU
3	C	4627	MET
3	C	4676	GLU
3	C	4689	THR
3	C	4720	VAL
3	C	4823	LEU
3	C	4966	ASP
3	D	35	LEU
3	D	73	LEU
3	D	164	ARG
3	D	169	LEU
3	D	227	MET
3	D	458	GLU
3	D	577	ILE
3	D	667	MET
3	D	870	ILE
3	D	892	THR
3	D	896	VAL
3	D	904	HIS
3	D	922	LEU

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Mol	Chain	Res	Type
3	D	935	LEU
3	D	1039	LEU
3	D	1071	ARG
3	D	1300	HIS
3	D	2173	GLN
3	D	2308	GLN
3	D	2312	MET
3	D	2597	LYS
3	D	2738	ARG
3	D	2806	ARG
3	D	2813	LEU
3	D	2870	GLU
3	D	2888	ARG
3	D	2894	LEU
3	D	2922	LYS
3	D	2924	GLN
3	D	2932	MET
3	D	2944	MET
3	D	2985	ARG
3	D	2986	VAL
3	D	3082	LYS
3	D	3108	GLU
3	D	3158	LEU
3	D	3184	GLU
3	D	3201	MET
3	D	3239	MET
3	D	3258	GLU
3	D	3333	THR
3	D	3394	VAL
3	D	3399	SER
3	D	3405	LEU
3	D	3409	TYR
3	D	3437	MET
3	D	3449	HIS
3	D	3590	GLU
3	D	3668	SER
3	D	3720	TYR
3	D	3850	GLN
3	D	3899	PHE
3	D	3910	THR
3	D	4001	MET
3	D	4121	GLU

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Mol	Chain	Res	Type
3	D	4139	ILE
3	D	4164	LEU
3	D	4166	LEU
3	D	4200	THR
3	D	4224	GLU
3	D	4583	SER
3	D	4627	MET
3	D	4676	GLU
3	D	4689	THR
3	D	4720	VAL
3	D	4966	ASP
3	D	4980	LEU
3	D	5000	GLU
3	B	35	LEU
3	B	73	LEU
3	B	164	ARG
3	B	496	VAL
3	B	577	ILE
3	B	667	MET
3	B	870	ILE
3	B	892	THR
3	B	896	VAL
3	B	904	HIS
3	B	935	LEU
3	B	960	MET
3	B	970	LEU
3	B	974	HIS
3	B	1071	ARG
3	B	1183	GLU
3	B	1299	GLN
3	B	1300	HIS
3	B	1931	LEU
3	B	2006	ILE
3	B	2228	MET
3	B	2308	GLN
3	B	2312	MET
3	B	2738	ARG
3	B	2790	MET
3	B	2806	ARG
3	B	2813	LEU
3	B	2870	GLU
3	B	2874	MET

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Mol	Chain	Res	Type
3	B	2888	ARG
3	B	2894	LEU
3	B	2922	LYS
3	B	2924	GLN
3	B	2932	MET
3	B	2985	ARG
3	B	2986	VAL
3	B	3108	GLU
3	B	3158	LEU
3	B	3201	MET
3	B	3239	MET
3	B	3258	GLU
3	B	3333	THR
3	B	3352	GLU
3	B	3399	SER
3	B	3405	LEU
3	B	3409	TYR
3	B	3437	MET
3	B	3668	SER
3	B	3762	ARG
3	B	3899	PHE
3	B	3905	THR
3	B	4121	GLU
3	B	4139	ILE
3	B	4164	LEU
3	B	4166	LEU
3	B	4200	THR
3	B	4224	GLU
3	B	4627	MET
3	B	4720	VAL
3	B	4818	MET
3	B	4823	LEU
3	B	4966	ASP
3	B	4980	LEU
2	H	26	HIS
2	H	30	MET
2	H	54	GLN
2	H	68	SER
2	H	78	THR
2	F	26	HIS
2	F	68	SER
2	F	78	THR

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Mol	Chain	Res	Type
2	G	26	HIS
2	G	30	MET
2	G	44	ASN
2	G	78	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (146) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	-1	HIS
1	K	-1	HIS
3	A	32	GLN
3	A	44	ASN
3	A	56	GLN
3	A	57	ASN
3	A	98	HIS
3	A	113	HIS
3	A	151	HIS
3	A	226	HIS
3	A	489	ASN
3	A	597	HIS
3	A	720	HIS
3	A	765	GLN
3	A	981	GLN
3	A	1220	GLN
3	A	1231	GLN
3	A	1299	GLN
3	A	1484	HIS
3	A	1665	HIS
3	A	1938	GLN
3	A	2693	GLN
3	A	2856	ASN
3	A	2858	GLN
3	A	2892	GLN
3	A	3128	ASN
3	A	3343	GLN
3	A	3418	ASN
3	A	3456	GLN
3	A	3523	ASN
3	A	3555	ASN
3	A	3558	HIS
3	A	3814	GLN
3	A	3850	GLN

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Mol	Chain	Res	Type
3	A	3914	ASN
3	A	4020	GLN
3	A	4109	GLN
3	A	4204	GLN
3	A	5015	GLN
3	C	44	ASN
3	C	56	GLN
3	C	57	ASN
3	C	79	GLN
3	C	98	HIS
3	C	113	HIS
3	C	151	HIS
3	C	190	GLN
3	C	226	HIS
3	C	308	HIS
3	C	489	ASN
3	C	597	HIS
3	C	720	HIS
3	C	765	GLN
3	C	1231	GLN
3	C	1660	GLN
3	C	1665	HIS
3	C	1938	GLN
3	C	2693	GLN
3	C	2788	HIS
3	C	2856	ASN
3	C	2858	GLN
3	C	3418	ASN
3	C	3456	GLN
3	C	3461	GLN
3	C	3523	ASN
3	C	3555	ASN
3	C	3699	HIS
3	C	3914	ASN
3	C	3946	GLN
3	C	4020	GLN
3	C	4043	GLN
3	C	4109	GLN
3	D	44	ASN
3	D	56	GLN
3	D	57	ASN
3	D	113	HIS

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Mol	Chain	Res	Type
3	D	151	HIS
3	D	181	HIS
3	D	226	HIS
3	D	489	ASN
3	D	597	HIS
3	D	720	HIS
3	D	765	GLN
3	D	1231	GLN
3	D	1660	GLN
3	D	1665	HIS
3	D	1938	GLN
3	D	2693	GLN
3	D	2780	ASN
3	D	2856	ASN
3	D	2858	GLN
3	D	2892	GLN
3	D	3128	ASN
3	D	3343	GLN
3	D	3418	ASN
3	D	3456	GLN
3	D	3461	GLN
3	D	3699	HIS
3	D	3814	GLN
3	D	3914	ASN
3	D	3946	GLN
3	D	3998	HIS
3	D	4020	GLN
3	D	4043	GLN
3	D	4054	ASN
3	D	4109	GLN
3	D	5035	GLN
3	B	44	ASN
3	B	56	GLN
3	B	57	ASN
3	B	113	HIS
3	B	151	HIS
3	B	181	HIS
3	B	226	HIS
3	B	489	ASN
3	B	597	HIS
3	B	720	HIS
3	B	765	GLN

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Mol	Chain	Res	Type
3	B	1660	GLN
3	B	1665	HIS
3	B	1938	GLN
3	B	2693	GLN
3	B	2773	ASN
3	B	2780	ASN
3	B	2856	ASN
3	B	2858	GLN
3	B	2892	GLN
3	B	3128	ASN
3	B	3343	GLN
3	B	3418	ASN
3	B	3456	GLN
3	B	3461	GLN
3	B	3523	ASN
3	B	3555	ASN
3	B	3558	HIS
3	B	3699	HIS
3	B	3761	GLN
3	B	3809	ASN
3	B	3814	GLN
3	B	3850	GLN
3	B	3914	ASN
3	B	3946	GLN
3	B	3960	GLN
3	B	4109	GLN
3	B	5015	GLN
3	B	5035	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
5	ATP	A	5602	-	32,33,33	0.31	0	48,52,52	0.41	0
5	ATP	B	5602	-	32,33,33	0.31	0	48,52,52	0.41	0
5	ATP	C	5602	-	32,33,33	0.31	0	48,52,52	0.42	0
5	ATP	D	5602	-	32,33,33	0.30	0	48,52,52	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	A	5602	-	-	2/22/38/38	0/3/3/3
5	ATP	B	5602	-	-	2/22/38/38	0/3/3/3
5	ATP	C	5602	-	-	2/22/38/38	0/3/3/3
5	ATP	D	5602	-	-	2/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	5602	ATP	O4'-C4'-C5'-O5'
5	A	5602	ATP	O4'-C4'-C5'-O5'
5	C	5602	ATP	O4'-C4'-C5'-O5'
5	D	5602	ATP	C3'-C4'-C5'-O5'
5	B	5602	ATP	O4'-C4'-C5'-O5'
5	B	5602	ATP	C3'-C4'-C5'-O5'
5	A	5602	ATP	C3'-C4'-C5'-O5'

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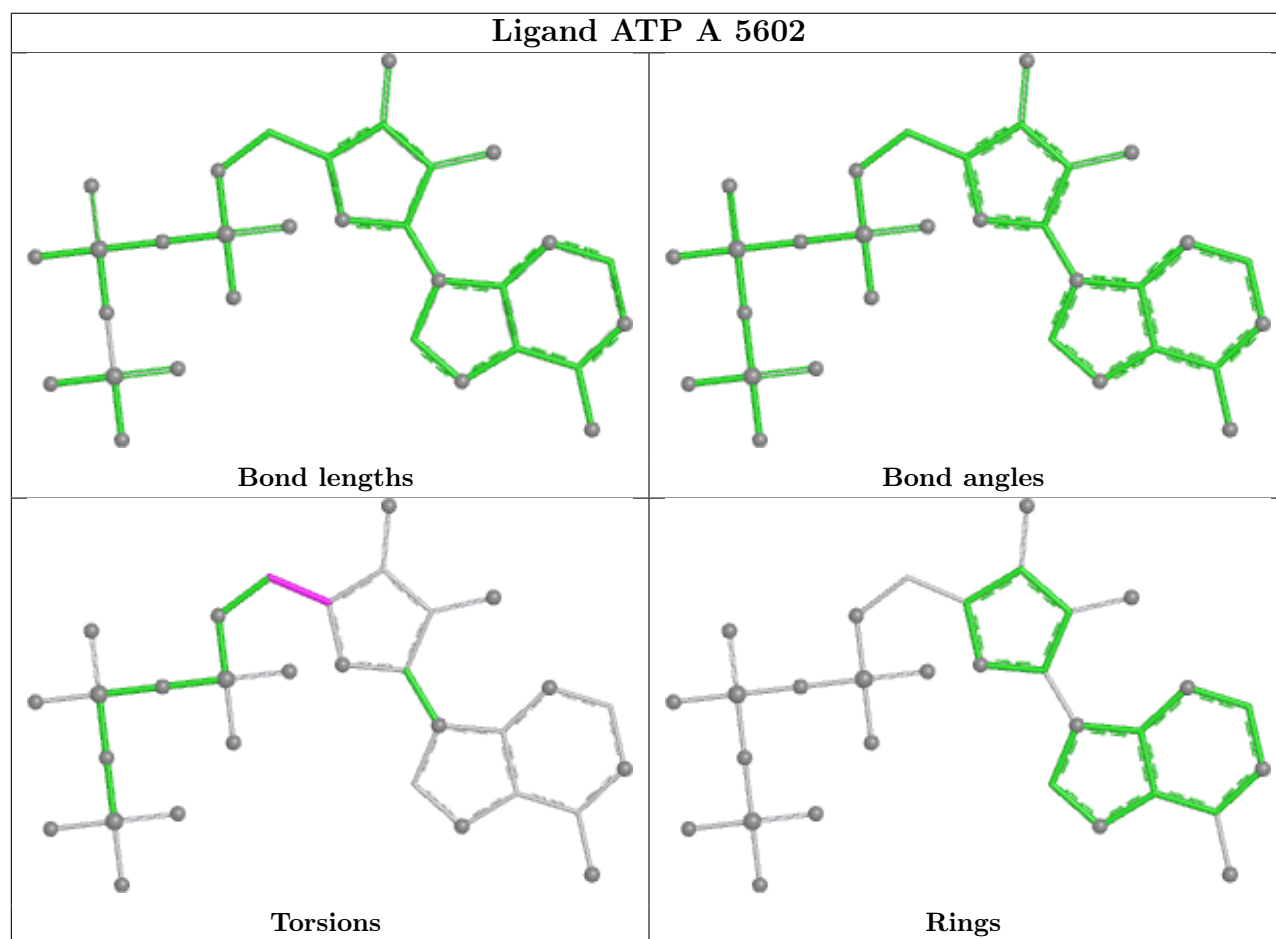
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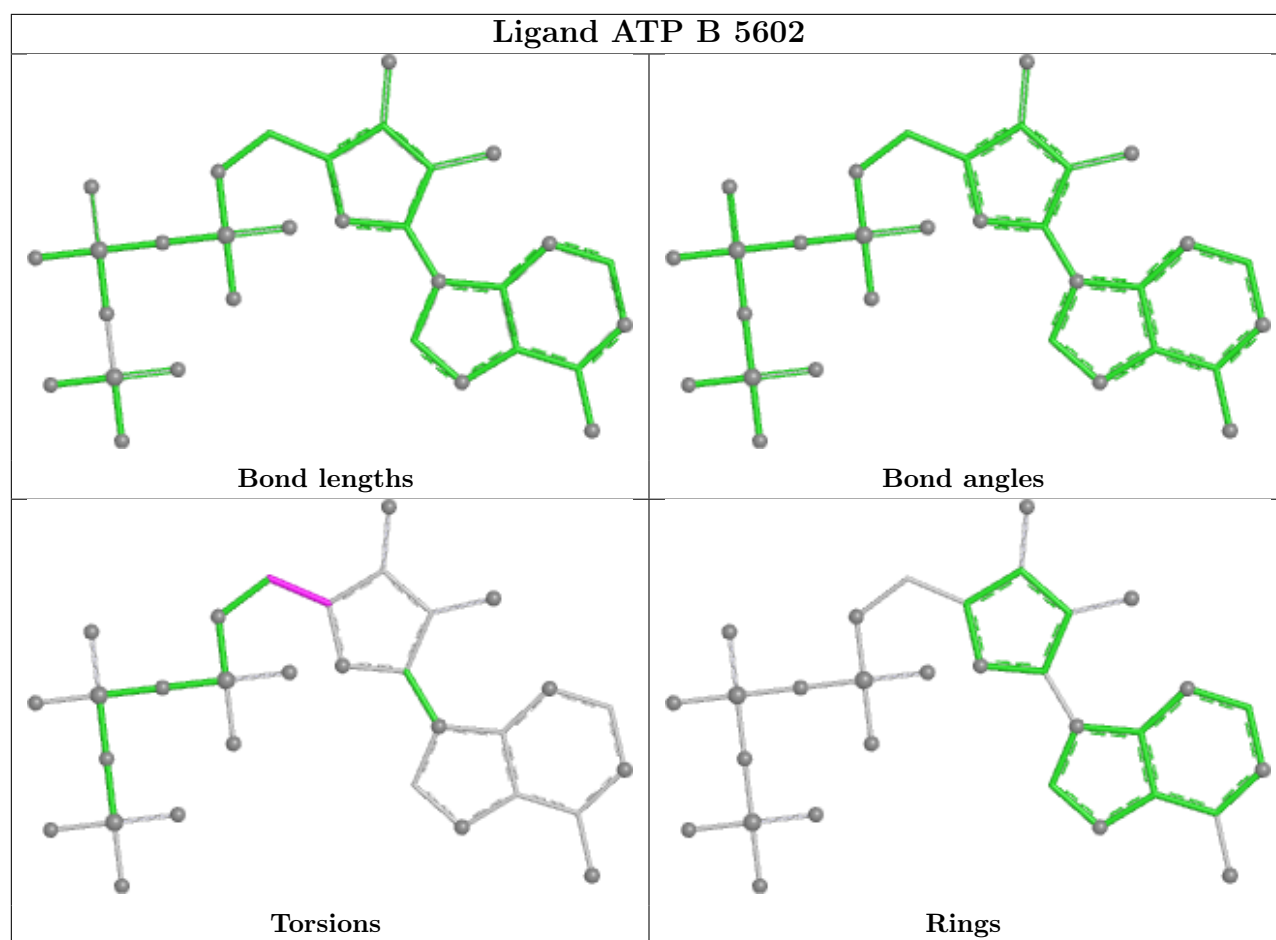
Mol	Chain	Res	Type	Atoms
5	C	5602	ATP	C3'-C4'-C5'-O5'

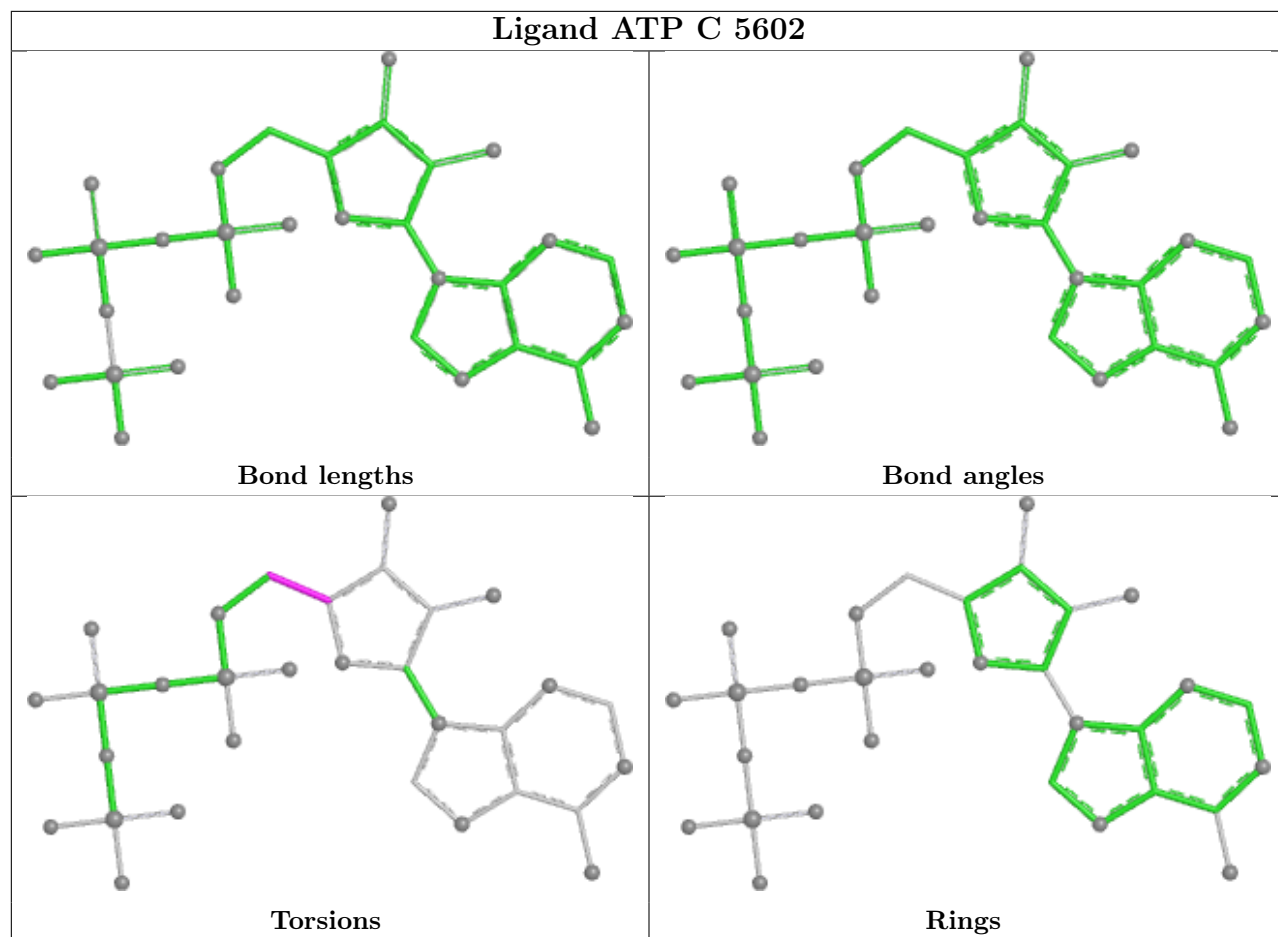
There are no ring outliers.

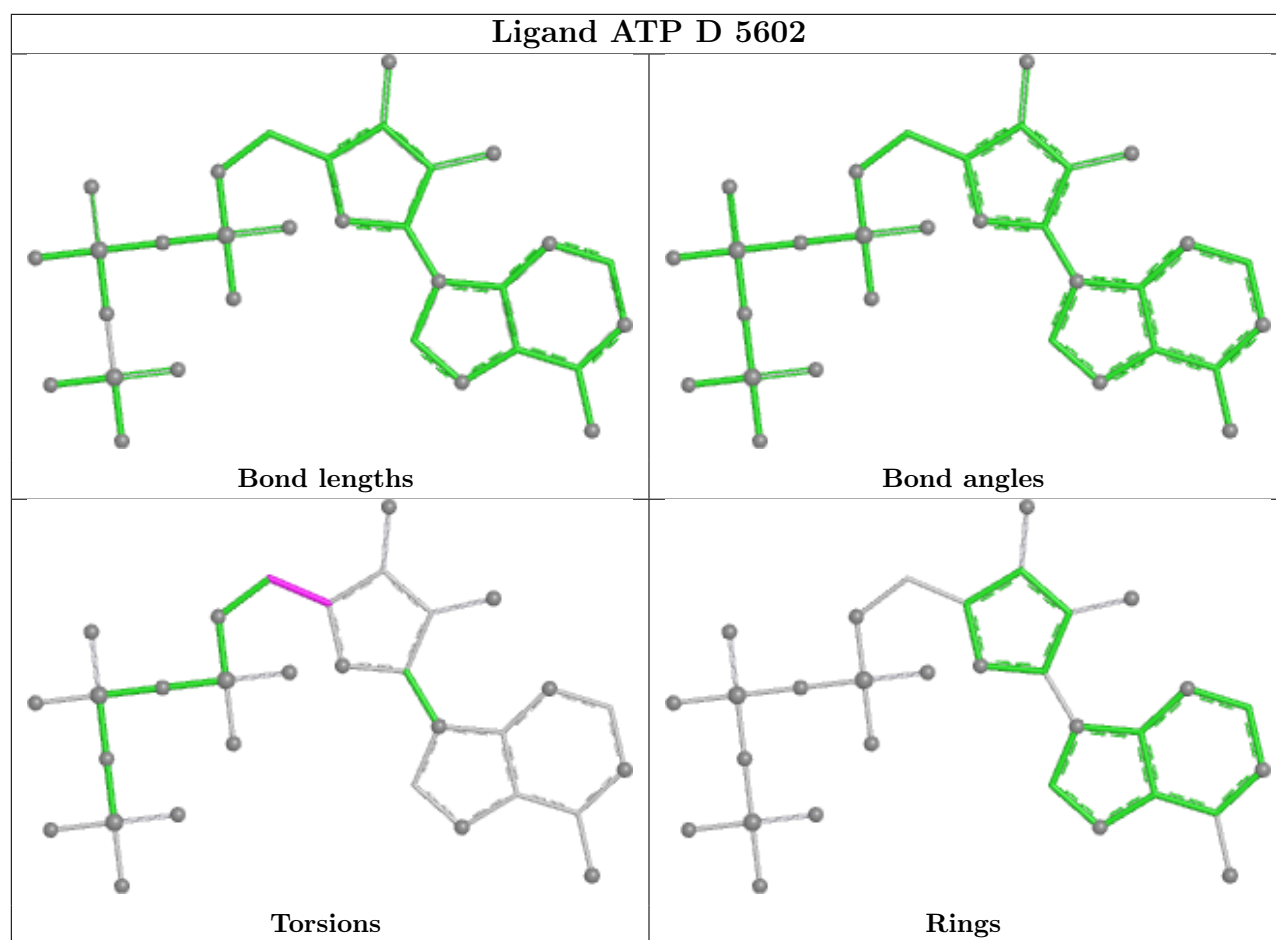
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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.

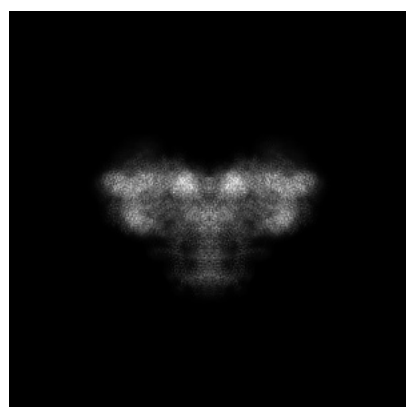
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74438. These allow visual inspection of the internal detail of the map and identification of artifacts.

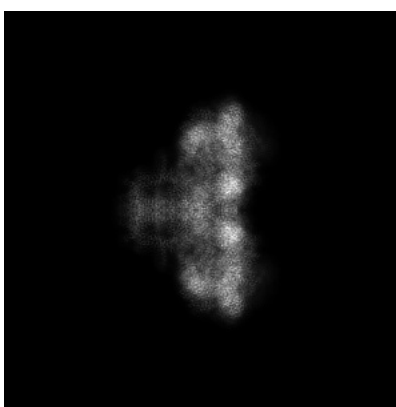
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

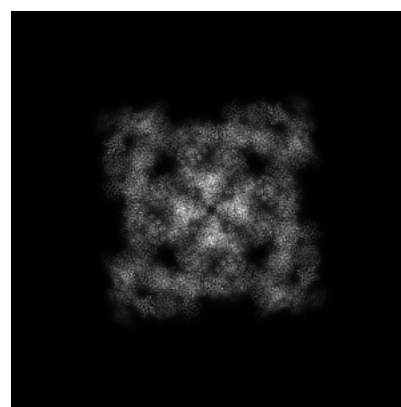
6.1.1 Primary map



X



Y

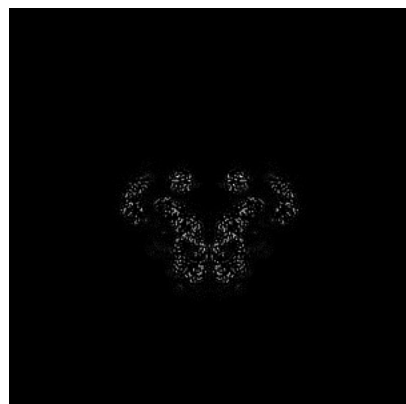


Z

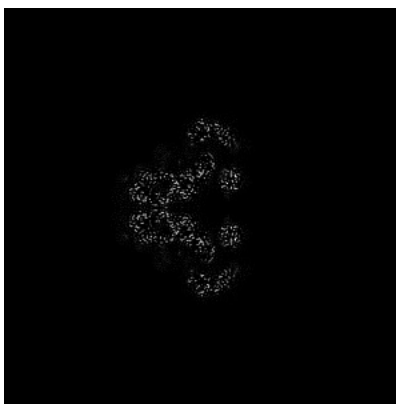
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

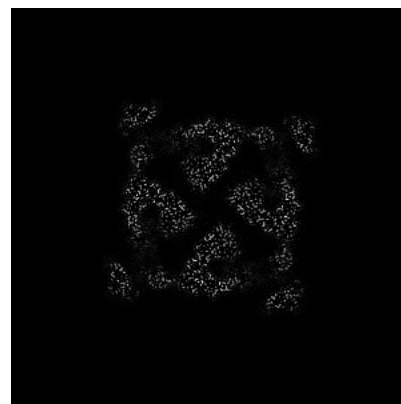
6.2.1 Primary map



X Index: 300



Y Index: 300

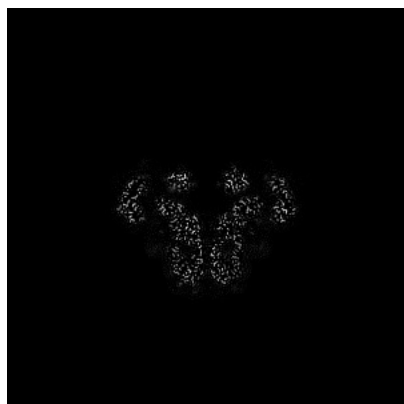


Z Index: 300

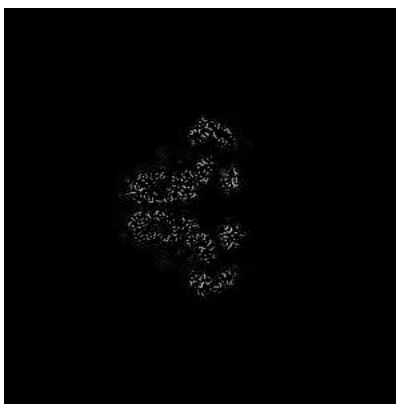
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

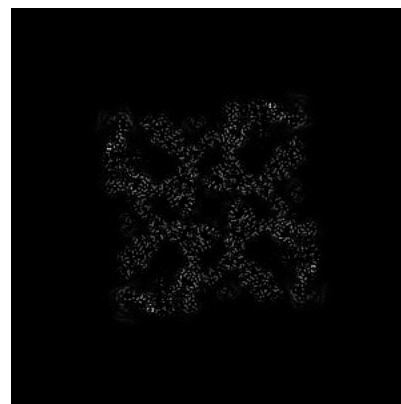
6.3.1 Primary map



X Index: 302



Y Index: 302

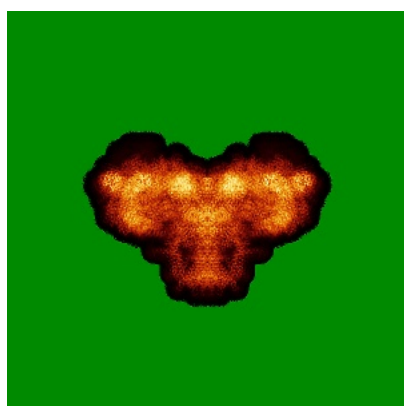


Z Index: 338

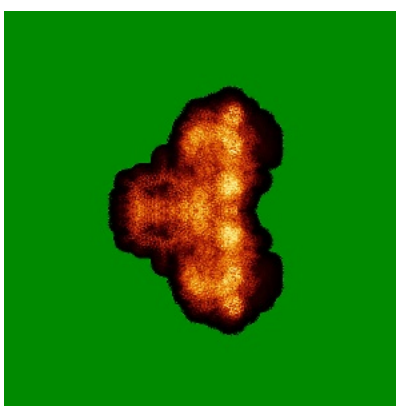
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

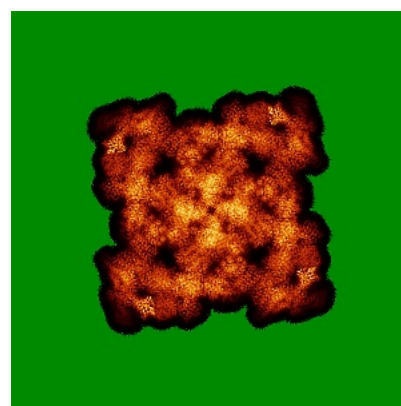
6.4.1 Primary map



X



Y

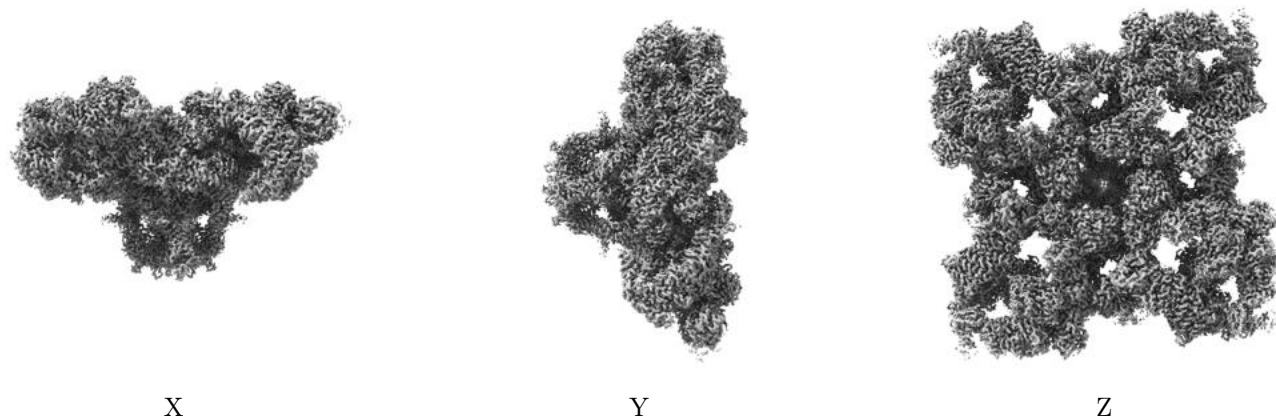


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

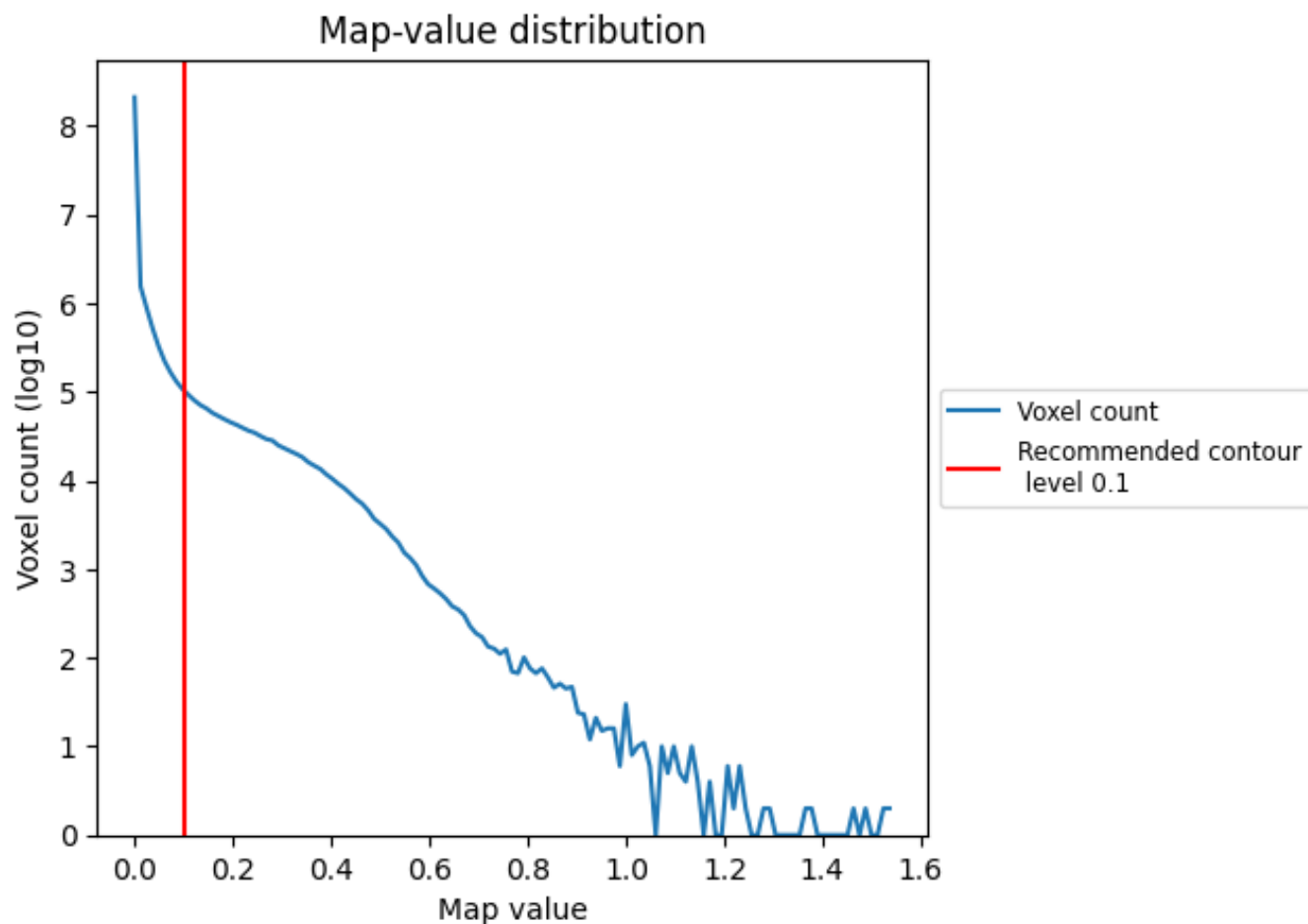
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

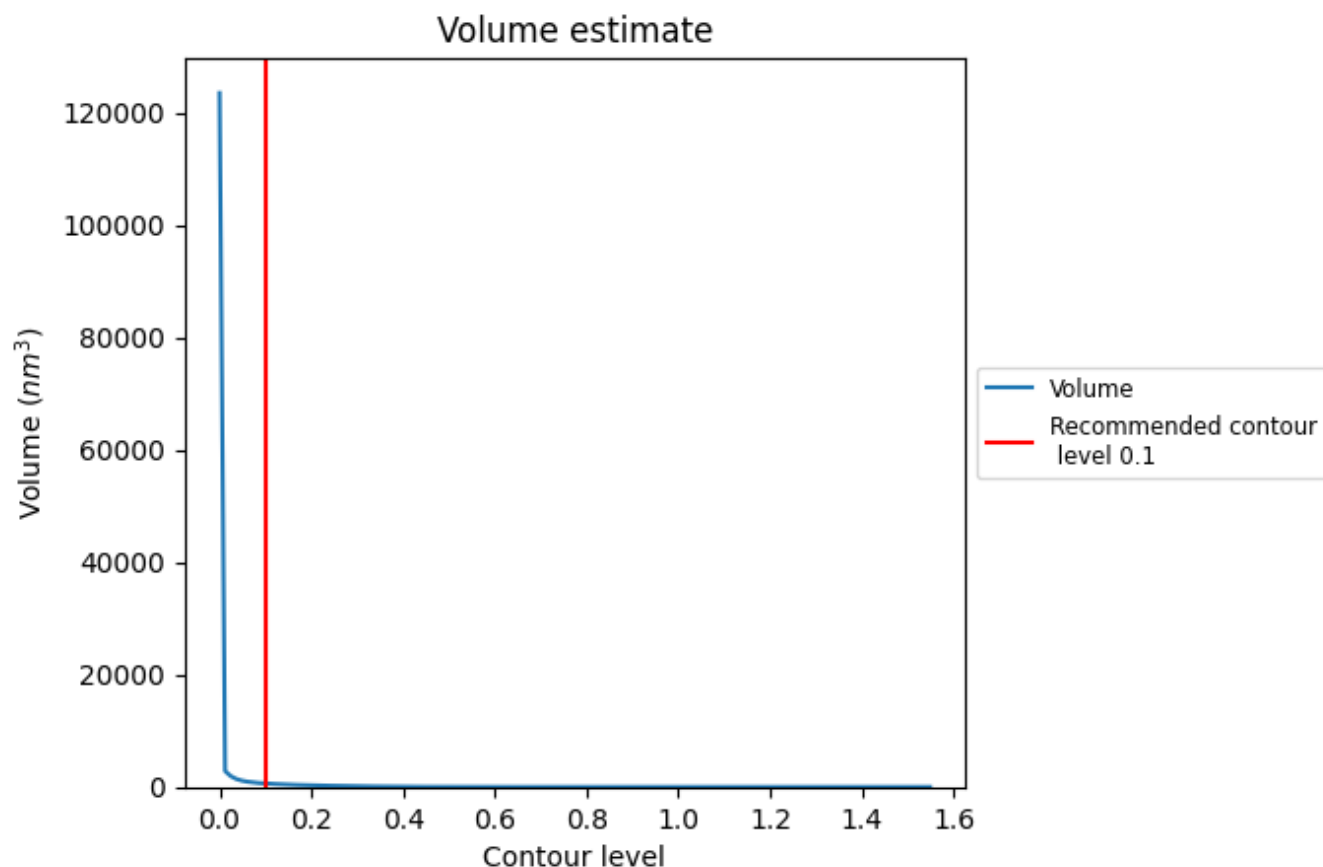
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

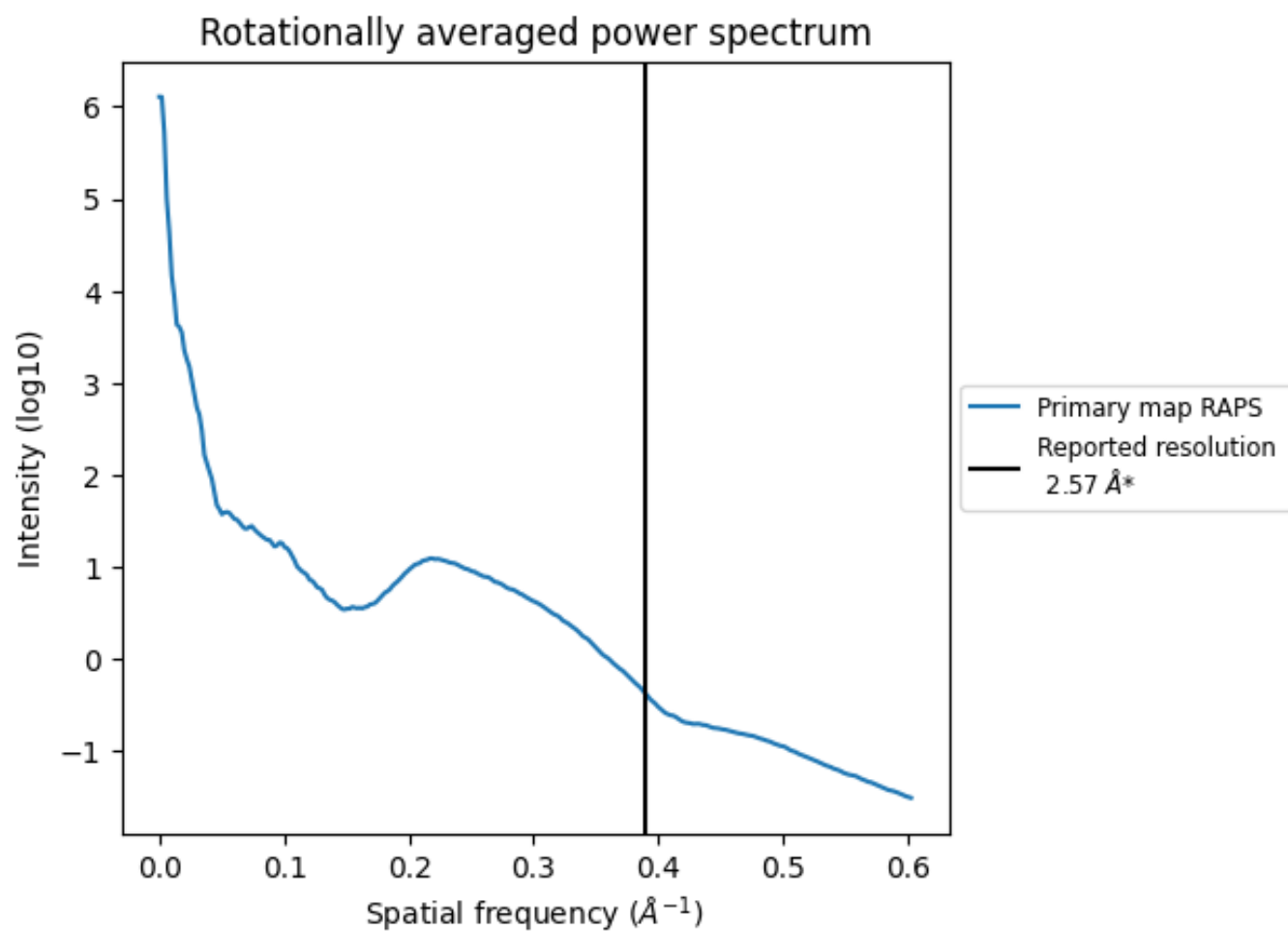
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 620 nm^3 ; this corresponds to an approximate mass of 560 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.389 Å⁻¹

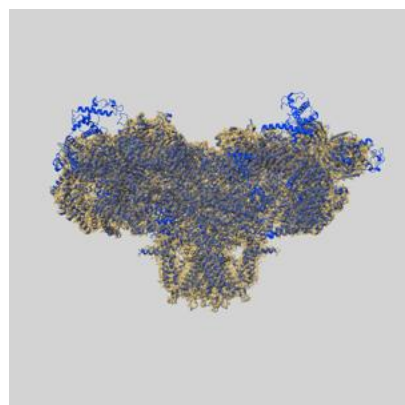
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

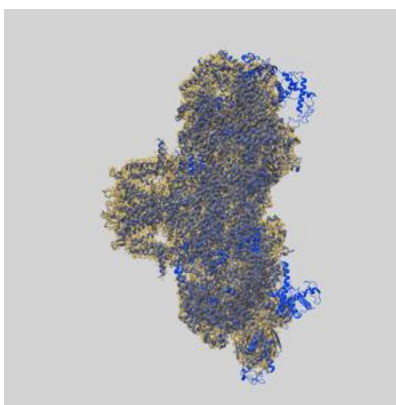
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-74438 and PDB model 9ZN8. Per-residue inclusion information can be found in section [3](#) on page [7](#).

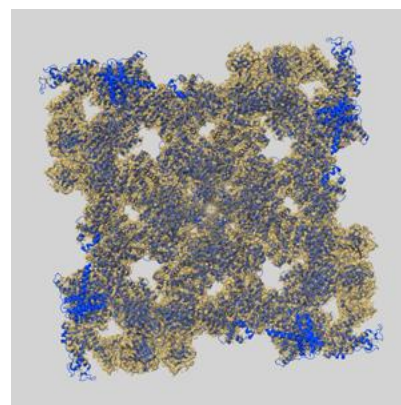
9.1 Map-model overlay [i](#)



X



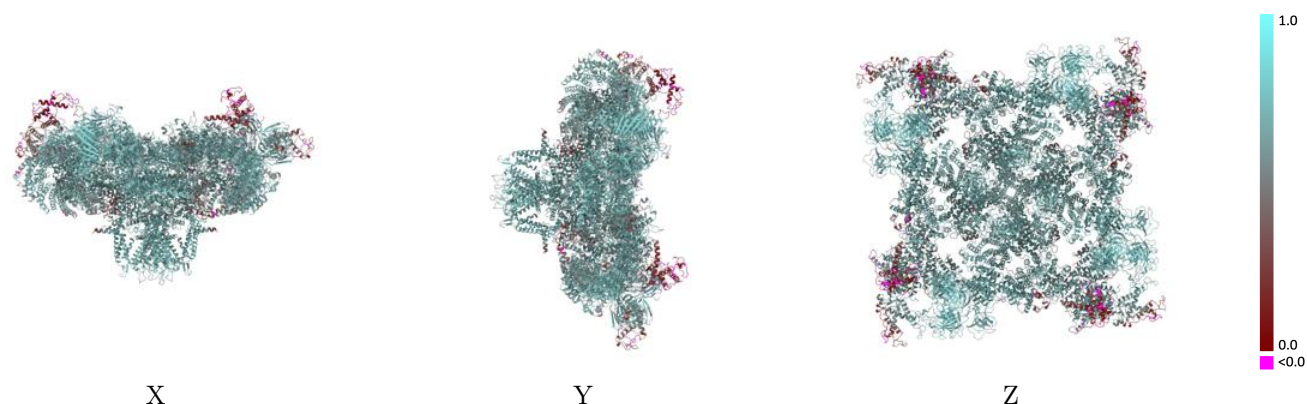
Y



Z

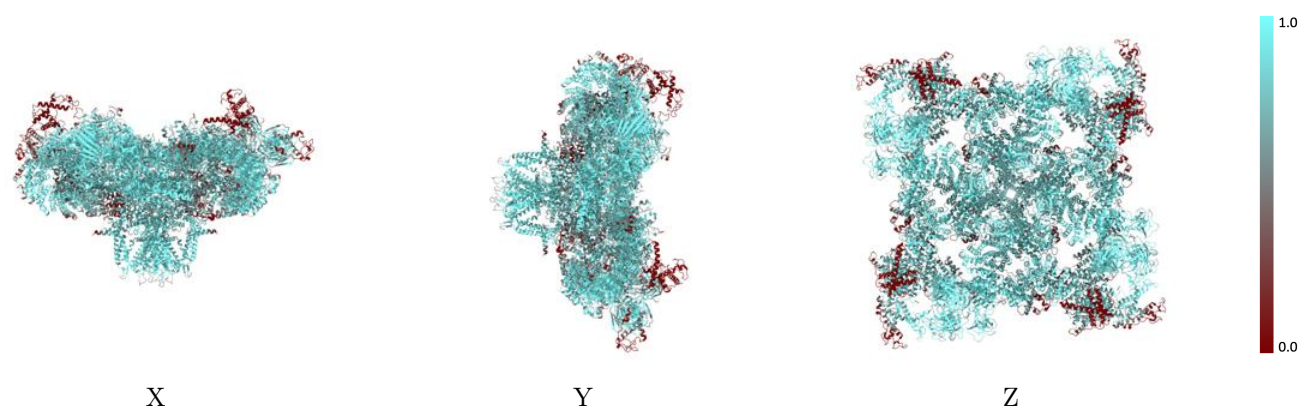
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



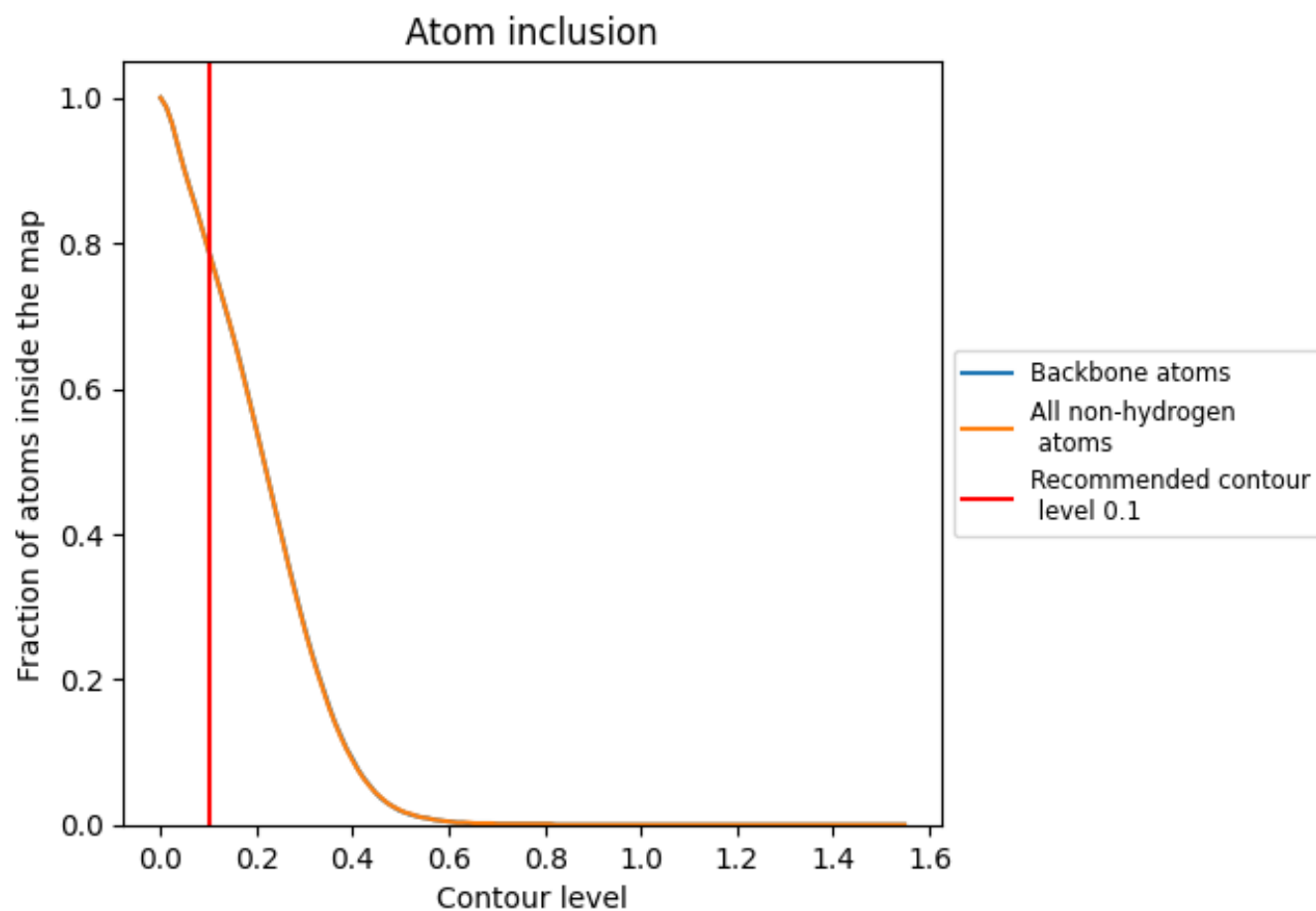
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7890	0.6200
A	0.8020	0.6230
B	0.8020	0.6230
C	0.8020	0.6230
D	0.8020	0.6240
E	0.8930	0.6690
F	0.8950	0.6660
G	0.8910	0.6660
H	0.8930	0.6670
I	0.4080	0.4860
J	0.4160	0.4870
K	0.4140	0.4840
L	0.4160	0.4840

1.0

0.0

<0.0