



wwPDB EM Map/Model Validation Report ⓘ

Oct 17, 2016 – 01:54 PM EDT

PDB ID : 5T9N
EMDB ID: : EMD-8373
Title : Structure of rabbit RyR1 (Ca²⁺-only dataset, class 2)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on : 2016-09-09
Resolution : 3.80 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

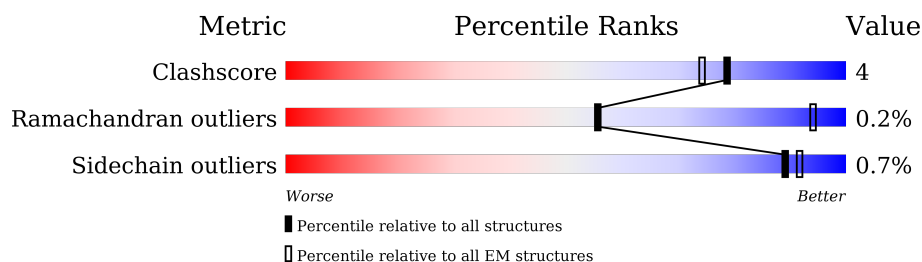
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	108	88% 11% .
1	F	108	88% 11% .
1	H	108	88% 11% .
1	J	108	88% 11% .
2	B	4676	81% 8% 11%
2	E	4676	81% 8% 11%
2	G	4676	81% 8% 11%
2	I	4676	81% 8% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 120756 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	E	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	I	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	G	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	G	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	


- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	G	1	Total 1	Ca 1	0
4	B	1	Total 1	Ca 1	0
4	I	1	Total 1	Ca 1	0
4	E	1	Total 1	Ca 1	0

3 Residue-property plots


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

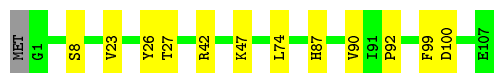
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 



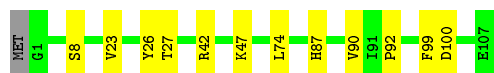
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A: 




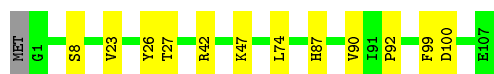
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 




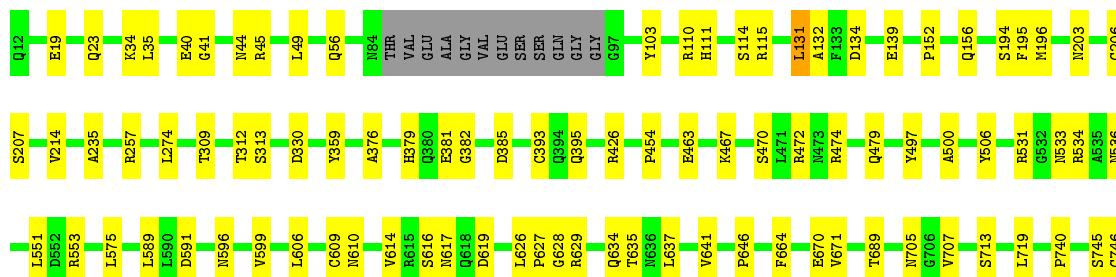
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 

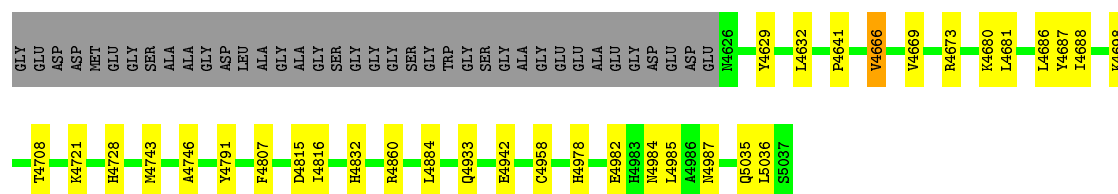


- Molecule 2: Ryanodine receptor 1

Chain B: 

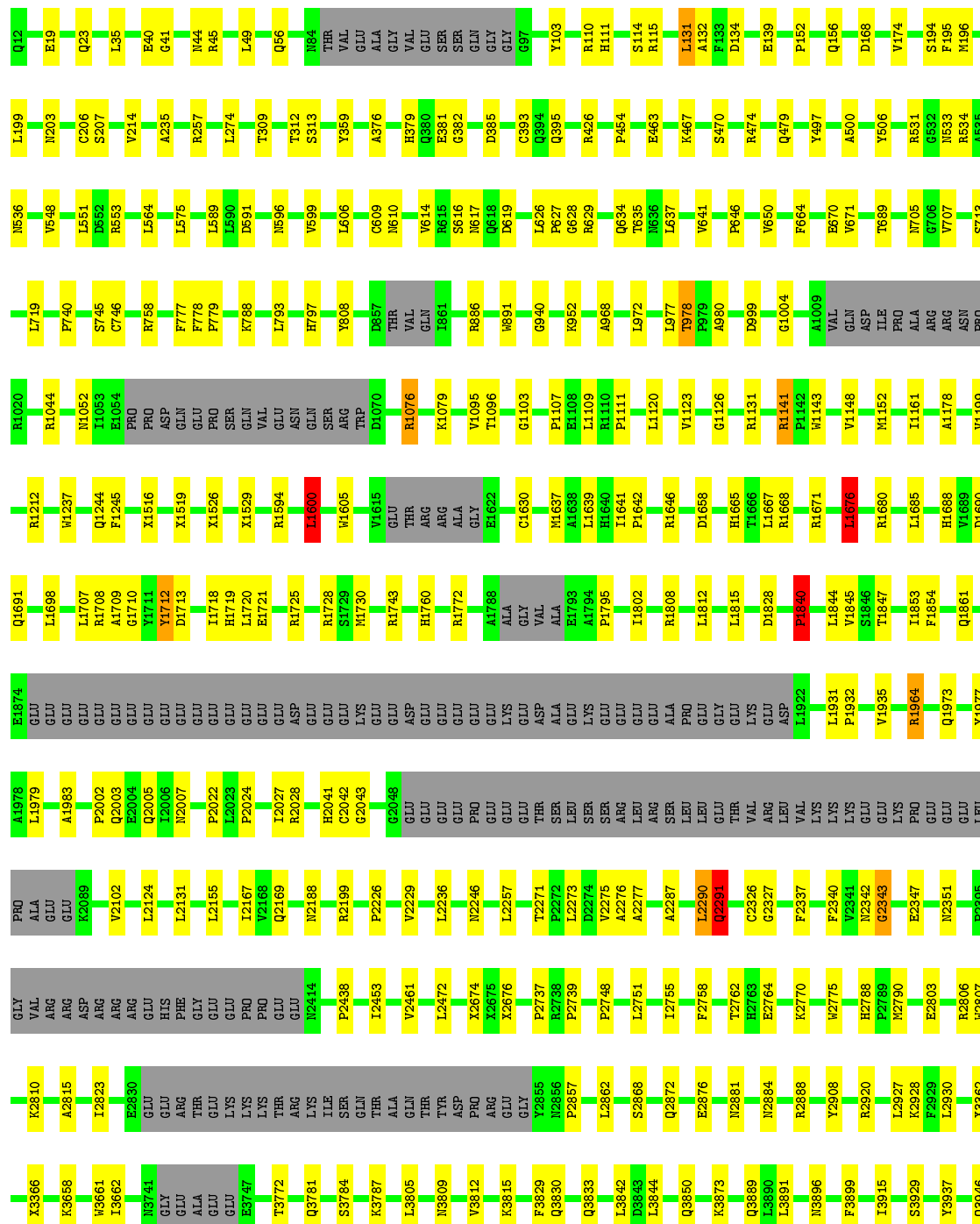




• Molecule 2: Ryanodine receptor 1

Chain E: 81% 8% 11%








GLU	PRO	GLU	LYS	ALA	ASP	GLU	ASN	GLY	GLY	LYS	GLU	GLU	VAL	PRO	GLU	ALA	PRO	PRO	GLU	PRO	PRO	LYS	LYS	ALA	PRO	PRO	SER	PRO	PRO	ALA	LYS	LYS	GLU	GLU	ALA	GLY	GLY	MET	GLU	P4540	M4553	L4567	L4577	Y4580	K4581	V4582	P4587	GLY	GLU	ASP	ASP
MET	GLU	GLY	SER	ALA	ALA	GLY	ASP	LEU	ALA	GLY	GLY	GLY	GLY	SER	GLY	GLY	SER	GLY	TRP	GLY	SER	GLY	ALA	GLU	GLU	ALA	GLU	GLY	ASP	GLU	ASP	GLU	N4626	L4632	P4641	V4666	V4669	R4673	K4680	L4681	L4686	Y4687	I4688	K4698	T4708	K4721	H4728				

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.31	0/834	0.52	0/1123
1	F	0.31	0/834	0.52	0/1123
1	H	0.31	0/834	0.52	0/1123
1	J	0.31	0/834	0.52	0/1123
2	B	0.31	0/25428	0.55	8/34534 (0.0%)
2	E	0.31	0/25428	0.55	8/34534 (0.0%)
2	G	0.31	0/25428	0.55	8/34534 (0.0%)
2	I	0.31	0/25428	0.55	8/34534 (0.0%)
All	All	0.31	0/105048	0.55	32/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	17
2	E	0	17
2	G	0	17
2	I	0	17
All	All	0	72

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	131	LEU	CA-CB-CG	8.36	134.52	115.30
2	B	131	LEU	CA-CB-CG	8.34	134.49	115.30
2	I	131	LEU	CA-CB-CG	8.34	134.49	115.30
2	G	131	LEU	CA-CB-CG	8.34	134.49	115.30
2	I	1600	LEU	CA-CB-CG	6.97	131.32	115.30
2	G	1600	LEU	CA-CB-CG	6.96	131.30	115.30
2	E	1600	LEU	CA-CB-CG	6.95	131.29	115.30
2	B	1600	LEU	CA-CB-CG	6.94	131.27	115.30
2	G	1676	LEU	CA-CB-CG	6.52	130.29	115.30
2	I	1676	LEU	CA-CB-CG	6.49	130.24	115.30
2	E	1676	LEU	CA-CB-CG	6.49	130.23	115.30
2	B	1676	LEU	CA-CB-CG	6.49	130.22	115.30
2	B	977	LEU	CA-CB-CG	5.36	127.62	115.30
2	I	977	LEU	CA-CB-CG	5.34	127.59	115.30
2	E	977	LEU	CA-CB-CG	5.34	127.59	115.30
2	G	977	LEU	CA-CB-CG	5.33	127.56	115.30
2	E	2290	LEU	CA-CB-CG	5.20	127.26	115.30
2	G	2290	LEU	CA-CB-CG	5.20	127.25	115.30
2	I	2290	LEU	CA-CB-CG	5.19	127.23	115.30
2	B	2290	LEU	CA-CB-CG	5.17	127.20	115.30
2	G	2291	GLN	C-N-CA	5.14	134.55	121.70
2	B	2291	GLN	C-N-CA	5.13	134.53	121.70
2	E	2291	GLN	C-N-CA	5.13	134.52	121.70
2	I	2291	GLN	C-N-CA	5.13	134.51	121.70
2	G	4985	LEU	CA-CB-CG	5.13	127.09	115.30
2	I	4985	LEU	CA-CB-CG	5.12	127.08	115.30
2	B	4985	LEU	CA-CB-CG	5.12	127.07	115.30
2	E	4985	LEU	CA-CB-CG	5.10	127.03	115.30
2	I	1667	LEU	CA-CB-CG	5.05	126.92	115.30
2	B	1667	LEU	CA-CB-CG	5.04	126.90	115.30
2	E	1667	LEU	CA-CB-CG	5.03	126.88	115.30
2	G	1667	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

All (72) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1712	TYR	Peptide
2	B	1795	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	2291	GLN	Peptide
2	B	2342	ASN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	312	THR	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide
2	E	1712	TYR	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	2291	GLN	Peptide
2	E	2342	ASN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	312	THR	Peptide
2	E	3971	GLY	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	Peptide
2	G	1712	TYR	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2342	ASN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide

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Mol	Chain	Res	Type	Group
2	G	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	Peptide
2	I	1712	TYR	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	2291	GLN	Peptide
2	I	2342	ASN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	312	THR	Peptide
2	I	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	6	0
1	F	818	0	824	7	0
1	H	818	0	824	6	0
1	J	818	0	824	6	0
2	B	29369	0	24723	198	0
2	E	29369	0	24722	194	0
2	G	29369	0	24722	196	0
2	I	29369	0	24722	198	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	120756	0	102185	789	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 4.

All (789) 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)
2:G:4958:CYS:SG	2:G:4978:HIS:CD2	2.67	0.87
2:I:4958:CYS:SG	2:I:4978:HIS:CD2	2.67	0.87
2:E:4958:CYS:SG	2:E:4978:HIS:CD2	2.67	0.87
2:B:4958:CYS:SG	2:B:4978:HIS:CD2	2.67	0.87
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.75	0.68
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.75	0.68
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.27	0.68
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.27	0.67
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.75	0.67
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.77	0.67
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.77	0.67
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.27	0.67
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.77	0.66
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.78	0.66
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.27	0.66
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.77	0.66
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.78	0.66
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.78	0.65
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.76	0.65
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.77	0.65
2:B:2764:GLU:HG3	2:B:2857:PRO:HB2	1.79	0.65
2:G:2764:GLU:HG3	2:G:2857:PRO:HB2	1.79	0.65
2:I:2764:GLU:HG3	2:I:2857:PRO:HB2	1.79	0.64
2:E:2764:GLU:HG3	2:E:2857:PRO:HB2	1.79	0.64
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.81	0.62
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.82	0.62
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.82	0.62
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.34	0.61
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.65	0.61
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.33	0.61
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.33	0.61
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.33	0.61
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.82	0.61
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.65	0.61
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.34	0.61
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.65	0.61
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.65	0.60
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.34	0.60
2:E:670:GLU:HG3	2:E:788:LYS:H	1.66	0.60
2:G:670:GLU:HG3	2:G:788:LYS:H	1.66	0.60
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.33	0.60
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.34	0.60
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.34	0.60
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.34	0.60
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.34	0.60
2:B:670:GLU:HG3	2:B:788:LYS:H	1.66	0.60
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.34	0.60
2:I:670:GLU:HG3	2:I:788:LYS:H	1.66	0.59
2:E:2131:LEU:HB3	2:E:3662:ILE:HD13	1.85	0.59
2:G:2131:LEU:HB3	2:G:3662:ILE:HD13	1.85	0.59
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.83	0.59
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.84	0.59
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	1.84	0.59
2:G:4184:MET:HB3	2:G:4190:ILE:HD13	1.85	0.59
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.85	0.59
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	1.85	0.59
2:I:2131:LEU:HB3	2:I:3662:ILE:HD13	1.85	0.59
2:B:2131:LEU:HB3	2:B:3662:ILE:HD13	1.85	0.58
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.85	0.58
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	1.85	0.58
2:B:4184:MET:HB3	2:B:4190:ILE:HD13	1.85	0.58
2:E:4184:MET:HB3	2:E:4190:ILE:HD13	1.85	0.58
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.85	0.58
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.69	0.58
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.68	0.58
2:B:609:CYS:SG	2:B:610:ASN:N	2.77	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:606:LEU:O	2:B:617:ASN:ND2	2.37	0.58
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.85	0.58
2:I:4184:MET:HB3	2:I:4190:ILE:HD13	1.85	0.58
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	1.84	0.57
2:I:41:GLY:O	2:I:45:ARG:NH1	2.37	0.57
2:I:609:CYS:SG	2:I:610:ASN:N	2.77	0.57
2:E:41:GLY:O	2:E:45:ARG:NH1	2.37	0.57
2:G:111:HIS:HD2	2:G:114:SER:H	1.51	0.57
2:G:606:LEU:O	2:G:617:ASN:ND2	2.37	0.57
2:I:111:HIS:HD2	2:I:114:SER:H	1.51	0.57
1:A:27:THR:HB	1:A:100:ASP:HB3	1.87	0.57
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.35	0.57
2:B:41:GLY:O	2:B:45:ARG:NH1	2.37	0.57
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.68	0.57
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.68	0.57
2:I:4832:HIS:NE2	2:I:4942:GLU:OE1	2.38	0.57
2:I:606:LEU:O	2:I:617:ASN:ND2	2.37	0.57
2:E:606:LEU:O	2:E:617:ASN:ND2	2.37	0.57
1:F:27:THR:HB	1:F:100:ASP:HB3	1.87	0.57
2:B:379:HIS:HD2	2:B:382:GLY:H	1.53	0.57
2:E:609:CYS:SG	2:E:610:ASN:N	2.77	0.57
1:J:27:THR:HB	1:J:100:ASP:HB3	1.87	0.57
2:B:4791:TYR:OH	2:B:4815:ASP:O	2.23	0.57
2:G:41:GLY:O	2:G:45:ARG:NH1	2.37	0.57
2:G:626:LEU:HG	2:G:628:GLY:H	1.70	0.57
2:I:626:LEU:HG	2:I:628:GLY:H	1.70	0.56
2:B:4832:HIS:NE2	2:B:4942:GLU:OE1	2.38	0.56
2:G:609:CYS:SG	2:G:610:ASN:N	2.77	0.56
2:I:379:HIS:HD2	2:I:382:GLY:H	1.53	0.56
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.88	0.56
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.87	0.56
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.35	0.56
2:B:111:HIS:HD2	2:B:114:SER:H	1.51	0.56
2:I:4791:TYR:OH	2:I:4815:ASP:O	2.23	0.56
2:B:626:LEU:HG	2:B:628:GLY:H	1.70	0.56
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.87	0.56
2:E:4791:TYR:OH	2:E:4815:ASP:O	2.23	0.56
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.88	0.56
2:G:1730:MET:O	2:G:1772:ARG:NH1	2.39	0.56
1:H:27:THR:HB	1:H:100:ASP:HB3	1.87	0.56
2:E:111:HIS:HD2	2:E:114:SER:H	1.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.87	0.56
2:E:1730:MET:O	2:E:1772:ARG:NH1	2.39	0.56
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.87	0.56
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.88	0.56
2:E:626:LEU:HG	2:E:628:GLY:H	1.70	0.56
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.87	0.56
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.87	0.55
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.88	0.55
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.78	0.55
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.39	0.55
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.88	0.55
2:G:379:HIS:HD2	2:G:382:GLY:H	1.53	0.55
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.87	0.55
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.39	0.55
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.88	0.55
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.78	0.55
2:G:4791:TYR:OH	2:G:4815:ASP:O	2.23	0.55
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.88	0.55
2:B:2347:GLU:O	2:B:2351:ASN:N	2.40	0.55
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.88	0.55
2:B:1730:MET:O	2:B:1772:ARG:NH1	2.39	0.55
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.89	0.55
2:G:2347:GLU:O	2:G:2351:ASN:N	2.40	0.55
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.87	0.55
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.89	0.55
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.88	0.55
2:I:1730:MET:O	2:I:1772:ARG:NH1	2.39	0.55
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.88	0.55
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.39	0.55
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.88	0.55
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.78	0.54
2:E:379:HIS:HD2	2:E:382:GLY:H	1.53	0.54
2:G:4152:GLU:OE1	2:G:4192:ARG:NH2	2.41	0.54
2:E:4832:HIS:NE2	2:E:4942:GLU:OE1	2.38	0.54
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.89	0.54
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.88	0.54
2:E:56:GLN:O	2:E:309:THR:OG1	2.26	0.54
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.89	0.54
2:I:2758:PHE:O	2:I:2762:THR:N	2.40	0.54
2:E:4152:GLU:OE1	2:E:4192:ARG:NH2	2.41	0.54
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:56:GLN:O	2:G:309:THR:OG1	2.26	0.54
2:I:2347:GLU:O	2:I:2351:ASN:N	2.40	0.54
2:G:132:ALA:HA	2:G:194:SER:HB2	1.89	0.54
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.90	0.54
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.90	0.54
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.39	0.54
2:I:132:ALA:HA	2:I:194:SER:HB2	1.89	0.54
2:B:132:ALA:HA	2:B:194:SER:HB2	1.89	0.54
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.35	0.54
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.90	0.54
2:G:1148:VAL:HG21	2:G:1212:ARG:HG2	1.90	0.54
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.90	0.54
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.90	0.54
2:I:4152:GLU:OE1	2:I:4192:ARG:NH2	2.41	0.54
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.90	0.53
2:B:2876:GLU:OE1	2:B:2920:ARG:NH2	2.41	0.53
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.90	0.53
2:E:132:ALA:HA	2:E:194:SER:HB2	1.89	0.53
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.90	0.53
2:G:309:THR:O	2:G:313:SER:OG	2.26	0.53
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.89	0.53
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.39	0.53
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.90	0.53
2:I:309:THR:O	2:I:313:SER:OG	2.26	0.53
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.39	0.53
2:G:2758:PHE:O	2:G:2762:THR:N	2.40	0.53
2:B:4152:GLU:OE1	2:B:4192:ARG:NH2	2.41	0.53
2:I:2876:GLU:OE1	2:I:2920:ARG:NH2	2.41	0.53
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.90	0.53
2:E:1148:VAL:HG21	2:E:1212:ARG:HG2	1.90	0.53
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.90	0.53
2:B:1148:VAL:HG21	2:B:1212:ARG:HG2	1.90	0.53
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.41	0.53
2:E:2876:GLU:OE1	2:E:2920:ARG:NH2	2.41	0.53
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.90	0.53
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.90	0.53
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.74	0.53
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.39	0.53
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.90	0.52
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.35	0.52
2:I:56:GLN:O	2:I:309:THR:OG1	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.90	0.52
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.91	0.52
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.42	0.52
2:G:23:GLN:OE1	2:G:203:ASN:ND2	2.42	0.52
2:G:2876:GLU:OE1	2:G:2920:ARG:NH2	2.41	0.52
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.90	0.52
2:I:1148:VAL:HG21	2:I:1212:ARG:HG2	1.90	0.52
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.42	0.52
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.42	0.52
2:B:56:GLN:O	2:B:309:THR:OG1	2.26	0.52
2:I:4933:GLN:NE2	2:G:4933:GLN:OE1	2.43	0.52
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.91	0.52
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.75	0.52
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.39	0.52
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.91	0.52
2:B:4978:HIS:ND1	2:B:4982:GLU:OE1	2.39	0.52
2:E:2758:PHE:O	2:E:2762:THR:N	2.40	0.52
2:E:309:THR:O	2:E:313:SER:OG	2.26	0.52
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.42	0.52
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.91	0.52
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.78	0.52
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.91	0.52
2:I:23:GLN:OE1	2:I:203:ASN:ND2	2.42	0.52
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.42	0.52
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.91	0.52
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.43	0.52
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.83	0.52
2:E:23:GLN:OE1	2:E:203:ASN:ND2	2.42	0.52
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.92	0.52
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.42	0.52
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.43	0.52
2:G:454:PRO:HG2	2:G:531:ARG:HH12	1.74	0.52
2:G:4832:HIS:NE2	2:G:4942:GLU:OE1	2.38	0.52
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.43	0.52
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.75	0.52
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.43	0.51
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.43	0.51
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.91	0.51
2:E:454:PRO:HG2	2:E:531:ARG:HH12	1.74	0.51
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.42	0.51
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:689:THR:H	2:G:778:PHE:HE2	1.58	0.51
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.75	0.51
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.43	0.51
2:I:4567:LEU:HD12	2:I:4816:ILE:HD12	1.93	0.51
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.42	0.51
2:B:4567:LEU:HD12	2:B:4816:ILE:HD12	1.93	0.51
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.43	0.51
2:B:454:PRO:HG2	2:B:531:ARG:HH12	1.74	0.51
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.83	0.51
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.83	0.51
2:E:2347:GLU:O	2:E:2351:ASN:N	2.40	0.51
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.91	0.51
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.83	0.51
2:E:4567:LEU:HD12	2:E:4816:ILE:HD12	1.93	0.51
2:G:1245:PHE:HD1	2:G:1600:LEU:HB3	1.76	0.51
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.92	0.51
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	1.93	0.51
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	1.93	0.51
2:E:1245:PHE:HD1	2:E:1600:LEU:HB3	1.76	0.51
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.42	0.51
2:B:2758:PHE:O	2:B:2762:THR:N	2.40	0.51
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.93	0.51
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.92	0.51
2:B:309:THR:O	2:B:313:SER:OG	2.26	0.51
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.75	0.51
2:G:4567:LEU:HD12	2:G:4816:ILE:HD12	1.93	0.51
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.41	0.51
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.92	0.51
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.43	0.51
2:B:4933:GLN:OE1	2:E:4933:GLN:NE2	2.43	0.51
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.39	0.51
2:I:4581:LYS:HD2	2:I:4632:LEU:HD22	1.93	0.51
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.41	0.50
2:I:689:THR:H	2:I:778:PHE:HE2	1.58	0.50
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.92	0.50
2:B:689:THR:H	2:B:778:PHE:HE2	1.58	0.50
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.92	0.50
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.77	0.50
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.92	0.50
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.93	0.50
2:I:4984:ASN:ND2	2:I:4987:ASN:OD1	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.93	0.50
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	1.93	0.50
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.77	0.50
2:B:4933:GLN:NE2	2:I:4933:GLN:OE1	2.44	0.50
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.93	0.50
2:B:4138:ASP:OD1	2:B:4138:ASP:N	2.44	0.50
2:E:4984:ASN:ND2	2:E:4987:ASN:OD1	2.38	0.50
2:E:689:THR:H	2:E:778:PHE:HE2	1.58	0.50
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.94	0.50
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.94	0.50
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.77	0.50
2:E:4581:LYS:HD2	2:E:4632:LEU:HD22	1.94	0.50
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.77	0.49
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.46	0.49
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	1.93	0.49
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.94	0.49
2:B:4581:LYS:HD2	2:B:4632:LEU:HD22	1.94	0.49
2:B:2236:LEU:HD23	2:B:2275:VAL:HG21	1.94	0.49
2:G:627:PRO:O	2:G:629:ARG:NH1	2.46	0.49
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.92	0.49
2:I:1245:PHE:HD1	2:I:1600:LEU:HB3	1.76	0.49
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.92	0.49
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.39	0.49
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.77	0.49
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.94	0.49
2:I:2236:LEU:HD23	2:I:2275:VAL:HG21	1.94	0.49
2:G:4581:LYS:HD2	2:G:4632:LEU:HD22	1.93	0.49
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.45	0.49
2:I:627:PRO:O	2:I:629:ARG:NH1	2.46	0.49
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.95	0.49
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.77	0.49
2:B:1245:PHE:HD1	2:B:1600:LEU:HB3	1.76	0.49
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.95	0.49
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.46	0.48
2:B:627:PRO:O	2:B:629:ARG:NH1	2.46	0.48
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.95	0.48
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.95	0.48
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.95	0.48
2:E:2236:LEU:HD23	2:E:2275:VAL:HG21	1.94	0.48
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.95	0.48
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.77	0.48
2:E:4978:HIS:ND1	2:E:4982:GLU:OE1	2.39	0.48
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	1.96	0.48
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.95	0.48
2:G:2236:LEU:HD23	2:G:2275:VAL:HG21	1.94	0.48
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	1.96	0.48
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.39	0.48
1:F:26:TYR:OH	1:F:42:ARG:NH2	2.47	0.48
2:G:999:ASP:O	2:G:1004:GLY:N	2.47	0.48
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	1.96	0.48
1:J:26:TYR:OH	1:J:42:ARG:NH2	2.47	0.48
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	1.95	0.48
2:B:940:GLY:O	2:B:1052:ASN:N	2.47	0.48
2:G:4984:ASN:ND2	2:G:4987:ASN:OD1	2.38	0.48
2:I:1131:ARG:NH1	2:I:1178:ALA:O	2.47	0.48
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.95	0.48
2:I:940:GLY:O	2:I:1052:ASN:N	2.47	0.48
2:I:999:ASP:O	2:I:1004:GLY:N	2.47	0.48
2:B:1131:ARG:NH1	2:B:1178:ALA:O	2.47	0.48
2:G:1516:UNK:N	2:G:1529:UNK:O	2.47	0.48
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.87	0.48
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.96	0.48
2:B:999:ASP:O	2:B:1004:GLY:N	2.47	0.48
2:E:940:GLY:O	2:E:1052:ASN:N	2.47	0.48
2:E:1131:ARG:NH1	2:E:1178:ALA:O	2.47	0.48
2:E:1244:GLN:OE1	2:E:1646:ARG:NH1	2.47	0.48
2:E:1516:UNK:N	2:E:1529:UNK:O	2.47	0.48
2:E:627:PRO:O	2:E:629:ARG:NH1	2.46	0.48
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.95	0.48
2:I:1244:GLN:OE1	2:I:1646:ARG:NH1	2.47	0.48
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.96	0.48
1:A:26:TYR:OH	1:A:42:ARG:NH2	2.47	0.48
2:B:1516:UNK:N	2:B:1529:UNK:O	2.47	0.48
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.95	0.48
2:G:1131:ARG:NH1	2:G:1178:ALA:O	2.47	0.48
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	1.95	0.48
2:G:614:VAL:HA	2:G:2169:GLN:HB3	1.96	0.48
2:I:1516:UNK:N	2:I:1529:UNK:O	2.47	0.48
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.87	0.47
2:E:359:TYR:HA	2:E:376:ALA:HA	1.96	0.47
2:E:999:ASP:O	2:E:1004:GLY:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1244:GLN:OE1	2:B:1646:ARG:NH1	2.47	0.47
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.80	0.47
2:E:614:VAL:HA	2:E:2169:GLN:HB3	1.96	0.47
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.96	0.47
2:G:2868:SER:O	2:G:2872:GLN:N	2.45	0.47
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	1.95	0.47
2:I:359:TYR:HA	2:I:376:ALA:HA	1.96	0.47
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.95	0.47
2:G:359:TYR:HA	2:G:376:ALA:HA	1.96	0.47
1:H:26:TYR:OH	1:H:42:ARG:NH2	2.47	0.47
2:I:1720:LEU:HD12	2:I:1847:THR:HG23	1.97	0.47
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.87	0.47
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.97	0.47
2:I:2868:SER:O	2:I:2872:GLN:N	2.45	0.47
2:B:359:TYR:HA	2:B:376:ALA:HA	1.96	0.47
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.95	0.47
2:G:1720:LEU:HD12	2:G:1847:THR:HG23	1.97	0.47
2:G:793:LEU:HD12	2:G:797:HIS:H	1.80	0.47
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.96	0.47
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.49	0.47
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.96	0.47
2:G:1244:GLN:OE1	2:G:1646:ARG:NH1	2.47	0.47
2:G:1973:GLN:O	2:G:1977:TYR:N	2.47	0.47
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.96	0.47
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.95	0.47
2:I:1815:LEU:HD22	2:I:1845:VAL:HG21	1.97	0.47
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.97	0.47
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.96	0.47
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.49	0.47
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.80	0.47
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	1.95	0.47
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.77	0.47
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	1.96	0.47
2:E:4138:ASP:N	2:E:4138:ASP:OD1	2.44	0.47
2:G:940:GLY:O	2:G:1052:ASN:N	2.47	0.47
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.95	0.47
2:E:4933:GLN:OE1	2:G:4933:GLN:NE2	2.46	0.47
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.96	0.47
2:E:1720:LEU:HD12	2:E:1847:THR:HG23	1.97	0.47
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.49	0.47
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.96	0.47
2:B:1815:LEU:HD22	2:B:1845:VAL:HG21	1.97	0.47
2:B:1973:GLN:O	2:B:1977:TYR:N	2.47	0.47
2:E:793:LEU:HD12	2:E:797:HIS:H	1.80	0.47
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.49	0.47
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.96	0.47
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.97	0.47
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.33	0.47
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.96	0.47
2:G:470:SER:O	2:G:474:ARG:NE	2.46	0.47
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.79	0.47
2:I:2908:TYR:OH	2:I:2920:ARG:NE	2.44	0.47
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.33	0.47
2:B:1720:LEU:HD12	2:B:1847:THR:HG23	1.97	0.46
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.33	0.46
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.81	0.46
2:G:614:VAL:HG22	2:G:616:SER:H	1.79	0.46
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.41	0.46
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.96	0.46
2:E:1973:GLN:O	2:E:1977:TYR:N	2.47	0.46
2:E:3809:ASN:HB3	2:E:3812:VAL:HG22	1.97	0.46
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.80	0.46
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.49	0.46
2:B:614:VAL:HA	2:B:2169:GLN:HB3	1.96	0.46
2:B:793:LEU:HD12	2:B:797:HIS:H	1.80	0.46
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.97	0.46
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.81	0.46
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.33	0.46
2:I:614:VAL:HG22	2:I:616:SER:H	1.79	0.46
2:B:614:VAL:HG22	2:B:616:SER:H	1.79	0.46
2:G:1815:LEU:HD22	2:G:1845:VAL:HG21	1.97	0.46
2:G:4138:ASP:N	2:G:4138:ASP:OD1	2.44	0.46
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.81	0.46
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.81	0.46
2:E:1815:LEU:HD22	2:E:1845:VAL:HG21	1.97	0.46
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.80	0.46
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.81	0.46
2:G:1840:PRO:O	2:G:1844:LEU:N	2.48	0.46
2:B:470:SER:O	2:B:474:ARG:NE	2.45	0.46
2:E:1808:ARG:HD2	2:E:1854:PHE:HA	1.98	0.46
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:793:LEU:HD12	2:I:797:HIS:H	1.80	0.46
2:E:1840:PRO:O	2:E:1844:LEU:N	2.48	0.46
2:E:614:VAL:HG22	2:E:616:SER:H	1.79	0.46
2:G:1808:ARG:HD2	2:G:1854:PHE:HA	1.98	0.46
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.51	0.46
2:I:1840:PRO:O	2:I:1844:LEU:N	2.48	0.46
2:I:614:VAL:HA	2:I:2169:GLN:HB3	1.96	0.46
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.51	0.45
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.49	0.45
2:B:3809:ASN:HB3	2:B:3812:VAL:HG22	1.97	0.45
2:B:235:ALA:HA	2:B:257:ARG:HD3	1.98	0.45
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.49	0.45
2:G:3809:ASN:HB3	2:G:3812:VAL:HG22	1.97	0.45
2:I:235:ALA:HA	2:I:257:ARG:HD3	1.98	0.45
2:I:4708:THR:O	2:I:4721:LYS:NZ	2.48	0.45
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.49	0.45
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.51	0.45
2:I:1808:ARG:HD2	2:I:1854:PHE:HA	1.98	0.45
2:I:379:HIS:CD2	2:I:381:GLU:H	2.35	0.45
2:I:4978:HIS:ND1	2:I:4982:GLU:OE1	2.39	0.45
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.99	0.45
2:E:235:ALA:HA	2:E:257:ARG:HD3	1.98	0.45
2:E:2868:SER:O	2:E:2872:GLN:N	2.45	0.45
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	1.99	0.45
2:G:379:HIS:CD2	2:G:381:GLU:H	2.35	0.45
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	1.98	0.45
2:I:1973:GLN:O	2:I:1977:TYR:N	2.47	0.45
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.51	0.45
2:I:3842:LEU:O	2:I:3929:SER:OG	2.35	0.45
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.98	0.45
2:B:134:ASP:OD1	2:B:134:ASP:N	2.49	0.45
2:B:2908:TYR:OH	2:B:2920:ARG:NE	2.44	0.45
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.51	0.45
2:G:4978:HIS:ND1	2:G:4982:GLU:OE1	2.39	0.45
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.98	0.45
2:I:4138:ASP:N	2:I:4138:ASP:OD1	2.44	0.45
2:I:4688:ILE:HG21	2:I:4728:HIS:HB3	1.99	0.45
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.99	0.45
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.51	0.45
2:B:1808:ARG:HD2	2:B:1854:PHE:HA	1.98	0.45
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.50	0.45
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.50	0.45
2:G:4036:VAL:HG11	2:G:5035:GLN:HB3	1.99	0.45
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.99	0.45
2:I:4036:VAL:HG11	2:I:5035:GLN:HB3	1.99	0.45
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.81	0.44
2:B:1840:PRO:O	2:B:1844:LEU:N	2.48	0.44
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.50	0.44
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.99	0.44
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.99	0.44
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.51	0.44
2:G:3842:LEU:O	2:G:3929:SER:OG	2.35	0.44
2:I:3809:ASN:HB3	2:I:3812:VAL:HG22	1.97	0.44
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.99	0.44
2:B:4036:VAL:HG11	2:B:5035:GLN:HB3	1.99	0.44
2:B:4059:LEU:HD13	2:B:4167:ALA:HB2	1.99	0.44
2:B:4688:ILE:HG21	2:B:4728:HIS:HB3	1.99	0.44
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.99	0.44
2:E:4059:LEU:HD13	2:E:4167:ALA:HB2	1.99	0.44
2:G:4577:LEU:HG	2:G:4580:TYR:HE2	1.83	0.44
2:I:4681:LEU:HD21	2:I:4687:TYR:HD2	1.82	0.44
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	1.99	0.44
2:E:134:ASP:N	2:E:134:ASP:OD1	2.49	0.44
2:E:4681:LEU:HD21	2:E:4687:TYR:HD2	1.82	0.44
2:E:4036:VAL:HG11	2:E:5035:GLN:HB3	1.99	0.44
2:G:134:ASP:OD1	2:G:134:ASP:N	2.49	0.44
2:G:235:ALA:HA	2:G:257:ARG:HD3	1.98	0.44
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.99	0.44
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.99	0.44
2:B:3842:LEU:O	2:B:3929:SER:OG	2.35	0.44
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.98	0.44
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.99	0.44
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	2.00	0.44
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	2.00	0.44
2:B:379:HIS:CD2	2:B:381:GLU:H	2.35	0.44
2:B:4629:TYR:OH	2:I:4860:ARG:NH2	2.49	0.44
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.98	0.44
2:E:978:THR:HB	2:E:980:ALA:H	1.82	0.44
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	1.99	0.44
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	2.00	0.44
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.99	0.44
2:B:385:ASP:HB2	2:I:156:GLN:HE21	1.83	0.44
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.82	0.44
2:E:379:HIS:CD2	2:E:381:GLU:H	2.35	0.44
2:G:1096:THR:HG23	2:G:1199:VAL:HG22	2.00	0.44
2:G:4092:ASP:OD1	2:G:4092:ASP:N	2.51	0.44
2:I:4059:LEU:HD13	2:I:4167:ALA:HB2	1.99	0.44
2:I:4228:ALA:O	2:I:4232:GLU:N	2.51	0.44
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.99	0.44
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	1.99	0.44
2:B:1096:THR:HG23	2:B:1199:VAL:HG22	2.00	0.44
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	2.00	0.44
2:B:4228:ALA:O	2:B:4232:GLU:N	2.51	0.44
2:B:4708:THR:O	2:B:4721:LYS:NZ	2.48	0.44
2:E:4233:LEU:HA	2:E:4236:SER:HB3	2.00	0.44
2:G:978:THR:HB	2:G:980:ALA:H	1.82	0.44
2:I:470:SER:O	2:I:474:ARG:NE	2.46	0.44
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	1.99	0.43
2:G:2024:PRO:O	2:G:2028:ARG:NE	2.47	0.43
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.82	0.43
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	2.00	0.43
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	2.00	0.43
2:I:4577:LEU:HG	2:I:4580:TYR:HE2	1.83	0.43
2:B:4577:LEU:HG	2:B:4580:TYR:HE2	1.83	0.43
2:E:3842:LEU:O	2:E:3929:SER:OG	2.35	0.43
2:B:4233:LEU:HA	2:B:4236:SER:HB3	2.00	0.43
2:B:596:ASN:HB3	2:B:599:VAL:HG22	2.01	0.43
2:B:978:THR:HB	2:B:980:ALA:H	1.82	0.43
2:E:1096:THR:HG23	2:E:1199:VAL:HG22	2.00	0.43
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	2.00	0.43
2:G:4228:ALA:O	2:G:4232:GLU:N	2.51	0.43
2:G:596:ASN:HB3	2:G:599:VAL:HG22	2.00	0.43
2:I:2024:PRO:O	2:I:2028:ARG:NE	2.47	0.43
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.99	0.43
2:I:596:ASN:HB3	2:I:599:VAL:HG22	2.00	0.43
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	2.00	0.43
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	2.01	0.43
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	2.00	0.43
2:G:2908:TYR:OH	2:G:2920:ARG:NE	2.44	0.43
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	2.00	0.43
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1096:THR:HG23	2:I:1199:VAL:HG22	2.00	0.43
2:I:134:ASP:OD1	2:I:134:ASP:N	2.49	0.43
2:I:1979:LEU:HA	2:I:1983:ALA:HB3	2.01	0.43
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	2.00	0.43
2:E:426:ARG:HB2	2:E:506:TYR:HA	2.01	0.43
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.99	0.43
2:B:426:ARG:HB2	2:B:506:TYR:HA	2.01	0.43
2:E:4251:ILE:HG22	2:E:4553:ASN:HD22	1.84	0.43
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	2.01	0.43
2:I:637:LEU:HD23	2:I:1637:MET:HB3	2.01	0.43
2:B:195:PHE:HB3	2:B:196:MET:HG2	2.00	0.43
2:B:1979:LEU:HA	2:B:1983:ALA:HB3	2.01	0.43
2:B:206:CYS:SG	2:B:207:SER:N	2.92	0.43
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.52	0.43
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.99	0.43
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	2.01	0.43
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.99	0.43
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.83	0.43
1:F:34:LYS:HD3	2:E:629:ARG:HD2	2.00	0.43
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	2.01	0.43
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.99	0.43
2:G:4708:THR:O	2:G:4721:LYS:NZ	2.48	0.43
2:E:4914:VAL:HG21	2:G:4884:LEU:HD11	2.01	0.43
2:G:637:LEU:HD23	2:G:1637:MET:HB3	2.01	0.43
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	2.00	0.43
2:G:195:PHE:HB3	2:G:196:MET:HG2	2.00	0.43
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.48	0.43
2:I:551:LEU:HD21	2:I:589:LEU:HD13	2.01	0.43
2:I:886:ARG:HB3	2:I:891:TRP:HB2	2.01	0.43
2:B:2102:VAL:HB	2:B:2124:LEU:HD12	2.01	0.43
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.48	0.43
2:E:596:ASN:HB3	2:E:599:VAL:HG22	2.00	0.43
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	2.00	0.43
2:G:1707:LEU:O	2:G:1709:ALA:N	2.52	0.43
2:E:156:GLN:HE21	2:G:385:ASP:HB2	1.84	0.43
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.84	0.43
2:I:2102:VAL:HB	2:I:2124:LEU:HD12	2.01	0.43
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.99	0.42
2:E:206:CYS:SG	2:E:207:SER:N	2.92	0.42
2:G:206:CYS:SG	2:G:207:SER:N	2.92	0.42
2:E:174:VAL:O	2:G:2452:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4059:LEU:HD13	2:G:4167:ALA:HB2	1.99	0.42
2:G:629:ARG:HD3	2:G:634:GLN:HG2	2.01	0.42
2:I:4092:ASP:OD1	2:I:4092:ASP:N	2.51	0.42
2:I:4233:LEU:HA	2:I:4236:SER:HB3	2.00	0.42
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	2.00	0.42
2:E:195:PHE:HB3	2:E:196:MET:HG2	2.00	0.42
2:E:1979:LEU:HA	2:E:1983:ALA:HB3	2.00	0.42
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.52	0.42
2:E:2908:TYR:OH	2:E:2920:ARG:NE	2.44	0.42
2:E:4092:ASP:N	2:E:4092:ASP:OD1	2.51	0.42
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.53	0.42
2:G:3362:UNK:O	2:G:3366:UNK:N	2.53	0.42
2:G:886:ARG:HB3	2:G:891:TRP:HB2	2.01	0.42
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.51	0.42
2:I:195:PHE:HB3	2:I:196:MET:HG2	2.00	0.42
2:I:4251:ILE:HG22	2:I:4553:ASN:HD22	1.84	0.42
2:B:2342:ASN:N	2:B:2342:ASN:OD1	2.41	0.42
2:B:4984:ASN:ND2	2:B:4987:ASN:OD1	2.38	0.42
2:B:637:LEU:HD23	2:B:1637:MET:HB3	2.01	0.42
2:E:3362:UNK:O	2:E:3366:UNK:N	2.53	0.42
2:G:4251:ILE:HG22	2:G:4553:ASN:HD22	1.84	0.42
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	2.01	0.42
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.84	0.42
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.53	0.42
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.52	0.42
2:G:4233:LEU:HA	2:G:4236:SER:HB3	2.00	0.42
2:I:206:CYS:SG	2:I:207:SER:N	2.92	0.42
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.52	0.42
2:I:3362:UNK:O	2:I:3366:UNK:N	2.53	0.42
2:I:978:THR:HB	2:I:980:ALA:H	1.82	0.42
2:B:1760:HIS:HE1	2:B:2041:HIS:HA	1.85	0.42
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	2.01	0.42
2:B:19:GLU:HB2	2:B:206:CYS:HB3	2.01	0.42
2:B:629:ARG:HD3	2:B:634:GLN:HG2	2.01	0.42
2:E:1707:LEU:O	2:E:1709:ALA:N	2.52	0.42
2:E:4228:ALA:O	2:E:4232:GLU:N	2.51	0.42
2:E:4708:THR:O	2:E:4721:LYS:NZ	2.48	0.42
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.85	0.42
2:G:479:GLN:HE21	2:G:536:ASN:ND2	2.18	0.42
2:B:1707:LEU:O	2:B:1709:ALA:N	2.52	0.42
2:B:551:LEU:HD21	2:B:589:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:551:LEU:HD21	2:E:589:LEU:HD13	2.01	0.42
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	2.00	0.42
2:I:1707:LEU:O	2:I:1709:ALA:N	2.52	0.42
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.53	0.42
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	2.01	0.42
2:G:19:GLU:HB2	2:G:206:CYS:HB3	2.01	0.42
2:G:3662:ILE:HG13	2:G:3662:ILE:H	1.73	0.42
2:B:1671:ARG:NH2	2:B:1713:ASP:HB3	2.35	0.42
2:B:886:ARG:HB3	2:B:891:TRP:HB2	2.01	0.42
2:E:168:ASP:HB3	2:E:199:LEU:HD22	2.02	0.42
2:E:2102:VAL:HB	2:E:2124:LEU:HD12	2.01	0.42
2:E:479:GLN:HE21	2:E:536:ASN:ND2	2.18	0.42
2:G:1979:LEU:HA	2:G:1983:ALA:HB3	2.00	0.42
2:G:2102:VAL:HB	2:G:2124:LEU:HD12	2.01	0.42
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.85	0.42
2:I:3891:LEU:HB3	2:I:3899:PHE:CE2	2.55	0.42
2:I:479:GLN:HE21	2:I:536:ASN:ND2	2.18	0.42
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.53	0.41
2:B:4092:ASP:OD1	2:B:4092:ASP:N	2.51	0.41
2:B:479:GLN:HE21	2:B:536:ASN:ND2	2.18	0.41
2:B:864:PRO:HA	2:B:865:PRO:HD3	1.92	0.41
2:E:637:LEU:HD23	2:E:1637:MET:HB3	2.01	0.41
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.32	0.41
2:G:551:LEU:HD21	2:G:589:LEU:HD13	2.01	0.41
2:I:19:GLU:HB2	2:I:206:CYS:HB3	2.01	0.41
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.85	0.41
2:B:3362:UNK:O	2:B:3366:UNK:N	2.53	0.41
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.84	0.41
2:G:168:ASP:HB3	2:G:199:LEU:HD22	2.02	0.41
2:G:1671:ARG:NH2	2:G:1713:ASP:HB3	2.35	0.41
2:G:4815:ASP:N	2:G:4815:ASP:OD1	2.53	0.41
2:G:426:ARG:HB2	2:G:506:TYR:HA	2.01	0.41
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	2.00	0.41
2:E:2788:HIS:CE1	2:E:2790:MET:HB2	2.56	0.41
2:B:4860:ARG:NH2	2:E:4629:TYR:OH	2.50	0.41
2:E:629:ARG:HD3	2:E:634:GLN:HG2	2.01	0.41
2:B:156:GLN:HE21	2:E:385:ASP:HB2	1.85	0.41
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	2.03	0.41
2:B:3891:LEU:HB3	2:B:3899:PHE:CE2	2.55	0.41
2:B:4884:LEU:HD11	2:I:4914:VAL:HG21	2.03	0.41
2:E:19:GLU:HB2	2:E:206:CYS:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	2.02	0.41
2:E:3891:LEU:HB3	2:E:3899:PHE:CE2	2.55	0.41
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.85	0.41
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	2.01	0.41
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.84	0.41
2:I:1760:HIS:HE1	2:I:2041:HIS:HA	1.85	0.41
2:I:426:ARG:HB2	2:I:506:TYR:HA	2.01	0.41
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	2.02	0.41
2:B:2788:HIS:CE1	2:B:2790:MET:HB2	2.56	0.41
2:E:591:ASP:O	2:E:1594:ARG:NH2	2.54	0.41
2:E:886:ARG:HB3	2:E:891:TRP:HB2	2.01	0.41
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	2.02	0.41
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	2.03	0.41
2:G:4201:ASN:HA	2:G:4204:GLN:HB3	2.03	0.41
2:G:582:HIS:O	2:G:585:SER:OG	2.29	0.41
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.02	0.41
2:B:3829:PHE:HD1	2:B:3915:ILE:HD11	1.86	0.41
2:E:2290:LEU:HG	2:E:2291:GLN:H	1.85	0.41
2:E:2815:ALA:HB3	2:E:2881:ASN:HD21	1.86	0.41
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.53	0.41
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	2.02	0.41
2:I:2290:LEU:HG	2:I:2291:GLN:H	1.86	0.41
2:I:330:ASP:N	2:I:330:ASP:OD1	2.54	0.41
2:I:3829:PHE:HD1	2:I:3915:ILE:HD11	1.86	0.41
2:I:3927:GLN:NE2	2:I:3988:ALA:O	2.50	0.41
2:B:2868:SER:O	2:B:2872:GLN:N	2.45	0.41
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	2.02	0.41
2:E:1658:ASP:N	2:E:1658:ASP:OD1	2.54	0.41
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.85	0.41
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	2.02	0.41
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	2.03	0.41
2:I:2788:HIS:CE1	2:I:2790:MET:HB2	2.56	0.41
2:B:214:VAL:HG12	2:B:274:LEU:HD12	2.03	0.41
2:B:4251:ILE:HG22	2:B:4553:ASN:HD22	1.84	0.41
2:E:1671:ARG:NH2	2:E:1713:ASP:HB3	2.35	0.41
2:G:3891:LEU:HB3	2:G:3899:PHE:CE2	2.55	0.41
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	2.01	0.41
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	2.02	0.41
2:B:2815:ALA:HB3	2:B:2881:ASN:HD21	1.86	0.41
2:E:1641:ILE:HA	2:E:1642:PRO:HD3	1.96	0.41
2:E:1760:HIS:HE1	2:E:2041:HIS:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2024:PRO:O	2:E:2028:ARG:NE	2.47	0.41
2:G:330:ASP:OD1	2:G:330:ASP:N	2.54	0.41
2:I:629:ARG:HD3	2:I:634:GLN:HG2	2.01	0.41
2:B:2024:PRO:O	2:B:2028:ARG:NE	2.47	0.41
2:B:2188:ASN:N	2:B:2188:ASN:OD1	2.54	0.41
2:B:2290:LEU:HG	2:B:2291:GLN:H	1.86	0.41
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	2.02	0.41
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	2.03	0.41
2:E:470:SER:O	2:E:474:ARG:NE	2.46	0.41
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	2.02	0.41
2:G:1676:LEU:HD23	2:G:2167:ILE:HG23	2.03	0.41
2:G:2788:HIS:CE1	2:G:2790:MET:HB2	2.55	0.41
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.86	0.41
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	2.02	0.41
2:I:4201:ASN:HA	2:I:4204:GLN:HB3	2.03	0.41
2:I:591:ASP:O	2:I:1594:ARG:NH2	2.54	0.41
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	2.02	0.41
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.52	0.41
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.85	0.41
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.03	0.41
2:I:2452:ARG:NH1	2:G:174:VAL:O	2.54	0.41
2:G:2815:ALA:HB3	2:G:2881:ASN:HD21	1.86	0.41
2:I:1725:ARG:HH21	2:I:1725:ARG:HD2	1.71	0.41
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.53	0.41
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.86	0.40
2:B:330:ASP:N	2:B:330:ASP:OD1	2.54	0.40
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	2.02	0.40
2:E:214:VAL:HG12	2:E:274:LEU:HD12	2.03	0.40
2:G:1658:ASP:OD1	2:G:1658:ASP:N	2.54	0.40
2:G:3829:PHE:HD1	2:G:3915:ILE:HD11	1.86	0.40
2:I:1671:ARG:NH2	2:I:1713:ASP:HB3	2.36	0.40
2:B:1131:ARG:HH12	2:B:1178:ALA:HB3	1.86	0.40
2:B:1658:ASP:N	2:B:1658:ASP:OD1	2.54	0.40
2:E:1141:ARG:HD2	2:E:1141:ARG:H	1.86	0.40
2:E:3844:LEU:HD23	2:E:3844:LEU:HA	1.92	0.40
2:G:1141:ARG:HD2	2:G:1141:ARG:H	1.86	0.40
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.51	0.40
2:I:168:ASP:HB3	2:I:199:LEU:HD22	2.02	0.40
2:I:2815:ALA:HB3	2:I:2881:ASN:HD21	1.86	0.40
2:I:3662:ILE:H	2:I:3662:ILE:HG13	1.73	0.40
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:591:ASP:O	2:B:1594:ARG:NH2	2.54	0.40
2:E:3829:PHE:HD1	2:E:3915:ILE:HD11	1.86	0.40
2:G:591:ASP:O	2:G:1594:ARG:NH2	2.54	0.40
2:G:2290:LEU:HG	2:G:2291:GLN:H	1.86	0.40
2:I:1131:ARG:HH12	2:I:1178:ALA:HB3	1.86	0.40
2:I:211:GLU:OE2	2:I:3907:THR:OG1	2.31	0.40
2:I:650:VAL:HB	2:I:777:PHE:HB2	2.04	0.40
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	2.04	0.40
2:B:2674:UNK:O	2:B:2676:UNK:N	2.54	0.40
2:B:23:GLN:HE21	2:B:34:LYS:HB3	1.87	0.40
2:E:548:VAL:HG12	2:E:564:LEU:HD22	2.04	0.40
2:E:650:VAL:HB	2:E:777:PHE:HB2	2.04	0.40
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.03	0.40
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	2.02	0.40
2:I:2437:ALA:HA	2:I:2438:PRO:HD3	1.93	0.40
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.48	0.40
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	2.04	0.40
2:B:4201:ASN:HA	2:B:4204:GLN:HB3	2.03	0.40
2:E:2674:UNK:O	2:E:2676:UNK:N	2.54	0.40
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	2.02	0.40
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.53	0.40
2:G:548:VAL:HG12	2:G:564:LEU:HD22	2.04	0.40
2:G:647:ASN:ND2	2:G:820:ARG:O	2.46	0.40
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	2.02	0.40
2:I:864:PRO:HA	2:I:865:PRO:HD3	1.92	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	A	105/108 (97%)	93 (89%)	12 (11%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	H	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	J	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	B	3235/4676 (69%)	2899 (90%)	330 (10%)	6 (0%)	52	86
2	E	3235/4676 (69%)	2899 (90%)	330 (10%)	6 (0%)	52	86
2	G	3235/4676 (69%)	2898 (90%)	331 (10%)	6 (0%)	52	86
2	I	3235/4676 (69%)	2899 (90%)	330 (10%)	6 (0%)	52	86
All	All	13360/19136 (70%)	11967 (90%)	1369 (10%)	24 (0%)	56	86

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	E	1708	ARG
2	I	1708	ARG
2	G	1708	ARG
2	B	1932	PRO
2	E	1932	PRO
2	I	1932	PRO
2	G	1932	PRO
2	B	1840	PRO
2	B	4641	PRO
2	E	1840	PRO
2	E	4641	PRO
2	I	1840	PRO
2	I	4641	PRO
2	G	1840	PRO
2	G	4641	PRO
2	E	2291	GLN
2	I	2291	GLN
2	G	2291	GLN
2	B	2291	GLN
2	B	2343	GLY
2	E	2343	GLY
2	I	2343	GLY
2	G	2343	GLY

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	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3202 (78%)	2476 (99%)	17 (1%)	88	95
2	E	2493/3202 (78%)	2476 (99%)	17 (1%)	88	95
2	G	2493/3202 (78%)	2476 (99%)	17 (1%)	88	95
2	I	2493/3202 (78%)	2476 (99%)	17 (1%)	88	95
All	All	10324/13164 (78%)	10256 (99%)	68 (1%)	89	95

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG
2	B	553	ARG
2	B	719	LEU
2	B	978	THR
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	2461	VAL
2	B	3787	LYS
2	B	3805	LEU
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	E	131	LEU
2	E	534	ARG

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Mol	Chain	Res	Type
2	E	553	ARG
2	E	719	LEU
2	E	978	THR
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	2461	VAL
2	E	3787	LYS
2	E	3805	LEU
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	719	LEU
2	I	978	THR
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	2461	VAL
2	I	3787	LYS
2	I	3805	LEU
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	719	LEU
2	G	978	THR
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG

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Mol	Chain	Res	Type
2	G	2461	VAL
2	G	3787	LYS
2	G	3805	LEU
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS
1	A	87	HIS
1	H	87	HIS
1	J	87	HIS
2	B	23	GLN
2	B	57	ASN
2	B	105	HIS
2	B	111	HIS
2	B	156	GLN
2	B	203	ASN
2	B	273	HIS
2	B	379	HIS
2	B	383	HIS
2	B	479	GLN
2	B	582	HIS
2	B	1158	ASN
2	B	1598	GLN
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	2005	GLN
2	B	2127	GLN
2	B	3771	HIS
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	4034	ASN
2	B	4120	ASN
2	B	4553	ASN
2	B	4806	ASN
2	E	23	GLN

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Mol	Chain	Res	Type
2	E	57	ASN
2	E	105	HIS
2	E	111	HIS
2	E	156	GLN
2	E	203	ASN
2	E	273	HIS
2	E	379	HIS
2	E	383	HIS
2	E	479	GLN
2	E	582	HIS
2	E	1158	ASN
2	E	1598	GLN
2	E	1688	HIS
2	E	1691	GLN
2	E	1693	GLN
2	E	1719	HIS
2	E	2005	GLN
2	E	2127	GLN
2	E	3771	HIS
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	4034	ASN
2	E	4120	ASN
2	E	4553	ASN
2	I	23	GLN
2	I	57	ASN
2	I	105	HIS
2	I	111	HIS
2	I	156	GLN
2	I	203	ASN
2	I	273	HIS
2	I	379	HIS
2	I	383	HIS
2	I	479	GLN
2	I	582	HIS
2	I	1158	ASN
2	I	1598	GLN
2	I	1691	GLN
2	I	1693	GLN
2	I	1719	HIS
2	I	2005	GLN

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Mol	Chain	Res	Type
2	I	2127	GLN
2	I	3771	HIS
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	4034	ASN
2	I	4120	ASN
2	I	4553	ASN
2	I	5003	HIS
2	G	23	GLN
2	G	57	ASN
2	G	105	HIS
2	G	111	HIS
2	G	156	GLN
2	G	203	ASN
2	G	273	HIS
2	G	379	HIS
2	G	383	HIS
2	G	479	GLN
2	G	582	HIS
2	G	1158	ASN
2	G	1598	GLN
2	G	1691	GLN
2	G	1693	GLN
2	G	1719	HIS
2	G	2005	GLN
2	G	2127	GLN
2	G	3771	HIS
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	4034	ASN
2	G	4120	ASN
2	G	4553	ASN
2	G	5003	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	G	12
2	B	12
2	I	12
2	E	12

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	3613:UNK	C	3639:THR	N	43.02
1	B	3613:UNK	C	3639:THR	N	43.01
1	E	3613:UNK	C	3639:THR	N	43.01
1	G	3613:UNK	C	3639:THR	N	42.96

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3163:UNK	C	3170:UNK	N	16.39
1	E	3163:UNK	C	3170:UNK	N	16.39
1	I	3163:UNK	C	3170:UNK	N	16.39
1	G	3163:UNK	C	3170:UNK	N	16.39
1	B	3468:UNK	C	3511:UNK	N	15.14
1	E	3468:UNK	C	3511:UNK	N	15.14
1	I	3468:UNK	C	3511:UNK	N	15.14
1	G	3468:UNK	C	3511:UNK	N	15.14
1	E	3063:UNK	C	3134:UNK	N	14.90
1	B	3063:UNK	C	3134:UNK	N	14.89
1	I	3063:UNK	C	3134:UNK	N	14.89
1	G	3063:UNK	C	3134:UNK	N	14.89
1	G	2703:UNK	C	2734:ASN	N	14.64
1	B	2703:UNK	C	2734:ASN	N	14.61
1	E	2703:UNK	C	2734:ASN	N	14.59
1	I	2703:UNK	C	2734:ASN	N	14.59
1	B	3236:UNK	C	3241:UNK	N	13.53
1	E	3236:UNK	C	3241:UNK	N	13.53
1	I	3236:UNK	C	3241:UNK	N	13.53
1	G	3236:UNK	C	3241:UNK	N	13.53
1	G	1564:UNK	C	1573:MET	N	12.52
1	B	1564:UNK	C	1573:MET	N	12.51
1	I	1564:UNK	C	1573:MET	N	12.51
1	E	1564:UNK	C	1573:MET	N	12.49
1	B	2976:UNK	C	2995:UNK	N	12.26
1	E	2976:UNK	C	2995:UNK	N	12.26
1	I	2976:UNK	C	2995:UNK	N	12.26
1	G	2976:UNK	C	2995:UNK	N	12.26
1	E	3254:UNK	C	3261:UNK	N	8.39
1	I	3254:UNK	C	3261:UNK	N	8.39
1	B	3254:UNK	C	3261:UNK	N	8.38
1	G	3254:UNK	C	3261:UNK	N	8.38
1	B	1297:UNK	C	1430:UNK	N	5.79
1	I	1297:UNK	C	1430:UNK	N	5.79
1	G	1297:UNK	C	1430:UNK	N	5.79
1	E	1297:UNK	C	1430:UNK	N	5.77
1	G	2939:ARG	C	2942:UNK	N	3.40
1	B	2939:ARG	C	2942:UNK	N	3.37
1	E	2939:ARG	C	2942:UNK	N	3.36
1	I	2939:ARG	C	2942:UNK	N	3.36
1	E	2479:LEU	C	2487:UNK	N	3.29
1	I	2479:LEU	C	2487:UNK	N	3.29

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	2479:LEU	C	2487:UNK	N	3.28
1	G	2479:LEU	C	2487:UNK	N	3.25