wwPDB EM Map/Model Validation Report (i)

Oct 17, 2016 – 07:14 PM EDT

PDB ID	:	5TAU
EMDB ID:	:	EMD-8385
Title	:	Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, class 3)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-10
Resolution	:	6.20 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

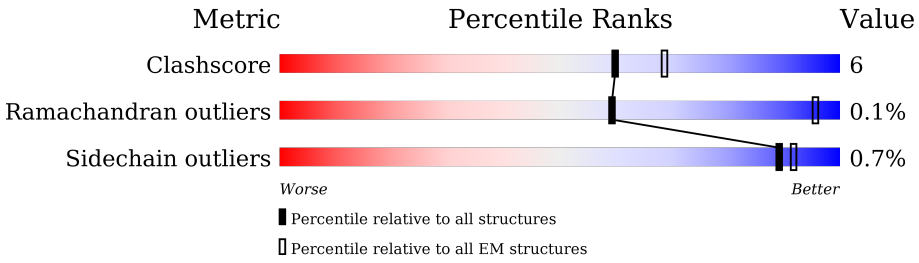
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.20 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	108	72% 27% .
1	F	108	69% 30% .
1	H	108	74% 25% .
1	J	108	72% 27% .
2	B	4416	83% 12% 5%
2	E	4416	83% 12% 5%
2	G	4416	83% 12% 5%
2	I	4416	82% 12% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121436 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.

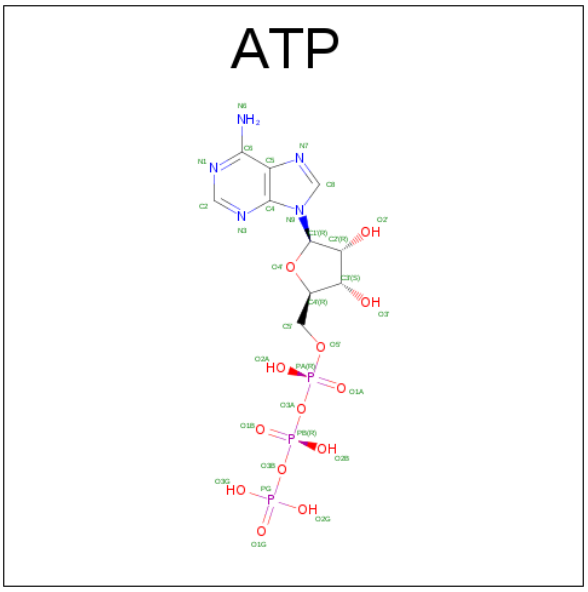
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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.

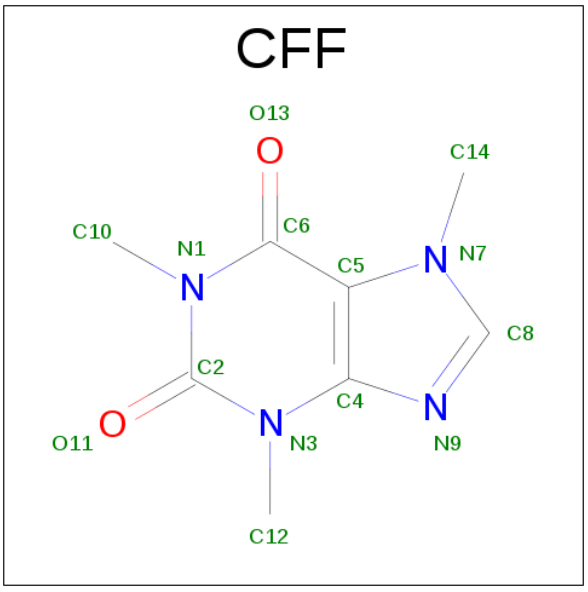
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29495	18683	5227	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29495	18683	5227	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29495	18683	5227	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29495	18683	5227	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

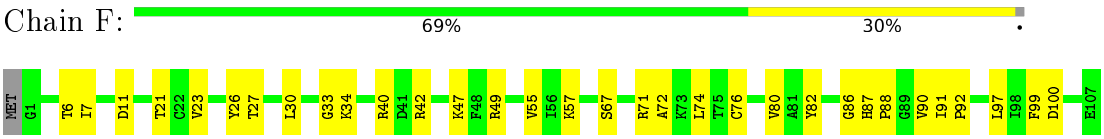
Mol	Chain	Residues	Atoms		AltConf
5	G	1	Total	Zn	0
			1	1	
5	B	1	Total	Zn	0
			1	1	
5	I	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

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.

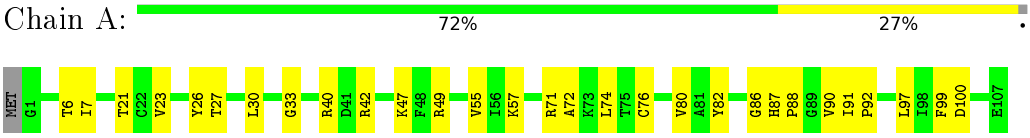
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



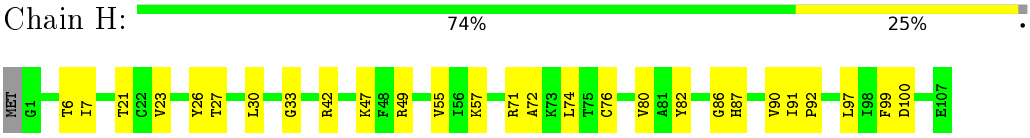
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



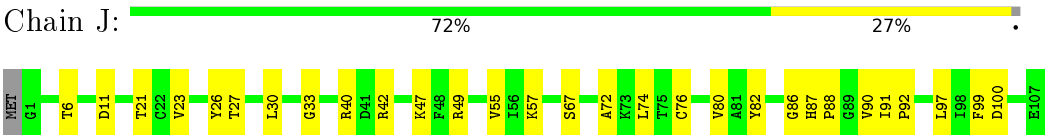
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



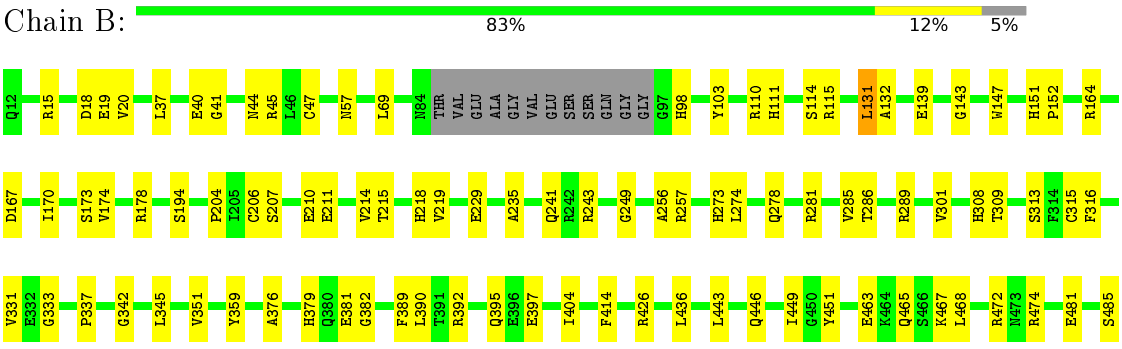
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

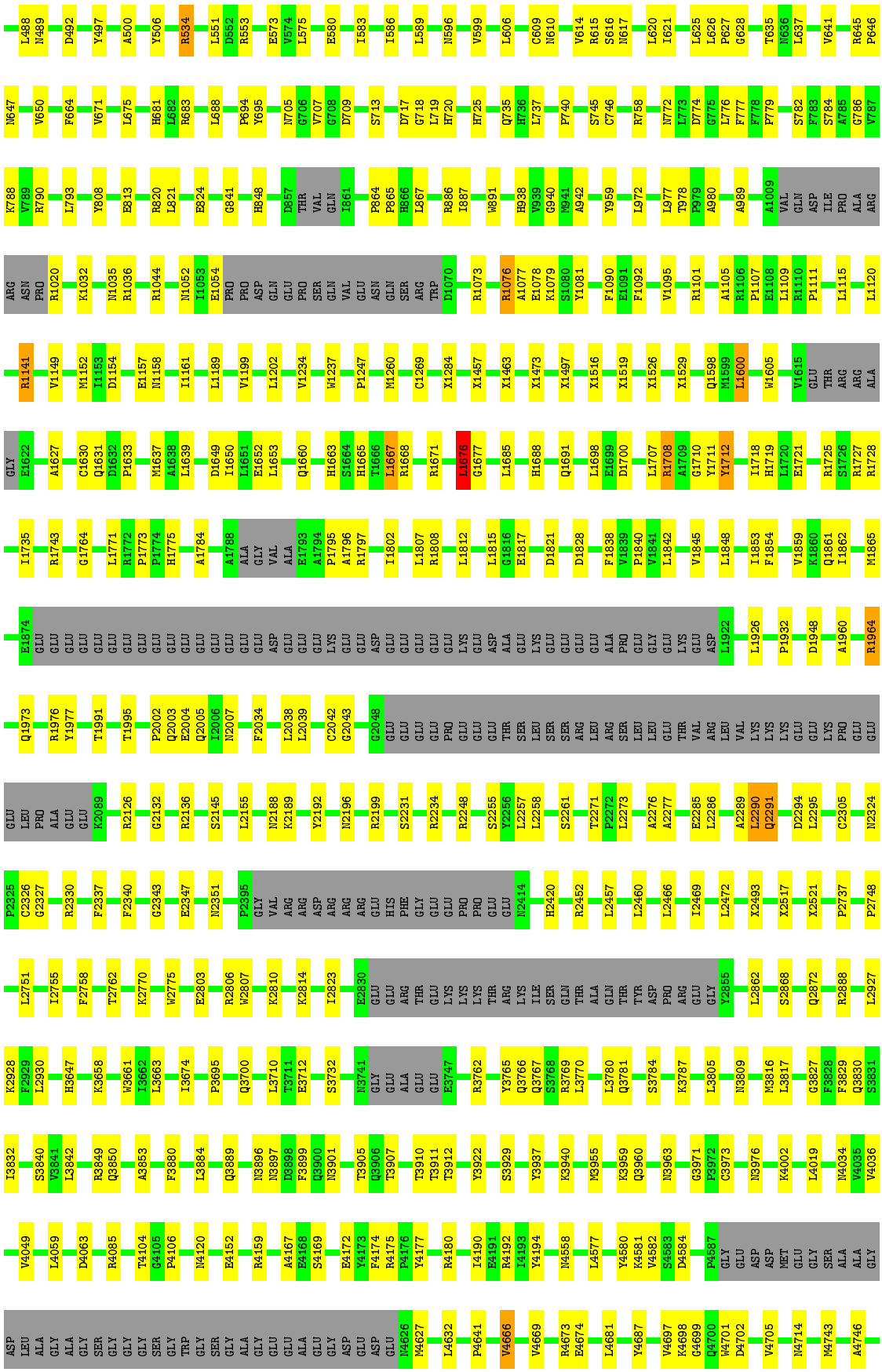
Chain J:

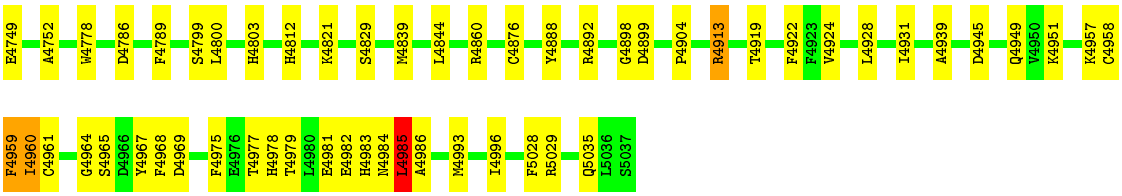


- Molecule 2: Ryanodine receptor 1

Chain B:

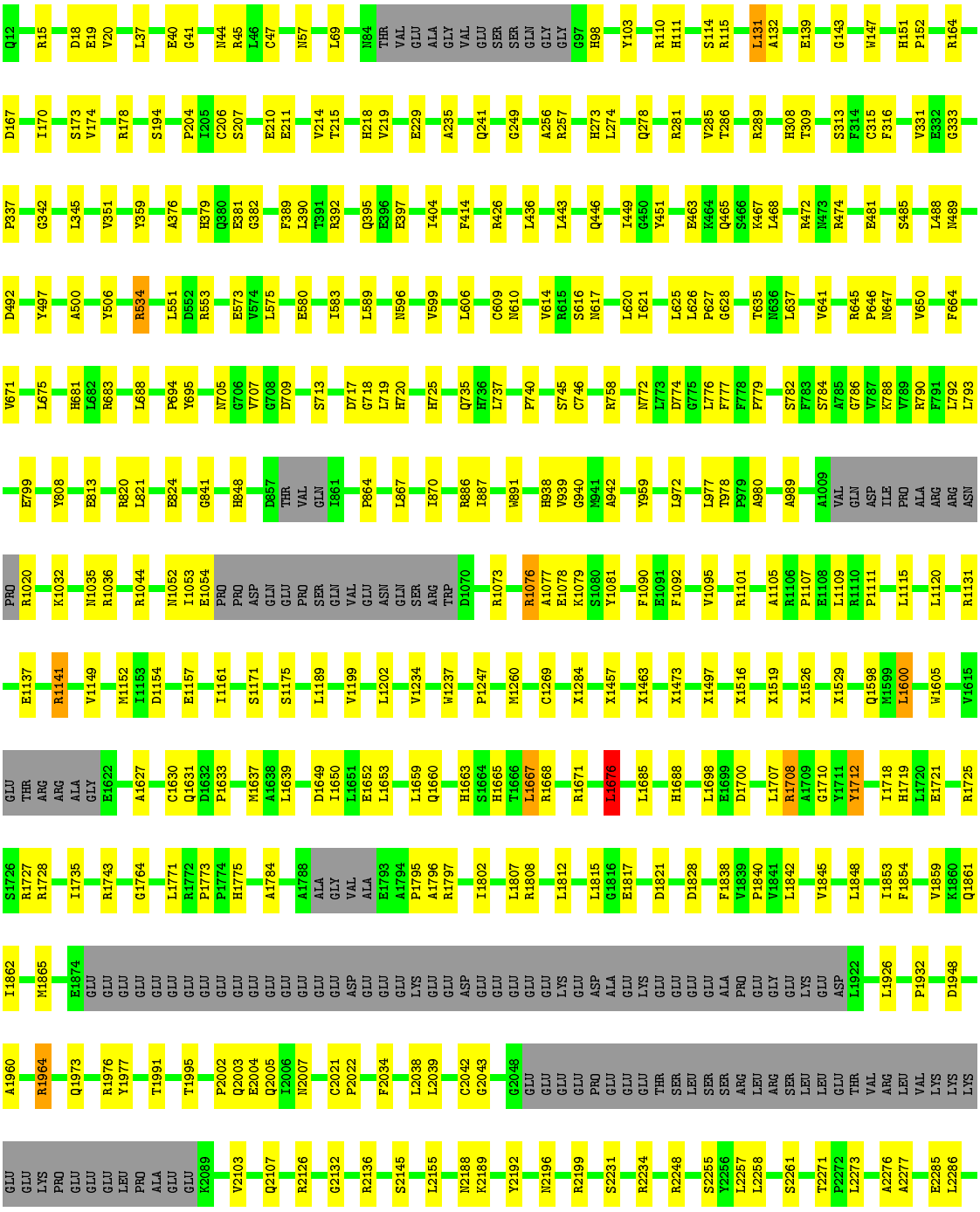


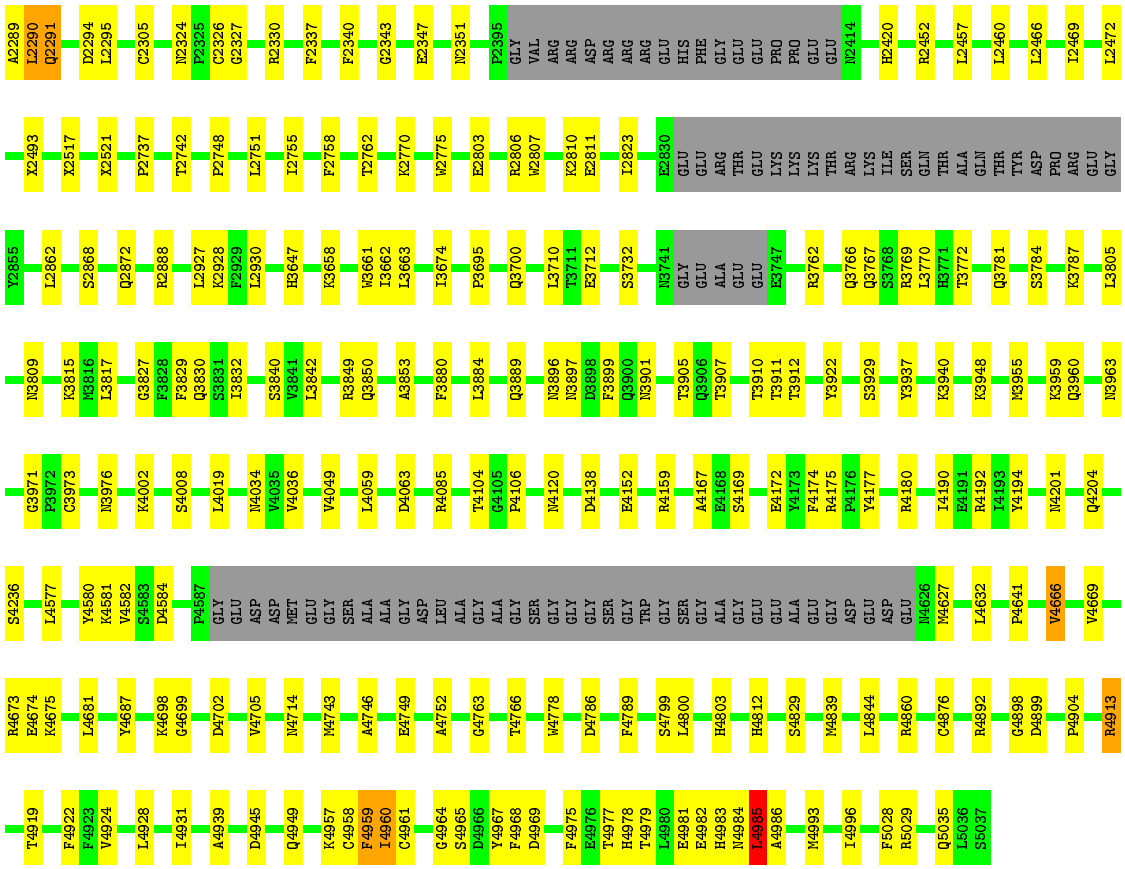




• Molecule 2: Ryanodine receptor 1

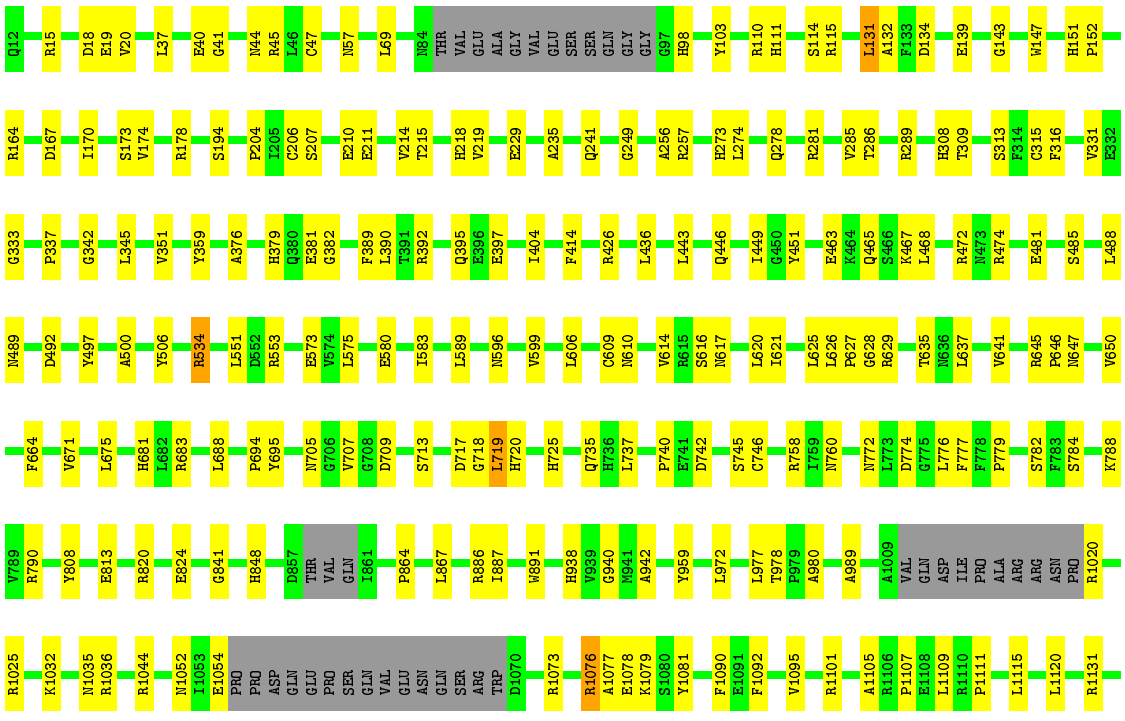
Chain I:

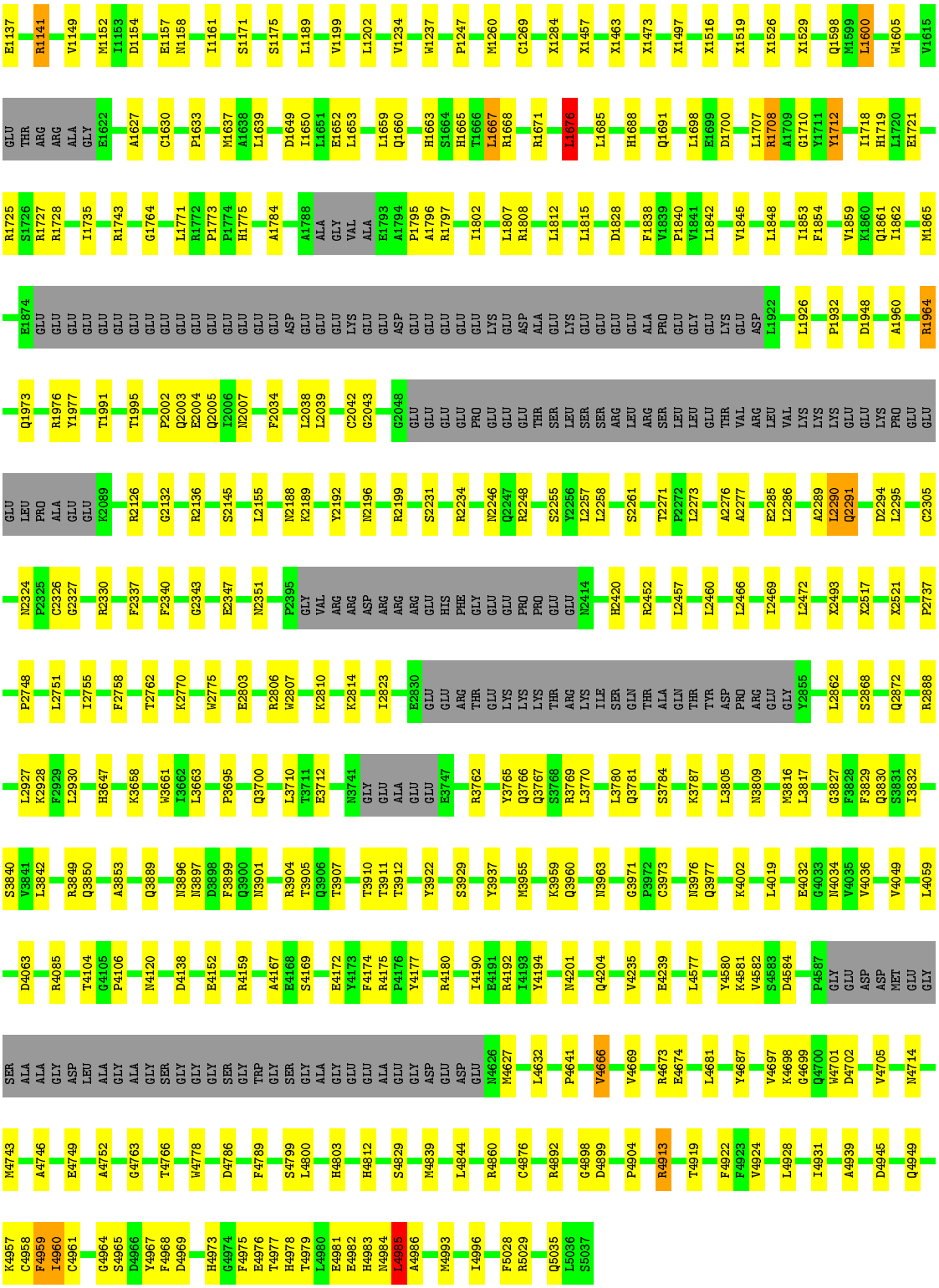




- Molecule 2: Ryanodine receptor 1

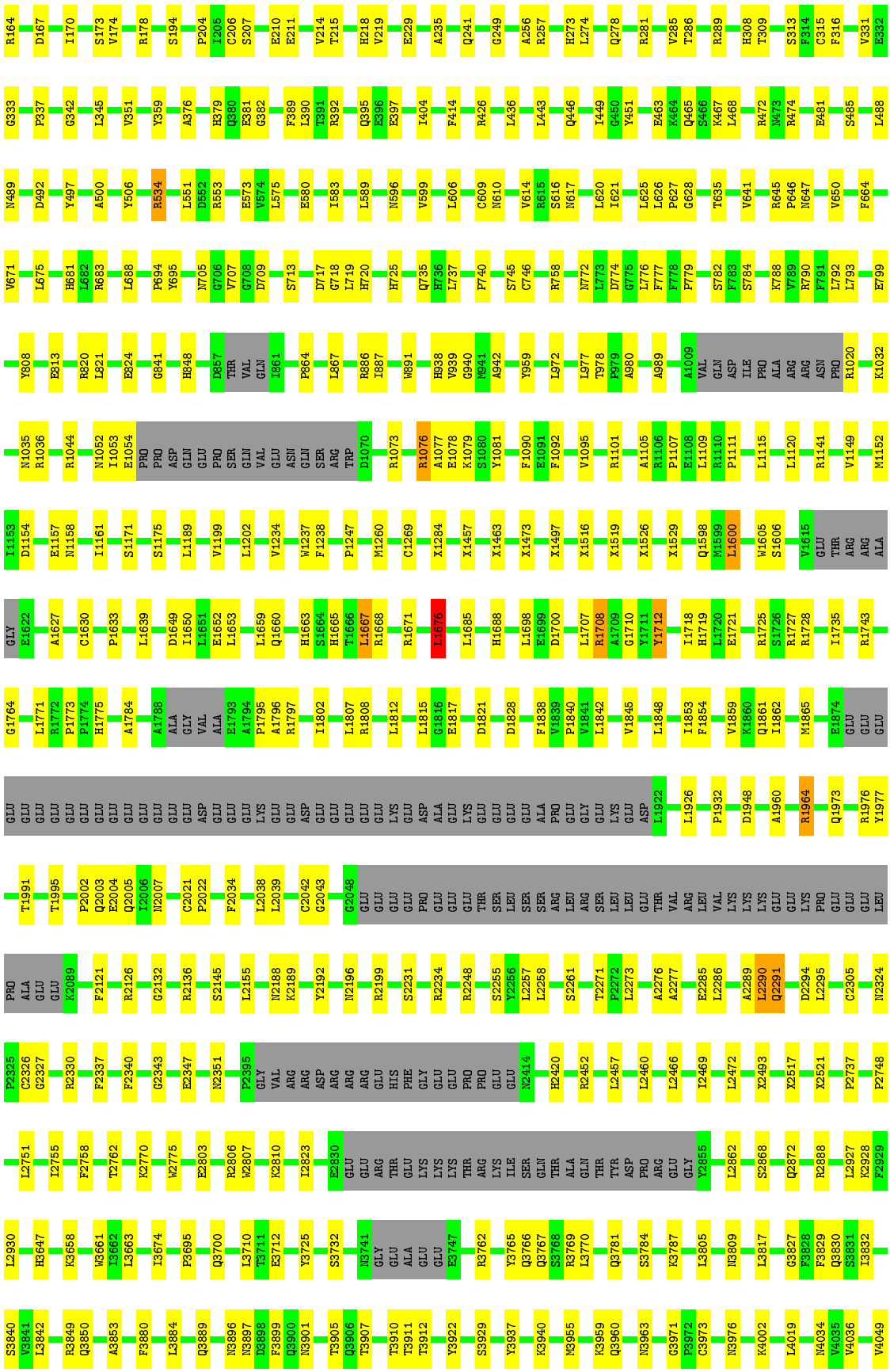
Chain E:

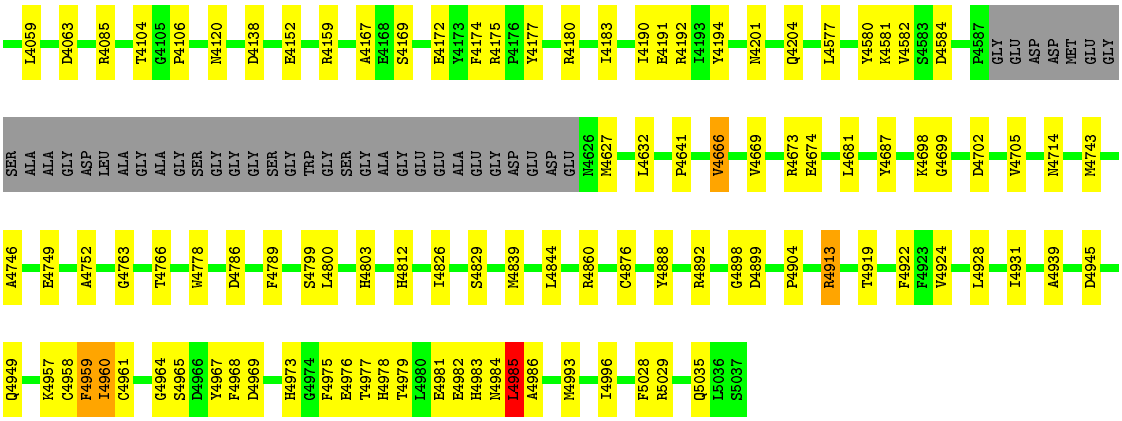




• Molecule 2: Ryanodine receptor 1

Chain G:




L4059 D4063 R4085 T4104 G4105 P4106 N4120 D4138 E4152 R4159 A4167 E4168 S4169 E4172 Y4173 F4174 R4175 P4176 Y4177 R4180 I4183 I4190 E4191 R4192 I4193 Y4194 N4201 Q4204 L4577 Y4580 K4581 V4582 S4583 D4584 P4587 GLY GLU ASP ASP MET GLU GLY
SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU N4626 M4627 L4632 P4641 V4666 V4669 R4673 E4674 L4681 Y4687 K4698 G4699 D4702 V4705 N4714 M4743
A4746 E4749 A4752 G4763 T4766 W4778 D4786 F4789 S4799 L4800 H4803 H4812 I4826 S4829 M4839 L4844 R4860 C4876 Y4888 R4892 G4898 D4899 P4904 R4913 T4919 F4922 F4923 V4924 L4928 I4931 A4939 D4945
Q4949 K4957 C4958 F4959 I4960 C4961 G4964 S4965 D4966 Y4967 F4968 D4969 H4973 G4974 F4975 E4976 T4977 H4978 T4979 L4980 E4981 E4982 H4983 N4984 L4985 A4986 M4993 I4996 F5028 R5029 Q5035 L5036 S5037

4 Experimental information (i)

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 ($e^-/Å^2$)	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: CFF, ZN, ATP

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	0.30	0/834	0.52	0/1123
1	F	0.30	0/834	0.52	0/1123
1	H	0.30	0/834	0.52	0/1123
1	J	0.30	0/834	0.52	0/1123
2	B	0.29	0/25424	0.53	8/34530 (0.0%)
2	E	0.29	0/25424	0.53	9/34530 (0.0%)
2	G	0.29	0/25424	0.53	8/34530 (0.0%)
2	I	0.29	0/25424	0.53	8/34530 (0.0%)
All	All	0.29	0/105032	0.53	33/142612 (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
2	B	0	13
2	E	0	13
2	G	0	13
2	I	0	13
All	All	0	52

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	131	LEU	CA-CB-CG	8.24	134.26	115.30
2	E	131	LEU	CA-CB-CG	8.24	134.25	115.30
2	I	131	LEU	CA-CB-CG	8.23	134.24	115.30
2	G	131	LEU	CA-CB-CG	8.23	134.22	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	4985	LEU	CA-CB-CG	7.85	133.36	115.30
2	G	4985	LEU	CA-CB-CG	7.85	133.35	115.30
2	B	4985	LEU	CA-CB-CG	7.84	133.33	115.30
2	I	4985	LEU	CA-CB-CG	7.82	133.29	115.30
2	E	1600	LEU	CA-CB-CG	6.92	131.21	115.30
2	B	1600	LEU	CA-CB-CG	6.90	131.17	115.30
2	I	1600	LEU	CA-CB-CG	6.90	131.17	115.30
2	G	1600	LEU	CA-CB-CG	6.90	131.16	115.30
2	G	1676	LEU	CA-CB-CG	6.54	130.34	115.30
2	B	1676	LEU	CA-CB-CG	6.53	130.32	115.30
2	I	1676	LEU	CA-CB-CG	6.52	130.31	115.30
2	E	1676	LEU	CA-CB-CG	6.52	130.29	115.30
2	G	977	LEU	CA-CB-CG	5.94	128.96	115.30
2	E	977	LEU	CA-CB-CG	5.93	128.94	115.30
2	B	977	LEU	CA-CB-CG	5.93	128.94	115.30
2	I	977	LEU	CA-CB-CG	5.93	128.94	115.30
2	I	2290	LEU	CA-CB-CG	5.65	128.30	115.30
2	E	2290	LEU	CA-CB-CG	5.65	128.29	115.30
2	B	2290	LEU	CA-CB-CG	5.64	128.27	115.30
2	G	2290	LEU	CA-CB-CG	5.63	128.25	115.30
2	G	1667	LEU	CA-CB-CG	5.36	127.63	115.30
2	I	1667	LEU	CA-CB-CG	5.36	127.62	115.30
2	E	1667	LEU	CA-CB-CG	5.35	127.60	115.30
2	B	1667	LEU	CA-CB-CG	5.34	127.59	115.30
2	I	688	LEU	CA-CB-CG	5.32	127.53	115.30
2	G	688	LEU	CA-CB-CG	5.30	127.50	115.30
2	B	688	LEU	CA-CB-CG	5.30	127.49	115.30
2	E	688	LEU	CA-CB-CG	5.29	127.47	115.30
2	E	719	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1712	TYR	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	2291	GLN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1712	TYR	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	2291	GLN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4666	VAL	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1712	TYR	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1712	TYR	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	2291	GLN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4666	VAL	Peptide

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Mol	Chain	Res	Type	Group
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide

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	A	818	0	824	18	0
1	F	818	0	824	20	0
1	H	818	0	824	15	0
1	J	818	0	824	17	0
2	B	29495	0	24734	313	0
2	E	29495	0	24734	312	0
2	G	29495	0	24734	310	0
2	I	29495	0	24734	314	0
3	B	31	0	12	1	0
3	E	31	0	12	1	0
3	G	31	0	12	1	0
3	I	31	0	12	1	0
4	B	14	0	10	0	0
4	E	14	0	10	0	0
4	G	14	0	10	0	0
4	I	14	0	10	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
All	All	121436	0	102320	1289	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 6.

All (1289) 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:B:4968:PHE:CZ	2:B:4978:HIS:CE1	2.60	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4968:PHE:CZ	2:E:4978:HIS:CE1	2.60	0.90
2:G:4968:PHE:CZ	2:G:4978:HIS:CE1	2.60	0.89
2:I:4968:PHE:CZ	2:I:4978:HIS:CE1	2.60	0.89
2:B:4975:PHE:O	2:B:4979:THR:HG23	1.86	0.76
2:E:4975:PHE:O	2:E:4979:THR:HG23	1.86	0.75
2:G:4975:PHE:O	2:G:4979:THR:HG23	1.86	0.75
2:I:4975:PHE:O	2:I:4979:THR:HG23	1.86	0.74
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.54	0.72
2:E:4960:ILE:HD13	2:E:4960:ILE:N	2.04	0.72
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.54	0.72
2:B:4960:ILE:HD13	2:B:4960:ILE:N	2.04	0.72
2:I:4960:ILE:N	2:I:4960:ILE:HD13	2.04	0.71
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.54	0.71
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.54	0.70
2:G:4960:ILE:N	2:G:4960:ILE:HD13	2.04	0.70
2:I:4978:HIS:HA	2:I:4982:GLU:HB2	1.75	0.69
2:E:4978:HIS:HA	2:E:4982:GLU:HB2	1.75	0.69
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.81	0.69
2:B:4978:HIS:HA	2:B:4982:GLU:HB2	1.75	0.69
2:E:379:HIS:HD2	2:E:382:GLY:H	1.40	0.69
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	2.81	0.68
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.58	0.68
2:B:379:HIS:HD2	2:B:382:GLY:H	1.40	0.68
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.58	0.68
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	2.81	0.68
2:E:4968:PHE:CE2	2:E:4978:HIS:CE1	2.81	0.68
2:G:4978:HIS:HA	2:G:4982:GLU:HB2	1.75	0.68
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.58	0.68
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.58	0.67
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.77	0.67
2:G:379:HIS:HD2	2:G:382:GLY:H	1.40	0.67
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.77	0.66
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.78	0.66
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.77	0.66
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.77	0.66
2:I:379:HIS:HD2	2:I:382:GLY:H	1.40	0.66
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.78	0.66
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.78	0.66
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.78	0.65
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.78	0.65
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.77	0.65
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.78	0.65
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.78	0.65
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.77	0.65
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.77	0.64
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.79	0.64
2:E:331:VAL:HG12	2:E:333:GLY:H	1.62	0.64
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.62	0.64
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.62	0.64
2:G:331:VAL:HG12	2:G:333:GLY:H	1.62	0.64
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.79	0.64
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.79	0.64
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.78	0.64
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.62	0.63
2:I:173:SER:HB3	2:I:178:ARG:H	1.64	0.63
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.81	0.63
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.81	0.63
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.81	0.63
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.62	0.63
2:B:173:SER:HB3	2:B:178:ARG:H	1.64	0.63
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.79	0.63
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.81	0.63
2:G:173:SER:HB3	2:G:178:ARG:H	1.64	0.63
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.81	0.63
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.81	0.63
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.32	0.62
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.82	0.62
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.81	0.62
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.82	0.62
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.32	0.62
2:B:331:VAL:HG12	2:B:333:GLY:H	1.62	0.62
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.32	0.62
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.80	0.62
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.80	0.62
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.32	0.62
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.82	0.62
2:E:173:SER:HB3	2:E:178:ARG:H	1.64	0.62
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.81	0.62
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.82	0.62
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.80	0.62
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.82	0.62
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.82	0.61
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.81	0.61
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.81	0.61
2:I:331:VAL:HG12	2:I:333:GLY:H	1.62	0.61
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.82	0.61
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.33	0.61
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.82	0.61
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.33	0.61
2:B:18:ASP:HB2	2:B:69:LEU:HD12	1.83	0.61
2:E:4968:PHE:CZ	2:E:4978:HIS:HE1	2.19	0.61
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.83	0.61
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.83	0.61
2:I:18:ASP:HB2	2:I:69:LEU:HD12	1.83	0.61
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.33	0.60
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.34	0.60
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.34	0.60
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.82	0.60
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.84	0.60
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.34	0.60
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.83	0.60
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.83	0.60
2:B:313:SER:HB3	2:B:351:VAL:HB	1.84	0.60
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.35	0.60
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.83	0.59
2:E:313:SER:HB3	2:E:351:VAL:HB	1.84	0.59
2:E:18:ASP:HB2	2:E:69:LEU:HD12	1.83	0.59
2:G:18:ASP:HB2	2:G:69:LEU:HD12	1.83	0.59
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.83	0.59
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.83	0.59
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.34	0.59
2:I:4844:LEU:HD13	2:I:4928:LEU:HG	1.84	0.59
2:B:111:HIS:HD2	2:B:114:SER:H	1.51	0.59
2:B:4844:LEU:HD13	2:B:4928:LEU:HG	1.85	0.59
2:B:4968:PHE:CZ	2:B:4978:HIS:HE1	2.19	0.59
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.35	0.59
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.84	0.59
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.34	0.59
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.82	0.59
1:F:6:THR:HA	1:F:72:ALA:HA	1.84	0.59
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4844:LEU:HD13	2:E:4928:LEU:HG	1.85	0.59
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.35	0.59
2:I:111:HIS:HD2	2:I:114:SER:H	1.51	0.59
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.84	0.59
2:G:111:HIS:HD2	2:G:114:SER:H	1.51	0.59
2:G:4844:LEU:HD13	2:G:4928:LEU:HG	1.84	0.59
2:E:111:HIS:HD2	2:E:114:SER:H	1.51	0.59
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.84	0.59
1:A:6:THR:HA	1:A:72:ALA:HA	1.84	0.59
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.83	0.59
1:J:6:THR:HA	1:J:72:ALA:HA	1.84	0.59
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.84	0.58
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.34	0.58
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.84	0.58
1:H:6:THR:HA	1:H:72:ALA:HA	1.84	0.58
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.35	0.58
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.36	0.58
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.84	0.58
2:E:4180:ARG:HH22	2:E:4981:GLU:HA	1.68	0.58
2:G:313:SER:HB3	2:G:351:VAL:HB	1.84	0.58
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.85	0.58
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.34	0.58
2:I:313:SER:HB3	2:I:351:VAL:HB	1.84	0.58
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.36	0.58
2:B:4190:ILE:HG21	2:B:5028:PHE:HA	1.86	0.58
2:B:609:CYS:SG	2:B:610:ASN:N	2.77	0.58
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.34	0.57
2:G:609:CYS:SG	2:G:610:ASN:N	2.77	0.57
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.85	0.57
2:B:2452:ARG:NH1	2:I:174:VAL:O	2.36	0.57
2:I:4180:ARG:HH22	2:I:4981:GLU:HA	1.68	0.57
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.38	0.57
2:E:609:CYS:SG	2:E:610:ASN:N	2.77	0.57
2:I:4190:ILE:HG21	2:I:5028:PHE:HA	1.86	0.57
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.87	0.57
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.87	0.57
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.85	0.57
2:I:609:CYS:SG	2:I:610:ASN:N	2.77	0.57
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.36	0.57
2:G:4180:ARG:HH22	2:G:4981:GLU:HA	1.68	0.57
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.85	0.57
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.38	0.57
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.38	0.56
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.87	0.56
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.70	0.56
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.70	0.56
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.34	0.56
2:B:4180:ARG:HH22	2:B:4981:GLU:HA	1.68	0.56
2:E:4190:ILE:HG21	2:E:5028:PHE:HA	1.86	0.56
2:G:4945:ASP:O	2:G:4949:GLN:NE2	2.38	0.56
2:B:4945:ASP:O	2:B:4949:GLN:NE2	2.38	0.56
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.87	0.56
2:G:4190:ILE:HG21	2:G:5028:PHE:HA	1.86	0.56
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.38	0.56
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.87	0.56
2:B:4899:ASP:OD1	2:E:4892:ARG:NH2	2.39	0.56
2:B:4892:ARG:NH2	2:I:4899:ASP:OD1	2.38	0.56
2:E:174:VAL:O	2:G:2452:ARG:NH1	2.38	0.56
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.71	0.56
2:I:4945:ASP:O	2:I:4949:GLN:NE2	2.38	0.56
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.71	0.56
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.87	0.56
2:I:2452:ARG:NH1	2:G:174:VAL:O	2.38	0.56
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.87	0.56
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.88	0.56
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.87	0.56
2:E:4945:ASP:O	2:E:4949:GLN:NE2	2.38	0.56
1:F:27:THR:HB	1:F:100:ASP:HB3	1.88	0.56
2:I:4892:ARG:NH2	2:G:4899:ASP:OD1	2.39	0.56
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.70	0.56
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.71	0.56
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.88	0.56
2:I:4968:PHE:CZ	2:I:4978:HIS:HE1	2.19	0.56
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.87	0.56
1:J:27:THR:HB	1:J:100:ASP:HB3	1.88	0.56
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.88	0.55
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.88	0.55
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.87	0.55
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.71	0.55
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.88	0.55
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.88	0.55
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.71	0.55
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.71	0.55
1:A:27:THR:HB	1:A:100:ASP:HB3	1.88	0.55
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.88	0.55
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.89	0.55
2:G:4829:SER:HB2	2:G:4939:ALA:HB1	1.88	0.55
2:G:621:ILE:O	2:G:625:LEU:N	2.40	0.55
1:F:26:TYR:OH	1:F:42:ARG:NH2	2.40	0.55
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.87	0.55
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.88	0.55
2:B:3897:ASN:O	2:B:3901:ASN:ND2	2.40	0.55
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.89	0.55
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.88	0.55
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.89	0.55
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.71	0.55
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.40	0.55
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.39	0.55
2:B:1808:ARG:HD2	2:B:1854:PHE:HA	1.89	0.55
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.88	0.55
2:E:4899:ASP:OD1	2:G:4892:ARG:NH2	2.40	0.55
2:G:4968:PHE:CZ	2:G:4978:HIS:HE1	2.19	0.55
1:H:27:THR:HB	1:H:100:ASP:HB3	1.88	0.55
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.87	0.55
2:I:4829:SER:HB2	2:I:4939:ALA:HB1	1.88	0.55
2:E:621:ILE:O	2:E:625:LEU:N	2.40	0.55
2:G:938:HIS:HB2	2:G:1054:GLU:HB2	1.89	0.55
2:I:1808:ARG:HD2	2:I:1854:PHE:HA	1.89	0.55
2:I:938:HIS:HB2	2:I:1054:GLU:HB2	1.89	0.55
2:B:3973:CYS:SG	2:B:3976:ASN:ND2	2.81	0.55
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.72	0.55
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.40	0.55
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.89	0.55
2:E:3897:ASN:O	2:E:3901:ASN:ND2	2.40	0.54
2:E:3973:CYS:SG	2:E:3976:ASN:ND2	2.80	0.54
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.88	0.54
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.41	0.54
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.72	0.54
2:E:4829:SER:HB2	2:E:4939:ALA:HB1	1.88	0.54
1:H:26:TYR:OH	1:H:42:ARG:NH2	2.40	0.54
1:J:26:TYR:OH	1:J:42:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.40	0.54
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.90	0.54
2:G:132:ALA:HA	2:G:194:SER:HB2	1.89	0.54
2:G:3973:CYS:SG	2:G:3976:ASN:ND2	2.81	0.54
2:I:132:ALA:HA	2:I:194:SER:HB2	1.89	0.54
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.72	0.54
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.40	0.54
2:I:3973:CYS:SG	2:I:3976:ASN:ND2	2.81	0.54
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.89	0.54
2:B:4829:SER:HB2	2:B:4939:ALA:HB1	1.88	0.54
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	1.90	0.54
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.40	0.54
2:G:3897:ASN:O	2:G:3901:ASN:ND2	2.40	0.54
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.72	0.54
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.89	0.54
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.40	0.54
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.89	0.54
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.90	0.54
2:E:683:ARG:NH1	2:E:707:VAL:O	2.39	0.54
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.88	0.54
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.41	0.54
1:A:26:TYR:OH	1:A:42:ARG:NH2	2.40	0.54
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.89	0.54
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.89	0.54
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.41	0.54
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.90	0.54
2:I:2420:HIS:ND1	2:I:2493:UNK:O	2.40	0.54
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.40	0.54
2:B:4786:ASP:OD2	2:B:4789:PHE:N	2.41	0.54
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.89	0.54
2:E:1808:ARG:HD2	2:E:1854:PHE:HA	1.89	0.54
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.40	0.54
2:I:621:ILE:O	2:I:625:LEU:N	2.40	0.54
2:B:2420:HIS:ND1	2:B:2493:UNK:O	2.40	0.54
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.40	0.54
2:I:3897:ASN:O	2:I:3901:ASN:ND2	2.40	0.54
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.90	0.54
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.90	0.54
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.90	0.54
2:B:938:HIS:HB2	2:B:1054:GLU:HB2	1.89	0.54
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1735:ILE:HG23	2:E:1771:LEU:HD23	1.90	0.54
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.72	0.54
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.41	0.54
2:B:621:ILE:O	2:B:625:LEU:N	2.40	0.54
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.41	0.54
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	1.90	0.54
2:E:132:ALA:HA	2:E:194:SER:HB2	1.89	0.53
2:E:938:HIS:HB2	2:E:1054:GLU:HB2	1.89	0.53
2:G:1735:ILE:HG23	2:G:1771:LEU:HD23	1.89	0.53
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.72	0.53
2:I:4786:ASP:OD2	2:I:4789:PHE:N	2.41	0.53
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.90	0.53
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.90	0.53
2:G:695:TYR:OH	2:G:1073:ARG:NH1	2.41	0.53
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.41	0.53
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	1.89	0.53
2:B:132:ALA:HA	2:B:194:SER:HB2	1.89	0.53
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.41	0.53
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.42	0.53
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.90	0.53
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	1.90	0.53
2:G:1808:ARG:HD2	2:G:1854:PHE:HA	1.89	0.53
2:G:4577:LEU:HG	2:G:4580:TYR:HE2	1.73	0.53
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.73	0.53
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.89	0.53
2:I:1735:ILE:HG23	2:I:1771:LEU:HD23	1.90	0.53
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.91	0.53
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.91	0.53
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.42	0.53
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.72	0.53
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.91	0.53
2:E:4584:ASP:HA	2:E:4627:MET:HA	1.91	0.53
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.90	0.53
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.91	0.53
2:I:4577:LEU:HG	2:I:4580:TYR:HE2	1.73	0.53
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.42	0.53
2:G:4584:ASP:HA	2:G:4627:MET:HA	1.91	0.53
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.90	0.53
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.72	0.53
2:B:534:ARG:NH2	2:B:573:GLU:OE2	2.42	0.53
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.36	0.53
2:I:683:ARG:NH1	2:I:707:VAL:O	2.39	0.53
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	1.92	0.52
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.90	0.52
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.91	0.52
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.90	0.52
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.90	0.52
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.91	0.52
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.91	0.52
2:I:1457:UNK:N	2:I:1497:UNK:O	2.43	0.52
2:E:1457:UNK:N	2:E:1497:UNK:O	2.43	0.52
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.91	0.52
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.40	0.52
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.91	0.52
2:G:4786:ASP:OD2	2:G:4789:PHE:N	2.41	0.52
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.42	0.52
2:G:645:ARG:N	2:G:824:GLU:O	2.41	0.52
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	1.91	0.52
2:I:4584:ASP:HA	2:I:4627:MET:HA	1.91	0.52
2:B:1457:UNK:N	2:B:1497:UNK:O	2.43	0.52
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	1.90	0.52
2:B:4584:ASP:HA	2:B:4627:MET:HA	1.91	0.52
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	1.92	0.52
2:G:683:ARG:NH1	2:G:707:VAL:O	2.39	0.52
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.91	0.52
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.91	0.52
2:E:4786:ASP:OD2	2:E:4789:PHE:N	2.41	0.52
2:G:111:HIS:CD2	2:G:114:SER:H	2.28	0.52
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.90	0.52
2:B:111:HIS:CD2	2:B:114:SER:H	2.28	0.52
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.83	0.52
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.43	0.52
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.92	0.52
2:E:451:TYR:O	2:E:474:ARG:NH1	2.43	0.52
1:A:55:VAL:HA	2:B:1784:ALA:HA	1.91	0.52
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.91	0.52
2:B:4577:LEU:HG	2:B:4580:TYR:HE2	1.73	0.52
2:I:111:HIS:CD2	2:I:114:SER:H	2.28	0.52
1:J:55:VAL:HA	2:I:1784:ALA:HA	1.90	0.52
2:E:534:ARG:NH2	2:E:573:GLU:OE2	2.42	0.52
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.43	0.52
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.90	0.52
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.83	0.52
2:I:534:ARG:NH2	2:I:573:GLU:OE2	2.42	0.52
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	1.92	0.51
2:G:451:TYR:O	2:G:474:ARG:NH1	2.43	0.51
2:I:451:TYR:O	2:I:474:ARG:NH1	2.43	0.51
2:B:4924:VAL:HA	2:B:4928:LEU:HD23	1.93	0.51
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.92	0.51
2:G:534:ARG:NH2	2:G:573:GLU:OE2	2.42	0.51
2:E:1838:PHE:HB3	2:E:1842:LEU:HD11	1.92	0.51
1:H:55:VAL:HA	2:G:1784:ALA:HA	1.92	0.51
2:G:978:THR:HB	2:G:980:ALA:H	1.75	0.51
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.91	0.51
1:J:87:HIS:H	1:J:91:ILE:HB	1.75	0.51
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.29	0.51
2:E:111:HIS:CD2	2:E:114:SER:H	2.28	0.51
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.27	0.51
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.43	0.51
2:I:978:THR:HB	2:I:980:ALA:H	1.75	0.51
2:B:3940:LYS:O	2:B:4002:LYS:NZ	2.41	0.51
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.91	0.51
1:F:87:HIS:H	1:F:91:ILE:HB	1.75	0.51
2:G:1838:PHE:HB3	2:G:1842:LEU:HD11	1.92	0.51
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.29	0.51
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.93	0.51
2:I:1838:PHE:HB3	2:I:1842:LEU:HD11	1.92	0.51
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.92	0.51
2:I:4928:LEU:HD13	2:I:4931:ILE:HD12	1.93	0.51
2:I:645:ARG:N	2:I:824:GLU:O	2.41	0.51
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.92	0.51
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.27	0.51
1:H:87:HIS:H	1:H:91:ILE:HB	1.75	0.51
2:B:451:TYR:O	2:B:474:ARG:NH1	2.43	0.51
2:B:978:THR:HB	2:B:980:ALA:H	1.75	0.51
2:E:1796:ALA:HB1	2:E:1797:ARG:HH21	1.76	0.51
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.91	0.51
2:G:1457:UNK:N	2:G:1497:UNK:O	2.43	0.51
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.43	0.51
2:I:241:GLN:O	2:I:289:ARG:NH1	2.38	0.51
1:A:87:HIS:H	1:A:91:ILE:HB	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1796:ALA:HB1	2:B:1797:ARG:HH21	1.76	0.51
2:B:1838:PHE:HB3	2:B:1842:LEU:HD11	1.92	0.51
2:B:465:GLN:HG3	2:B:3710:LEU:HB3	1.93	0.51
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.91	0.51
2:E:978:THR:HB	2:E:980:ALA:H	1.75	0.51
2:I:465:GLN:HG3	2:I:3710:LEU:HB3	1.93	0.51
2:E:2758:PHE:O	2:E:2762:THR:N	2.44	0.51
2:E:4928:LEU:HD13	2:E:4931:ILE:HD12	1.93	0.51
2:G:485:SER:O	2:G:489:ASN:N	2.40	0.51
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.93	0.51
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.93	0.50
2:E:465:GLN:HG3	2:E:3710:LEU:HB3	1.93	0.50
2:E:4924:VAL:HA	2:E:4928:LEU:HD23	1.93	0.50
2:G:1815:LEU:HD22	2:G:1845:VAL:HG21	1.94	0.50
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.93	0.50
2:I:1796:ALA:HB1	2:I:1797:ARG:HH21	1.76	0.50
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.93	0.50
2:B:214:VAL:HG12	2:B:274:LEU:HD12	1.94	0.50
2:E:214:VAL:HG12	2:E:274:LEU:HD12	1.93	0.50
2:G:1796:ALA:HB1	2:G:1797:ARG:HH21	1.76	0.50
2:G:465:GLN:HG3	2:G:3710:LEU:HB3	1.93	0.50
2:G:4928:LEU:HD13	2:G:4931:ILE:HD12	1.93	0.50
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.93	0.50
2:E:1815:LEU:HD22	2:E:1845:VAL:HG21	1.94	0.50
2:E:2457:LEU:HD23	2:E:2460:LEU:HD12	1.94	0.50
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.93	0.50
2:G:214:VAL:HG12	2:G:274:LEU:HD12	1.93	0.50
1:A:21:THR:HA	1:A:49:ARG:HA	1.93	0.50
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.94	0.50
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.93	0.50
2:G:647:ASN:ND2	2:G:820:ARG:O	2.43	0.50
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.29	0.50
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.94	0.50
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.29	0.50
2:E:647:ASN:ND2	2:E:820:ARG:O	2.43	0.50
2:G:4924:VAL:HA	2:G:4928:LEU:HD23	1.93	0.50
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.94	0.50
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.94	0.50
2:B:647:ASN:ND2	2:B:820:ARG:O	2.43	0.50
2:I:4059:LEU:HD13	2:I:4167:ALA:HB2	1.94	0.50
1:J:21:THR:HA	1:J:49:ARG:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:ARG:HD3	2:B:98:HIS:HB3	1.93	0.50
2:E:2290:LEU:HB3	2:E:3849:ARG:HH12	1.77	0.50
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.93	0.50
2:I:214:VAL:HG12	2:I:274:LEU:HD12	1.94	0.50
2:B:2457:LEU:HD23	2:B:2460:LEU:HD12	1.94	0.50
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.94	0.50
2:B:2290:LEU:HB3	2:B:3849:ARG:HH12	1.77	0.50
2:B:776:LEU:HG	2:B:848:HIS:HA	1.94	0.50
2:G:813:GLU:OE2	2:G:1020:ARG:N	2.45	0.50
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.83	0.50
2:G:241:GLN:O	2:G:289:ARG:NH1	2.38	0.50
2:I:315:CYS:SG	2:I:316:PHE:N	2.85	0.50
2:I:772:ASN:ND2	2:I:774:ASP:OD2	2.45	0.50
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.93	0.49
2:E:3766:GLN:O	2:E:3770:LEU:N	2.45	0.49
2:E:645:ARG:N	2:E:824:GLU:O	2.41	0.49
2:G:2457:LEU:HD23	2:G:2460:LEU:HD12	1.94	0.49
1:H:21:THR:HA	1:H:49:ARG:HA	1.93	0.49
2:I:2347:GLU:O	2:I:2351:ASN:N	2.34	0.49
2:I:4924:VAL:HA	2:I:4928:LEU:HD23	1.93	0.49
2:B:315:CYS:SG	2:B:316:PHE:N	2.85	0.49
2:B:4898:GLY:O	2:E:4892:ARG:NH2	2.45	0.49
2:E:485:SER:O	2:E:489:ASN:N	2.40	0.49
2:E:4898:GLY:O	2:G:4892:ARG:NH2	2.45	0.49
2:E:650:VAL:HB	2:E:777:PHE:HB2	1.94	0.49
2:G:2290:LEU:HB3	2:G:3849:ARG:HH12	1.77	0.49
2:G:4059:LEU:HD13	2:G:4167:ALA:HB2	1.94	0.49
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.93	0.49
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.41	0.49
2:E:315:CYS:SG	2:E:316:PHE:N	2.85	0.49
2:G:15:ARG:HD3	2:G:98:HIS:HB3	1.93	0.49
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.94	0.49
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.94	0.49
2:B:2758:PHE:O	2:B:2762:THR:N	2.44	0.49
2:B:4928:LEU:HD13	2:B:4931:ILE:HD12	1.93	0.49
2:E:813:GLU:OE2	2:E:1020:ARG:N	2.45	0.49
2:E:4059:LEU:HD13	2:E:4167:ALA:HB2	1.94	0.49
2:E:776:LEU:HG	2:E:848:HIS:HA	1.94	0.49
2:I:1815:LEU:HD22	2:I:1845:VAL:HG21	1.94	0.49
2:G:2758:PHE:O	2:G:2762:THR:N	2.44	0.49
2:G:315:CYS:SG	2:G:316:PHE:N	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4892:ARG:NH2	2:I:4898:GLY:O	2.46	0.49
2:B:2255:SER:HA	2:B:2258:LEU:HB3	1.94	0.49
2:E:4957:LYS:HG2	2:E:4964:GLY:HA2	1.95	0.49
1:F:21:THR:HA	1:F:49:ARG:HA	1.93	0.49
2:I:2868:SER:O	2:I:2872:GLN:N	2.43	0.49
2:B:4965:SER:O	2:B:4969:ASP:N	2.45	0.49
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.93	0.49
2:G:4965:SER:O	2:G:4969:ASP:N	2.45	0.49
2:G:650:VAL:HB	2:G:777:PHE:HB2	1.94	0.49
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.94	0.49
2:I:2290:LEU:HB3	2:I:3849:ARG:HH12	1.77	0.49
2:I:4965:SER:O	2:I:4969:ASP:N	2.45	0.49
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.78	0.49
2:B:1815:LEU:HD22	2:B:1845:VAL:HG21	1.94	0.49
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.86	0.49
2:B:650:VAL:HB	2:B:777:PHE:HB2	1.94	0.49
2:E:772:ASN:ND2	2:E:774:ASP:OD2	2.45	0.49
2:E:15:ARG:HD3	2:E:98:HIS:HB3	1.93	0.49
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.94	0.49
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.93	0.49
2:I:650:VAL:HB	2:I:777:PHE:HB2	1.94	0.49
2:I:813:GLU:OE2	2:I:1020:ARG:N	2.45	0.49
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.78	0.49
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.94	0.49
2:B:3766:GLN:O	2:B:3770:LEU:N	2.45	0.49
2:B:772:ASN:ND2	2:B:774:ASP:OD2	2.45	0.49
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.83	0.49
2:E:2255:SER:HA	2:E:2258:LEU:HB3	1.94	0.49
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.94	0.49
2:E:485:SER:HA	2:E:488:LEU:HB2	1.95	0.49
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	1.95	0.49
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.93	0.49
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.46	0.49
2:G:2255:SER:HA	2:G:2258:LEU:HB3	1.94	0.49
2:G:485:SER:HA	2:G:488:LEU:HB2	1.95	0.49
2:I:15:ARG:HD3	2:I:98:HIS:HB3	1.93	0.49
2:I:2457:LEU:HD23	2:I:2460:LEU:HD12	1.94	0.49
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.46	0.49
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.46	0.49
2:I:4892:ARG:NH2	2:G:4898:GLY:O	2.46	0.49
2:I:2255:SER:HA	2:I:2258:LEU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.86	0.49
2:E:1516:UNK:N	2:E:1529:UNK:O	2.46	0.48
2:E:211:GLU:OE2	2:E:3907:THR:OG1	2.31	0.48
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.86	0.48
1:F:55:VAL:HA	2:E:1784:ALA:HA	1.94	0.48
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.46	0.48
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.86	0.48
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.93	0.48
2:G:776:LEU:HG	2:G:848:HIS:HA	1.94	0.48
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.93	0.48
2:B:614:VAL:HG22	2:B:616:SER:H	1.78	0.48
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.95	0.48
2:G:1516:UNK:N	2:G:1529:UNK:O	2.46	0.48
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.94	0.48
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.46	0.48
2:I:485:SER:O	2:I:489:ASN:N	2.40	0.48
2:B:813:GLU:OE2	2:B:1020:ARG:N	2.45	0.48
2:B:1284:UNK:HA	2:B:1463:UNK:HA	1.96	0.48
2:B:1516:UNK:N	2:B:1529:UNK:O	2.46	0.48
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	1.96	0.48
2:B:683:ARG:NH1	2:B:707:VAL:O	2.39	0.48
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.46	0.48
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.94	0.48
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.78	0.48
2:I:1865:MET:SD	2:I:1865:MET:N	2.86	0.48
2:I:485:SER:HA	2:I:488:LEU:HB2	1.95	0.48
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.96	0.48
2:B:4059:LEU:HD13	2:B:4167:ALA:HB2	1.94	0.48
2:B:4957:LYS:HG2	2:B:4964:GLY:HA2	1.95	0.48
2:G:211:GLU:OE2	2:G:3907:THR:OG1	2.31	0.48
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	1.95	0.48
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.94	0.48
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.94	0.48
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.94	0.48
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.96	0.48
2:G:772:ASN:ND2	2:G:774:ASP:OD2	2.45	0.48
2:B:241:GLN:O	2:B:289:ARG:NH1	2.38	0.48
2:E:1865:MET:SD	2:E:1865:MET:N	2.87	0.48
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.94	0.48
2:E:4919:THR:HA	2:E:4922:PHE:HD2	1.79	0.48
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:776:LEU:HG	2:I:848:HIS:HA	1.94	0.48
2:I:647:ASN:ND2	2:I:820:ARG:O	2.43	0.48
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.96	0.48
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.47	0.48
2:E:1991:THR:O	2:E:1995:THR:OG1	2.32	0.48
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	1.96	0.48
2:E:614:VAL:HG22	2:E:616:SER:H	1.78	0.48
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.95	0.48
2:G:4800:LEU:HA	2:G:4803:HIS:HD2	1.79	0.48
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.95	0.48
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.95	0.48
2:G:1991:THR:O	2:G:1995:THR:OG1	2.32	0.48
2:I:1516:UNK:N	2:I:1529:UNK:O	2.46	0.48
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.79	0.48
2:I:614:VAL:HG22	2:I:616:SER:H	1.78	0.48
2:B:1865:MET:SD	2:B:1865:MET:N	2.87	0.48
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.79	0.48
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.47	0.48
2:G:4919:THR:HA	2:G:4922:PHE:HD2	1.79	0.48
2:I:4957:LYS:HG2	2:I:4964:GLY:HA2	1.95	0.48
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	1.95	0.48
2:I:1284:UNK:HA	2:I:1463:UNK:HA	1.96	0.48
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.96	0.48
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.96	0.47
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	1.96	0.47
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.46	0.47
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.96	0.47
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.79	0.47
2:G:4957:LYS:HG2	2:G:4964:GLY:HA2	1.95	0.47
2:G:614:VAL:HG22	2:G:616:SER:H	1.78	0.47
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.41	0.47
2:B:211:GLU:OE2	2:B:3907:THR:OG1	2.31	0.47
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.96	0.47
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.96	0.47
2:E:1284:UNK:HA	2:E:1463:UNK:HA	1.96	0.47
2:E:4965:SER:O	2:E:4969:ASP:N	2.45	0.47
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.47	0.47
2:G:3940:LYS:O	2:G:4002:LYS:NZ	2.41	0.47
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.96	0.47
2:I:1105:ALA:N	2:I:1189:LEU:O	2.48	0.47
2:I:1808:ARG:NH1	2:I:1853:ILE:O	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4919:THR:HA	2:B:4922:PHE:HD2	1.79	0.47
2:B:4960:ILE:H	2:B:4960:ILE:HD13	1.79	0.47
2:E:4800:LEU:HA	2:E:4803:HIS:HD2	1.79	0.47
2:I:4919:THR:HA	2:I:4922:PHE:HD2	1.79	0.47
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.96	0.47
2:B:485:SER:HA	2:B:488:LEU:HB2	1.95	0.47
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.96	0.47
2:G:143:GLY:HA3	2:G:147:TRP:HE1	1.80	0.47
2:G:1865:MET:SD	2:G:1865:MET:N	2.87	0.47
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.96	0.47
2:I:1865:MET:HB3	2:I:1926:LEU:HB2	1.96	0.47
2:I:3842:LEU:O	2:I:3929:SER:OG	2.33	0.47
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	1.96	0.47
2:B:4961:CYS:HB3	2:B:4983:HIS:CE1	2.49	0.47
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.47	0.47
2:I:3827:GLY:HA2	2:I:3830:GLN:HE21	1.79	0.47
2:I:596:ASN:HB3	2:I:599:VAL:HG22	1.97	0.47
2:B:1991:THR:O	2:B:1995:THR:OG1	2.32	0.47
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.79	0.47
2:I:1991:THR:O	2:I:1995:THR:OG1	2.32	0.47
2:I:3766:GLN:O	2:I:3770:LEU:N	2.45	0.47
2:B:1105:ALA:N	2:B:1189:LEU:O	2.48	0.47
2:B:488:LEU:O	2:B:492:ASP:N	2.45	0.47
2:E:1865:MET:HB3	2:E:1926:LEU:HB2	1.96	0.47
2:E:4961:CYS:HB3	2:E:4983:HIS:CE1	2.49	0.47
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.78	0.47
2:G:4961:CYS:HB3	2:G:4983:HIS:CE1	2.49	0.47
2:I:2758:PHE:O	2:I:2762:THR:N	2.44	0.47
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	1.95	0.47
2:B:4800:LEU:HA	2:B:4803:HIS:HD2	1.79	0.47
2:G:1284:UNK:HA	2:G:1463:UNK:HA	1.96	0.47
2:G:3827:GLY:HA2	2:G:3830:GLN:HE21	1.79	0.47
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	1.96	0.47
2:G:596:ASN:HB3	2:G:599:VAL:HG22	1.97	0.47
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.80	0.47
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.47	0.47
2:B:3842:LEU:O	2:B:3929:SER:OG	2.33	0.47
2:B:596:ASN:HB3	2:B:599:VAL:HG22	1.97	0.47
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.96	0.47
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.96	0.47
2:I:4800:LEU:HA	2:I:4803:HIS:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4961:CYS:HB3	2:I:4983:HIS:CE1	2.49	0.47
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.97	0.47
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.48	0.47
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.48	0.47
2:E:551:LEU:HD11	2:E:589:LEU:HD13	1.97	0.47
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	1.96	0.47
2:G:151:HIS:HB2	2:G:170:ILE:HB	1.97	0.47
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.41	0.47
2:G:1865:MET:HB3	2:G:1926:LEU:HB2	1.96	0.47
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.96	0.47
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.97	0.47
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	1.96	0.47
2:B:3840:SER:O	2:B:3922:TYR:OH	2.33	0.47
2:E:151:HIS:HB2	2:E:170:ILE:HB	1.97	0.47
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.49	0.47
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.80	0.47
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	1.96	0.47
2:I:143:GLY:HA3	2:I:147:TRP:HE1	1.80	0.47
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.96	0.47
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.46	0.47
2:I:211:GLU:OE2	2:I:3907:THR:OG1	2.31	0.47
2:B:1865:MET:HB3	2:B:1926:LEU:HB2	1.96	0.46
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.49	0.46
2:E:1032:LYS:O	2:E:1036:ARG:N	2.47	0.46
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.48	0.46
2:G:4960:ILE:H	2:G:4960:ILE:HD13	1.79	0.46
2:G:551:LEU:HD11	2:G:589:LEU:HD13	1.97	0.46
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	1.97	0.46
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.80	0.46
2:B:345:LEU:HD23	2:B:389:PHE:HB3	1.97	0.46
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.96	0.46
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	1.97	0.46
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.96	0.46
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.47	0.46
2:B:1808:ARG:NH1	2:B:1853:ILE:O	2.42	0.46
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.96	0.46
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	1.98	0.46
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.80	0.46
2:E:2196:ASN:OD1	2:E:2199:ARG:NH1	2.41	0.46
2:E:241:GLN:O	2:E:289:ARG:NH1	2.38	0.46
2:E:488:LEU:O	2:E:492:ASP:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:345:LEU:HD23	2:G:389:PHE:HB3	1.98	0.46
2:G:3842:LEU:O	2:G:3929:SER:OG	2.33	0.46
2:I:151:HIS:HB2	2:I:170:ILE:HB	1.97	0.46
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.48	0.46
2:I:4960:ILE:CD1	2:I:4985:LEU:HD23	2.46	0.46
2:E:1105:ALA:N	2:E:1189:LEU:O	2.48	0.46
2:E:345:LEU:HD23	2:E:389:PHE:HB3	1.98	0.46
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.47	0.46
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.80	0.46
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	1.98	0.46
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.96	0.46
2:I:3767:GLN:HA	2:I:3770:LEU:HB2	1.97	0.46
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	1.97	0.46
2:I:551:LEU:HD11	2:I:589:LEU:HD13	1.97	0.46
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	1.97	0.46
2:E:3842:LEU:O	2:E:3929:SER:OG	2.33	0.46
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.96	0.46
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.48	0.46
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	1.98	0.46
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.97	0.46
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.47	0.46
2:E:2347:GLU:O	2:E:2351:ASN:N	2.34	0.46
2:E:3840:SER:O	2:E:3922:TYR:OH	2.33	0.46
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	1.97	0.46
2:I:345:LEU:HD23	2:I:389:PHE:HB3	1.98	0.46
2:B:151:HIS:HB2	2:B:170:ILE:HB	1.97	0.46
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.97	0.46
2:E:342:GLY:N	2:E:390:LEU:O	2.49	0.46
2:E:596:ASN:HB3	2:E:599:VAL:HG22	1.97	0.46
2:G:4960:ILE:CD1	2:G:4985:LEU:HD23	2.46	0.46
2:I:342:GLY:N	2:I:390:LEU:O	2.49	0.46
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	1.98	0.46
2:E:4960:ILE:CD1	2:E:4985:LEU:HD23	2.46	0.46
2:G:3766:GLN:O	2:G:3770:LEU:N	2.45	0.46
2:G:3840:SER:O	2:G:3922:TYR:OH	2.33	0.46
2:E:3827:GLY:HA2	2:E:3830:GLN:HE21	1.79	0.46
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	1.97	0.46
2:G:488:LEU:O	2:G:492:ASP:N	2.45	0.46
1:A:30:LEU:HD23	1:A:33:GLY:HA3	1.98	0.45
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.34	0.45
2:B:3827:GLY:HA2	2:B:3830:GLN:HE21	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4172:GLU:HA	2:B:4175:ARG:HE	1.81	0.45
2:E:2868:SER:O	2:E:2872:GLN:N	2.43	0.45
2:E:3767:GLN:HA	2:E:3770:LEU:HB2	1.98	0.45
2:E:4172:GLU:HA	2:E:4175:ARG:HE	1.81	0.45
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.97	0.45
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.80	0.45
2:G:3767:GLN:HA	2:G:3770:LEU:HB2	1.97	0.45
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	1.97	0.45
2:I:4799:SER:HA	2:I:4812:HIS:HE1	1.82	0.45
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.97	0.45
2:B:4960:ILE:CD1	2:B:4985:LEU:HD23	2.46	0.45
2:B:864:PRO:HD2	2:B:867:LEU:HD12	1.98	0.45
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.81	0.45
2:I:790:ARG:HG2	2:I:1627:ALA:HA	1.98	0.45
2:I:446:GLN:HA	2:I:449:ILE:HD12	1.99	0.45
2:I:864:PRO:HD2	2:I:867:LEU:HD12	1.98	0.45
1:J:30:LEU:HD23	1:J:33:GLY:HA3	1.98	0.45
2:B:4984:ASN:C	2:B:4986:ALA:H	2.20	0.45
2:B:551:LEU:HD11	2:B:589:LEU:HD13	1.97	0.45
2:B:940:GLY:O	2:B:1052:ASN:N	2.50	0.45
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.99	0.45
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.48	0.45
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	1.97	0.45
2:B:4799:SER:HA	2:B:4812:HIS:HE1	1.82	0.45
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.81	0.45
2:G:1707:LEU:HG	2:G:1708:ARG:HG3	1.98	0.45
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.99	0.45
2:G:4888:TYR:O	2:G:4892:ARG:NE	2.39	0.45
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.97	0.45
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.46	0.45
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.82	0.45
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.34	0.45
2:G:4581:LYS:HD2	2:G:4632:LEU:HD22	1.99	0.45
2:G:4799:SER:HA	2:G:4812:HIS:HE1	1.82	0.45
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.35	0.45
2:I:359:TYR:HA	2:I:376:ALA:HA	1.98	0.45
2:B:1707:LEU:HG	2:B:1708:ARG:HG3	1.98	0.45
2:B:4581:LYS:HD2	2:B:4632:LEU:HD22	1.99	0.45
2:E:446:GLN:HA	2:E:449:ILE:HD12	1.99	0.45
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.97	0.45
2:B:1090:PHE:HD2	2:B:1202:LEU:HD11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:940:GLY:O	2:E:1052:ASN:N	2.50	0.45
2:E:2132:GLY:O	2:E:2136:ARG:N	2.50	0.45
2:E:864:PRO:HD2	2:E:867:LEU:HD12	1.98	0.45
1:F:30:LEU:HD23	1:F:33:GLY:HA3	1.98	0.45
2:G:342:GLY:N	2:G:390:LEU:O	2.49	0.45
2:G:446:GLN:HA	2:G:449:ILE:HD12	1.99	0.45
2:I:1707:LEU:HG	2:I:1708:ARG:HG3	1.98	0.45
2:I:940:GLY:O	2:I:1052:ASN:N	2.50	0.45
2:B:3767:GLN:HA	2:B:3770:LEU:HB2	1.98	0.45
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.81	0.45
2:G:864:PRO:HD2	2:G:867:LEU:HD12	1.98	0.45
2:E:1090:PHE:HD2	2:E:1202:LEU:HD11	1.82	0.45
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.99	0.45
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.97	0.45
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.82	0.45
2:B:1032:LYS:O	2:B:1036:ARG:N	2.47	0.45
2:B:790:ARG:HG2	2:B:1627:ALA:HA	1.98	0.45
2:B:2347:GLU:O	2:B:2351:ASN:N	2.34	0.45
2:B:446:GLN:HA	2:B:449:ILE:HD12	1.99	0.45
2:E:790:ARG:HG2	2:E:1627:ALA:HA	1.98	0.45
2:E:606:LEU:O	2:E:617:ASN:ND2	2.50	0.45
2:G:1247:PRO:HA	2:G:1598:GLN:HA	1.98	0.45
2:G:790:ARG:HG2	2:G:1627:ALA:HA	1.98	0.45
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.34	0.45
2:G:4172:GLU:HA	2:G:4175:ARG:HE	1.81	0.45
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.29	0.45
2:G:4702:ASP:HA	2:G:4778:TRP:HE1	1.82	0.45
1:H:30:LEU:HD23	1:H:33:GLY:HA3	1.98	0.45
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.41	0.45
2:I:4581:LYS:HD2	2:I:4632:LEU:HD22	1.99	0.45
2:B:1650:ILE:HG13	2:B:1707:LEU:HD21	1.99	0.44
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.99	0.44
2:B:342:GLY:N	2:B:390:LEU:O	2.49	0.44
2:B:4888:TYR:O	2:B:4892:ARG:NE	2.39	0.44
2:E:359:TYR:HA	2:E:376:ALA:HA	1.98	0.44
2:E:4581:LYS:HD2	2:E:4632:LEU:HD22	1.99	0.44
2:G:1105:ALA:N	2:G:1189:LEU:O	2.47	0.44
2:G:1973:GLN:O	2:G:1977:TYR:N	2.48	0.44
2:G:235:ALA:HA	2:G:257:ARG:HD3	1.99	0.44
2:I:4172:GLU:HA	2:I:4175:ARG:HE	1.81	0.44
2:I:4702:ASP:HA	2:I:4778:TRP:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1247:PRO:HA	2:E:1598:GLN:HA	1.98	0.44
2:E:4799:SER:HA	2:E:4812:HIS:HE1	1.82	0.44
2:G:940:GLY:O	2:G:1052:ASN:N	2.50	0.44
2:I:1247:PRO:HA	2:I:1598:GLN:HA	1.98	0.44
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.53	0.44
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.81	0.44
2:I:4174:PHE:HA	2:I:4177:TYR:HD2	1.83	0.44
2:B:359:TYR:HA	2:B:376:ALA:HA	1.98	0.44
2:B:3889:GLN:HE22	2:B:3963:ASN:HB3	1.83	0.44
2:B:4968:PHE:CE2	2:B:4978:HIS:ND1	2.86	0.44
2:E:206:CYS:SG	2:E:207:SER:N	2.91	0.44
2:E:3695:PRO:HB2	2:E:3700:GLN:HG3	2.00	0.44
2:E:4174:PHE:HA	2:E:4177:TYR:HD2	1.83	0.44
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.53	0.44
2:G:4174:PHE:HA	2:G:4177:TYR:HD2	1.83	0.44
2:I:1090:PHE:HD2	2:I:1202:LEU:HD11	1.82	0.44
2:I:4984:ASN:C	2:I:4986:ALA:H	2.20	0.44
2:B:206:CYS:SG	2:B:207:SER:N	2.91	0.44
2:B:243:ARG:NH1	2:B:301:VAL:O	2.42	0.44
2:B:3695:PRO:HB2	2:B:3700:GLN:HG3	2.00	0.44
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.81	0.44
2:B:468:LEU:HB3	2:B:472:ARG:HH12	1.83	0.44
2:B:4702:ASP:HA	2:B:4778:TRP:HE1	1.82	0.44
2:E:1707:LEU:HG	2:E:1708:ARG:HG3	1.98	0.44
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.82	0.44
2:E:4968:PHE:CE2	2:E:4978:HIS:ND1	2.86	0.44
2:G:4984:ASN:C	2:G:4986:ALA:H	2.20	0.44
2:B:1247:PRO:HA	2:B:1598:GLN:HA	1.98	0.44
2:E:1973:GLN:O	2:E:1977:TYR:N	2.48	0.44
2:G:1650:ILE:HG13	2:G:1707:LEU:HD21	2.00	0.44
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.46	0.44
2:G:606:LEU:O	2:G:617:ASN:ND2	2.50	0.44
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.99	0.44
2:I:3695:PRO:HB2	2:I:3700:GLN:HG3	2.00	0.44
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.47	0.44
2:I:3889:GLN:HE22	2:I:3963:ASN:HB3	1.83	0.44
2:B:485:SER:O	2:B:489:ASN:N	2.40	0.44
2:E:2034:PHE:O	2:E:2038:LEU:N	2.51	0.44
2:E:4702:ASP:HA	2:E:4778:TRP:HE1	1.82	0.44
2:E:468:LEU:HB3	2:E:472:ARG:HH12	1.83	0.44
2:E:709:ASP:HA	2:E:725:HIS:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2868:SER:O	2:G:2872:GLN:N	2.43	0.44
2:G:3695:PRO:HB2	2:G:3700:GLN:HG3	2.00	0.44
2:G:359:TYR:HA	2:G:376:ALA:HA	1.98	0.44
2:G:4201:ASN:ND2	2:G:4204:GLN:OE1	2.48	0.44
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.83	0.44
2:I:1650:ILE:HG13	2:I:1707:LEU:HD21	1.99	0.44
2:I:2034:PHE:O	2:I:2038:LEU:N	2.51	0.44
2:I:606:LEU:O	2:I:617:ASN:ND2	2.50	0.44
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.52	0.44
2:B:404:ILE:HG21	2:B:481:GLU:HG3	2.00	0.44
2:E:2286:LEU:HA	2:E:2289:ALA:HB3	2.00	0.44
2:E:4984:ASN:C	2:E:4986:ALA:H	2.20	0.44
2:G:4968:PHE:CE2	2:G:4978:HIS:ND1	2.86	0.44
2:I:4201:ASN:ND2	2:I:4204:GLN:OE1	2.48	0.44
2:I:404:ILE:HG21	2:I:481:GLU:HG3	2.00	0.44
2:B:1802:ILE:HG21	2:B:1807:LEU:HD22	1.99	0.44
2:B:3766:GLN:HA	2:B:3769:ARG:HG2	2.00	0.44
2:B:606:LEU:O	2:B:617:ASN:ND2	2.50	0.44
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.37	0.44
2:E:1659:LEU:O	2:E:1663:HIS:N	2.47	0.44
2:E:707:VAL:HG23	2:E:713:SER:HB2	2.00	0.44
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.83	0.44
2:G:1859:VAL:HA	2:G:1862:ILE:HG12	2.00	0.44
2:G:2347:GLU:O	2:G:2351:ASN:N	2.34	0.44
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.00	0.44
2:I:1802:ILE:HG21	2:I:1807:LEU:HD22	1.99	0.44
2:I:1948:ASP:OD1	2:I:2126:ARG:NH2	2.50	0.44
2:B:215:THR:HG22	2:B:273:HIS:HA	2.00	0.44
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.46	0.44
2:B:4961:CYS:HB3	2:B:4983:HIS:HE1	1.82	0.44
2:B:709:ASP:HA	2:B:725:HIS:H	1.82	0.44
2:B:645:ARG:N	2:B:824:GLU:O	2.41	0.44
2:E:1802:ILE:HG21	2:E:1807:LEU:HD22	1.99	0.44
2:E:3889:GLN:HE22	2:E:3963:ASN:HB3	1.83	0.44
2:G:1090:PHE:HD2	2:G:1202:LEU:HD11	1.82	0.44
2:G:1948:ASP:OD1	2:G:2126:ARG:NH2	2.50	0.44
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.83	0.44
2:G:404:ILE:HG21	2:G:481:GLU:HG3	2.00	0.44
2:I:1663:HIS:O	2:I:1667:LEU:N	2.50	0.44
2:B:3829:PHE:HA	2:B:3832:ILE:HD12	2.00	0.43
2:B:4993:MET:HA	2:B:4996:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1078:GLU:HB3	2:E:1081:TYR:HD2	1.83	0.43
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.52	0.43
2:G:1802:ILE:HG21	2:G:1807:LEU:HD22	1.99	0.43
2:I:3840:SER:O	2:I:3922:TYR:OH	2.33	0.43
2:I:4960:ILE:HD13	2:I:4960:ILE:H	1.79	0.43
2:B:1859:VAL:HA	2:B:1862:ILE:HG12	2.00	0.43
2:B:2286:LEU:HA	2:B:2289:ALA:HB3	2.00	0.43
2:B:4063:ASP:OD1	2:B:4169:SER:OG	2.36	0.43
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	2.00	0.43
2:E:404:ILE:HG21	2:E:481:GLU:HG3	2.00	0.43
2:G:1032:LYS:O	2:G:1036:ARG:N	2.47	0.43
2:G:4063:ASP:OD1	2:G:4169:SER:OG	2.36	0.43
2:I:206:CYS:SG	2:I:207:SER:N	2.91	0.43
2:I:2257:LEU:O	2:I:2261:SER:N	2.51	0.43
2:I:235:ALA:HA	2:I:257:ARG:HD3	1.99	0.43
2:I:3817:LEU:HD22	2:I:3899:PHE:HB2	2.00	0.43
2:I:4977:THR:HG22	2:I:4981:GLU:HB2	2.01	0.43
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.99	0.43
2:B:681:HIS:HB3	2:B:784:SER:HB3	2.00	0.43
2:E:1650:ILE:HG13	2:E:1707:LEU:HD21	1.99	0.43
2:E:4063:ASP:OD1	2:E:4169:SER:OG	2.36	0.43
2:G:206:CYS:SG	2:G:207:SER:N	2.91	0.43
2:G:468:LEU:HB3	2:G:472:ARG:HH12	1.83	0.43
2:I:2517:UNK:O	2:I:2521:UNK:N	2.52	0.43
2:B:4174:PHE:HA	2:B:4177:TYR:HD2	1.83	0.43
2:B:41:GLY:O	2:B:45:ARG:NH1	2.52	0.43
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.83	0.43
2:E:4961:CYS:HB3	2:E:4983:HIS:HE1	1.82	0.43
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.00	0.43
2:I:2039:LEU:HA	2:I:2042:CYS:HB3	2.01	0.43
2:I:3766:GLN:HA	2:I:3769:ARG:HG2	2.00	0.43
2:I:4063:ASP:OD1	2:I:4169:SER:OG	2.36	0.43
2:I:709:ASP:HA	2:I:725:HIS:H	1.82	0.43
2:B:1078:GLU:HB3	2:B:1081:TYR:HD2	1.83	0.43
2:B:1817:GLU:O	2:B:1821:ASP:N	2.51	0.43
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.84	0.43
2:B:707:VAL:HG23	2:B:713:SER:HB2	2.00	0.43
2:E:1171:SER:OG	2:E:1175:SER:N	2.45	0.43
2:E:1269:CYS:HA	2:E:1473:UNK:HA	2.01	0.43
2:E:1808:ARG:NH1	2:E:1853:ILE:O	2.42	0.43
2:E:235:ALA:HA	2:E:257:ARG:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4977:THR:HG22	2:E:4981:GLU:HB2	2.01	0.43
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.84	0.43
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.41	0.43
2:G:3766:GLN:HA	2:G:3769:ARG:HG2	2.00	0.43
2:G:3905:THR:HA	2:G:3912:THR:HG23	2.00	0.43
2:G:4977:THR:HG22	2:G:4981:GLU:HB2	2.01	0.43
2:I:1154:ASP:HB3	2:I:1157:GLU:HB3	2.01	0.43
2:I:164:ARG:N	2:I:167:ASP:OD2	2.52	0.43
2:I:4904:PRO:HB3	2:I:4913:ARG:HD2	2.00	0.43
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.83	0.43
2:B:3817:LEU:HD22	2:B:3899:PHE:HB2	2.00	0.43
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.99	0.43
2:E:2517:UNK:O	2:E:2521:UNK:N	2.52	0.43
2:E:41:GLY:O	2:E:45:ARG:NH1	2.52	0.43
1:F:92:PRO:HD3	2:E:627:PRO:HB2	2.01	0.43
2:G:1154:ASP:HB3	2:G:1157:GLU:HB3	2.01	0.43
2:G:2132:GLY:O	2:G:2136:ARG:N	2.50	0.43
2:G:4180:ARG:HH11	2:G:4192:ARG:HH12	1.67	0.43
2:G:4904:PRO:HB3	2:G:4913:ARG:HD2	2.00	0.43
2:I:1032:LYS:O	2:I:1036:ARG:N	2.47	0.43
2:I:468:LEU:HB3	2:I:472:ARG:HH12	1.83	0.43
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	2.00	0.43
1:J:87:HIS:HA	1:J:88:PRO:HD3	1.89	0.43
2:B:1154:ASP:HB3	2:B:1157:GLU:HB3	2.01	0.43
2:B:218:HIS:HB3	2:B:392:ARG:HD3	2.01	0.43
2:B:2257:LEU:O	2:B:2261:SER:N	2.51	0.43
2:E:215:THR:HG22	2:E:273:HIS:HA	2.00	0.43
2:E:4993:MET:HA	2:E:4996:ILE:HB	2.00	0.43
2:G:3829:PHE:HA	2:G:3832:ILE:HD12	2.00	0.43
2:I:1817:GLU:O	2:I:1821:ASP:N	2.51	0.43
2:I:4968:PHE:CE2	2:I:4978:HIS:ND1	2.86	0.43
2:B:2517:UNK:O	2:B:2521:UNK:N	2.52	0.43
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	2.01	0.43
2:B:4180:ARG:HH11	2:B:4192:ARG:HH12	1.67	0.43
2:E:1663:HIS:O	2:E:1667:LEU:N	2.50	0.43
2:E:278:GLN:N	2:E:315:CYS:SG	2.92	0.43
2:E:4036:VAL:HG11	2:E:5035:GLN:HB3	2.01	0.43
2:G:2286:LEU:HA	2:G:2289:ALA:HB3	2.00	0.43
2:G:2517:UNK:O	2:G:2521:UNK:N	2.52	0.43
1:H:7:ILE:N	1:H:71:ARG:O	2.49	0.43
2:I:215:THR:HG22	2:I:273:HIS:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:41:GLY:O	2:I:45:ARG:NH1	2.52	0.43
2:I:4961:CYS:HB3	2:I:4983:HIS:HE1	1.83	0.43
2:I:681:HIS:HB3	2:I:784:SER:HB3	2.00	0.43
2:I:707:VAL:HG23	2:I:713:SER:HB2	2.00	0.43
2:B:164:ARG:N	2:B:167:ASP:OD2	2.52	0.43
2:B:4958:CYS:HB2	3:B:5101:ATP:N6	2.34	0.43
2:B:4977:THR:HG22	2:B:4981:GLU:HB2	2.01	0.43
2:E:164:ARG:N	2:E:167:ASP:OD2	2.52	0.43
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.84	0.43
2:E:218:HIS:HB3	2:E:392:ARG:HD3	2.01	0.43
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	2.01	0.43
2:E:4904:PRO:HB3	2:E:4913:ARG:HD2	2.00	0.43
1:F:7:ILE:N	1:F:71:ARG:O	2.49	0.43
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	2.00	0.43
2:G:218:HIS:HB3	2:G:392:ARG:HD3	2.01	0.43
2:G:379:HIS:CD2	2:G:381:GLU:H	2.37	0.43
2:G:4967:TYR:HE2	2:G:5029:ARG:HG3	1.84	0.43
2:G:4958:CYS:HB2	3:G:5101:ATP:N6	2.34	0.43
2:I:2286:LEU:HA	2:I:2289:ALA:HB3	2.00	0.43
2:I:3905:THR:HA	2:I:3912:THR:HG23	2.00	0.43
2:I:4958:CYS:HB2	3:I:5101:ATP:N6	2.34	0.43
2:B:2132:GLY:O	2:B:2136:ARG:N	2.50	0.43
2:E:1154:ASP:HB3	2:E:1157:GLU:HB3	2.01	0.43
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	2.01	0.43
2:E:2257:LEU:O	2:E:2261:SER:N	2.51	0.43
2:E:4180:ARG:HH11	2:E:4192:ARG:HH12	1.67	0.43
2:G:1269:CYS:HA	2:G:1473:UNK:HA	2.01	0.43
2:G:1659:LEU:O	2:G:1663:HIS:N	2.47	0.43
2:G:2257:LEU:O	2:G:2261:SER:N	2.51	0.43
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	2.01	0.43
2:G:41:GLY:O	2:G:45:ARG:NH1	2.52	0.43
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.83	0.43
2:I:1269:CYS:HA	2:I:1473:UNK:HA	2.01	0.43
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.84	0.43
2:I:379:HIS:CD2	2:I:381:GLU:H	2.37	0.43
2:I:4967:TYR:HE2	2:I:5029:ARG:HG3	1.84	0.43
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	2.00	0.42
2:B:3905:THR:HA	2:B:3912:THR:HG23	2.00	0.42
2:B:4957:LYS:HZ3	2:B:4957:LYS:HB2	1.84	0.42
2:E:2039:LEU:HA	2:E:2042:CYS:HB3	2.01	0.42
2:E:3766:GLN:HA	2:E:3769:ARG:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:379:HIS:CD2	2:E:381:GLU:H	2.37	0.42
2:E:4958:CYS:HB2	3:E:5101:ATP:N6	2.34	0.42
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.99	0.42
2:G:164:ARG:N	2:G:167:ASP:OD2	2.52	0.42
2:G:2039:LEU:HA	2:G:2042:CYS:HB3	2.01	0.42
2:G:215:THR:HG22	2:G:273:HIS:HA	2.00	0.42
2:I:3940:LYS:O	2:I:4002:LYS:NZ	2.41	0.42
2:I:4180:ARG:HH11	2:I:4192:ARG:HH12	1.67	0.42
2:I:4236:SER:HG	2:I:4675:LYS:HZ1	1.60	0.42
2:I:488:LEU:O	2:I:492:ASP:N	2.45	0.42
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.84	0.42
2:G:1078:GLU:HB3	2:G:1081:TYR:HD2	1.83	0.42
2:G:3817:LEU:HD22	2:G:3899:PHE:HB2	2.00	0.42
2:G:4183:ILE:O	2:G:4191:GLU:N	2.43	0.42
2:I:1859:VAL:HA	2:I:1862:ILE:HG12	2.00	0.42
2:I:2132:GLY:O	2:I:2136:ARG:N	2.50	0.42
2:I:2327:GLY:HA2	2:I:2330:ARG:HD3	2.00	0.42
2:I:4959:PHE:HD2	2:I:4960:ILE:HD13	1.84	0.42
2:B:278:GLN:N	2:B:315:CYS:SG	2.92	0.42
2:B:379:HIS:CD2	2:B:381:GLU:H	2.37	0.42
2:B:4904:PRO:HB3	2:B:4913:ARG:HD2	2.00	0.42
2:E:2327:GLY:HA2	2:E:2330:ARG:HD3	2.00	0.42
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.54	0.42
2:E:3829:PHE:HA	2:E:3832:ILE:HD12	2.00	0.42
2:E:4960:ILE:H	2:E:4960:ILE:HD13	1.79	0.42
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.85	0.42
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.84	0.42
2:G:278:GLN:N	2:G:315:CYS:SG	2.92	0.42
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.84	0.42
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	2.01	0.42
2:I:4960:ILE:HD12	2:I:4985:LEU:HD23	2.02	0.42
2:I:4993:MET:HA	2:I:4996:ILE:HB	2.00	0.42
2:B:2034:PHE:O	2:B:2038:LEU:N	2.51	0.42
2:B:235:ALA:HA	2:B:257:ARG:HD3	1.99	0.42
2:B:4036:VAL:HG11	2:B:5035:GLN:HB3	2.01	0.42
2:B:4951:LYS:HB3	2:B:4951:LYS:HE2	1.91	0.42
2:B:4959:PHE:HD2	2:B:4960:ILE:HD13	1.84	0.42
2:E:4138:ASP:N	2:E:4138:ASP:OD1	2.52	0.42
2:G:2327:GLY:HA2	2:G:2330:ARG:HD3	2.00	0.42
2:G:709:ASP:HA	2:G:725:HIS:H	1.83	0.42
2:I:3829:PHE:HA	2:I:3832:ILE:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1269:CYS:HA	2:B:1473:UNK:HA	2.01	0.42
2:B:2039:LEU:HA	2:B:2042:CYS:HB3	2.01	0.42
2:B:2231:SER:HA	2:B:2234:ARG:HG2	2.01	0.42
2:B:2868:SER:O	2:B:2872:GLN:N	2.43	0.42
2:E:1131:ARG:N	2:E:1137:GLU:O	2.53	0.42
2:I:218:HIS:HB3	2:I:392:ARG:HD3	2.01	0.42
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.54	0.42
2:B:1973:GLN:HA	2:B:1976:ARG:HB3	2.02	0.42
2:E:1077:ALA:HB1	2:E:1234:VAL:HG11	2.02	0.42
1:F:11:ASP:OD1	1:F:67:SER:OG	2.28	0.42
1:F:34:LYS:HD3	2:E:629:ARG:HD2	2.00	0.42
1:F:57:LYS:HB2	1:F:80:VAL:HB	2.02	0.42
2:G:395:GLN:HG3	2:G:397:GLU:H	1.85	0.42
2:G:4959:PHE:HD2	2:G:4960:ILE:HD13	1.84	0.42
2:G:4993:MET:HA	2:G:4996:ILE:HB	2.00	0.42
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.85	0.42
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	2.02	0.42
2:B:256:ALA:HB1	2:B:286:THR:HG21	2.02	0.42
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.84	0.42
2:E:3817:LEU:HD22	2:E:3899:PHE:HB2	2.00	0.42
2:E:718:GLY:HA3	2:E:737:LEU:HA	2.02	0.42
2:G:2034:PHE:O	2:G:2038:LEU:N	2.51	0.42
2:G:4826:ILE:O	2:G:4829:SER:OG	2.33	0.42
1:A:57:LYS:HB2	1:A:80:VAL:HB	2.02	0.42
2:B:2327:GLY:HA2	2:B:2330:ARG:HD3	2.00	0.42
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	2.00	0.42
2:E:256:ALA:HB1	2:E:286:THR:HG21	2.02	0.42
2:E:3905:THR:HA	2:E:3912:THR:HG23	2.00	0.42
2:E:4201:ASN:ND2	2:E:4204:GLN:OE1	2.48	0.42
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	2.02	0.42
1:F:40:ARG:NH2	2:E:675:LEU:O	2.52	0.42
2:G:1171:SER:OG	2:G:1175:SER:N	2.46	0.42
2:G:1817:GLU:O	2:G:1821:ASP:N	2.51	0.42
2:G:2231:SER:HA	2:G:2234:ARG:HG2	2.01	0.42
2:G:718:GLY:HA3	2:G:737:LEU:HA	2.02	0.42
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.41	0.42
2:B:2810:LYS:O	2:B:2814:LYS:N	2.48	0.42
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.54	0.42
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	2.02	0.42
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.85	0.42
2:G:4961:CYS:HB3	2:G:4983:HIS:HE1	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2021:CYS:HA	2:I:2022:PRO:HD3	1.93	0.42
2:I:2231:SER:HA	2:I:2234:ARG:HG2	2.01	0.42
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.85	0.42
2:B:4697:VAL:O	2:B:4701:TRP:N	2.53	0.42
1:A:40:ARG:NH2	2:B:675:LEU:O	2.52	0.42
2:E:4681:LEU:HD21	2:E:4687:TYR:HD2	1.85	0.42
2:G:4960:ILE:HD12	2:G:4985:LEU:HD23	2.02	0.42
2:G:707:VAL:HG23	2:G:713:SER:HB2	2.00	0.42
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	2.02	0.42
2:B:395:GLN:HG3	2:B:397:GLU:H	1.85	0.41
2:G:2145:SER:HB2	2:G:3647:HIS:CE1	2.55	0.41
2:G:4036:VAL:HG11	2:G:5035:GLN:HB3	2.01	0.41
2:I:1659:LEU:O	2:I:1663:HIS:N	2.47	0.41
2:I:1973:GLN:HA	2:I:1976:ARG:HB3	2.02	0.41
2:I:2145:SER:HB2	2:I:3647:HIS:CE1	2.55	0.41
2:I:2248:ARG:NH2	2:I:2285:GLU:OE1	2.53	0.41
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.02	0.41
2:B:2145:SER:HB2	2:B:3647:HIS:CE1	2.55	0.41
2:B:2248:ARG:NH2	2:B:2285:GLU:OE1	2.53	0.41
2:B:414:PHE:HE1	2:B:436:LEU:HB3	1.85	0.41
2:E:414:PHE:HE1	2:E:436:LEU:HB3	1.85	0.41
2:E:4959:PHE:HD2	2:E:4960:ILE:HD13	1.84	0.41
2:E:626:LEU:HG	2:E:628:GLY:H	1.84	0.41
2:G:1973:GLN:HA	2:G:1976:ARG:HB3	2.02	0.41
2:G:4138:ASP:OD1	2:G:4138:ASP:N	2.52	0.41
2:I:626:LEU:HG	2:I:628:GLY:H	1.84	0.41
2:B:1077:ALA:HB1	2:B:1234:VAL:HG11	2.02	0.41
2:B:626:LEU:HG	2:B:628:GLY:H	1.84	0.41
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	2.02	0.41
2:E:2248:ARG:NH2	2:E:2285:GLU:OE1	2.54	0.41
2:G:256:ALA:HB1	2:G:286:THR:HG21	2.02	0.41
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.54	0.41
2:I:395:GLN:HG3	2:I:397:GLU:H	1.85	0.41
2:I:4036:VAL:HG11	2:I:5035:GLN:HB3	2.01	0.41
2:I:709:ASP:HB3	2:I:725:HIS:CE1	2.56	0.41
2:B:2305:CYS:O	2:B:2324:ASN:ND2	2.54	0.41
2:B:4960:ILE:HD12	2:B:4985:LEU:HD23	2.02	0.41
2:B:4967:TYR:HE2	2:B:5029:ARG:HG3	1.84	0.41
2:E:2231:SER:HA	2:E:2234:ARG:HG2	2.01	0.41
2:E:2145:SER:HB2	2:E:3647:HIS:CE1	2.55	0.41
2:E:4697:VAL:O	2:E:4701:TRP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4705:VAL:HB	2:G:4778:TRP:CG	2.56	0.41
1:H:57:LYS:HB2	1:H:80:VAL:HB	2.02	0.41
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	2.02	0.41
2:B:1101:ARG:HH21	2:B:1115:LEU:HB3	1.85	0.41
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.85	0.41
2:B:709:ASP:HB3	2:B:725:HIS:CE1	2.56	0.41
2:E:134:ASP:N	2:E:134:ASP:OD1	2.54	0.41
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.85	0.41
2:E:2810:LYS:O	2:E:2814:LYS:N	2.48	0.41
2:E:4967:TYR:HE2	2:E:5029:ARG:HG3	1.84	0.41
2:G:1101:ARG:HH21	2:G:1115:LEU:HB3	1.85	0.41
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	2.03	0.41
2:G:3959:LYS:O	2:G:3963:ASN:ND2	2.54	0.41
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	2.02	0.41
2:I:1973:GLN:O	2:I:1977:TYR:N	2.48	0.41
2:I:2103:VAL:O	2:I:2107:GLN:N	2.48	0.41
1:J:57:LYS:HB2	1:J:80:VAL:HB	2.01	0.41
2:B:1973:GLN:O	2:B:1977:TYR:N	2.48	0.41
2:B:3674:ILE:HG13	2:B:3732:SER:HB3	2.03	0.41
2:E:580:GLU:HG3	2:E:620:LEU:HD22	2.03	0.41
2:E:637:LEU:HD23	2:E:1637:MET:HB3	2.02	0.41
1:F:87:HIS:HA	1:F:88:PRO:HD3	1.89	0.41
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	2.02	0.41
2:G:414:PHE:HE1	2:G:436:LEU:HB3	1.85	0.41
2:I:256:ALA:HB1	2:I:286:THR:HG21	2.02	0.41
2:I:414:PHE:HE1	2:I:436:LEU:HB3	1.85	0.41
2:I:4681:LEU:HD21	2:I:4687:TYR:HD2	1.85	0.41
2:I:580:GLU:HG3	2:I:620:LEU:HD22	2.03	0.41
2:B:3880:PHE:O	2:B:3884:LEU:N	2.54	0.41
2:E:4763:GLY:O	2:E:4766:THR:OG1	2.29	0.41
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	2.02	0.41
2:G:20:VAL:HG12	2:G:204:PRO:HA	2.03	0.41
2:G:939:VAL:HG22	2:G:1053:ILE:HG23	2.03	0.41
2:I:1101:ARG:HH21	2:I:1115:LEU:HB3	1.85	0.41
2:I:1131:ARG:N	2:I:1137:GLU:O	2.53	0.41
2:I:1077:ALA:HB1	2:I:1234:VAL:HG11	2.02	0.41
2:I:3948:LYS:NZ	2:I:4008:SER:O	2.54	0.41
1:A:7:ILE:N	1:A:71:ARG:O	2.49	0.41
2:B:3959:LYS:O	2:B:3963:ASN:ND2	2.54	0.41
2:B:4960:ILE:CD1	2:B:4960:ILE:N	2.73	0.41
2:B:718:GLY:HA3	2:B:737:LEU:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1101:ARG:HH21	2:E:1115:LEU:HB3	1.85	0.41
2:E:3959:LYS:O	2:E:3963:ASN:ND2	2.54	0.41
2:E:4235:VAL:O	2:E:4239:GLU:N	2.44	0.41
2:E:4960:ILE:HD12	2:E:4985:LEU:HD23	2.02	0.41
2:G:1077:ALA:HB1	2:G:1234:VAL:HG11	2.02	0.41
2:G:2466:LEU:HD23	2:G:2469:ILE:HD12	2.03	0.41
2:G:37:LEU:HD11	2:G:47:CYS:HB3	2.03	0.41
2:G:792:LEU:HD22	2:G:799:GLU:H	1.86	0.41
2:I:2196:ASN:OD1	2:I:2199:ARG:NH1	2.41	0.41
1:J:82:TYR:O	1:J:86:GLY:N	2.54	0.41
2:E:1141:ARG:HD2	2:E:1141:ARG:H	1.86	0.41
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	2.02	0.41
2:E:37:LEU:HD11	2:E:47:CYS:HB3	2.03	0.41
2:E:709:ASP:HB3	2:E:725:HIS:CE1	2.56	0.41
2:G:1105:ALA:O	2:G:1189:LEU:N	2.54	0.41
2:G:3880:PHE:O	2:G:3884:LEU:N	2.54	0.41
2:G:580:GLU:HG3	2:G:620:LEU:HD22	2.03	0.41
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.86	0.41
2:I:37:LEU:HD11	2:I:47:CYS:HB3	2.03	0.41
2:I:4138:ASP:N	2:I:4138:ASP:OD1	2.52	0.41
1:J:40:ARG:NH2	2:I:675:LEU:O	2.54	0.41
1:A:82:TYR:O	1:A:86:GLY:N	2.54	0.41
2:B:3765:TYR:HD2	2:B:3769:ARG:HH21	1.69	0.41
2:B:583:ILE:H	2:B:583:ILE:HG13	1.71	0.41
2:E:20:VAL:HG12	2:E:204:PRO:HA	2.03	0.41
2:G:1238:PHE:O	2:G:1606:SER:N	2.45	0.41
2:G:709:ASP:HB3	2:G:725:HIS:CE1	2.56	0.41
2:I:2466:LEU:HD23	2:I:2469:ILE:HD12	2.03	0.41
2:I:4705:VAL:HB	2:I:4778:TRP:CG	2.56	0.41
2:B:37:LEU:HD11	2:B:47:CYS:HB3	2.03	0.41
2:E:1973:GLN:HA	2:E:1976:ARG:HB3	2.02	0.41
2:E:395:GLN:HG3	2:E:397:GLU:H	1.85	0.41
2:G:2248:ARG:NH2	2:G:2285:GLU:OE1	2.53	0.41
2:G:3674:ILE:HG13	2:G:3732:SER:HB3	2.03	0.41
2:I:939:VAL:HG22	2:I:1053:ILE:HG23	2.03	0.41
2:B:786:GLY:HA2	2:B:1631:GLN:HA	2.03	0.40
2:B:2466:LEU:HD23	2:B:2469:ILE:HD12	2.03	0.40
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	2.02	0.40
2:B:793:LEU:HD22	2:B:821:LEU:HD13	2.04	0.40
2:E:2305:CYS:O	2:E:2324:ASN:ND2	2.54	0.40
1:F:82:TYR:O	1:F:86:GLY:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2121:PHE:O	2:G:3725:TYR:OH	2.39	0.40
2:G:309:THR:O	2:G:313:SER:OG	2.39	0.40
2:I:637:LEU:HD23	2:I:1637:MET:HB3	2.03	0.40
2:I:2742:THR:OG1	2:I:2811:GLU:OE1	2.35	0.40
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.29	0.40
2:I:786:GLY:HA2	2:I:1631:GLN:HA	2.03	0.40
2:B:1663:HIS:NE2	2:B:1711:TYR:OH	2.39	0.40
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	2.02	0.40
2:B:20:VAL:HG12	2:B:204:PRO:HA	2.03	0.40
2:B:4821:LYS:HE2	2:B:4821:LYS:HB3	1.96	0.40
2:B:637:LEU:HD23	2:B:1637:MET:HB3	2.03	0.40
2:E:1948:ASP:OD1	2:E:2126:ARG:NH2	2.50	0.40
2:E:4928:LEU:HA	2:E:4931:ILE:HD12	2.03	0.40
2:G:1154:ASP:O	2:G:1158:ASN:N	2.54	0.40
2:G:2021:CYS:HA	2:G:2022:PRO:HD3	1.93	0.40
2:G:2305:CYS:O	2:G:2324:ASN:ND2	2.54	0.40
1:H:82:TYR:O	1:H:86:GLY:N	2.54	0.40
2:I:1171:SER:OG	2:I:1175:SER:N	2.45	0.40
2:I:20:VAL:HG12	2:I:204:PRO:HA	2.03	0.40
2:I:3880:PHE:O	2:I:3884:LEU:N	2.54	0.40
2:I:793:LEU:HD22	2:I:821:LEU:HD13	2.04	0.40
1:J:11:ASP:OD1	1:J:67:SER:OG	2.28	0.40
2:B:4558:ASN:N	2:B:4558:ASN:OD1	2.54	0.40
2:E:309:THR:O	2:E:313:SER:OG	2.39	0.40
2:E:3765:TYR:HD2	2:E:3769:ARG:HH21	1.69	0.40
2:E:3901:ASN:OD1	2:E:3904:ARG:NH1	2.50	0.40
2:G:4928:LEU:HA	2:G:4931:ILE:HD12	2.03	0.40
2:I:2305:CYS:O	2:I:2324:ASN:ND2	2.54	0.40
2:I:278:GLN:N	2:I:315:CYS:SG	2.92	0.40
2:I:379:HIS:CD2	2:I:382:GLY:H	2.30	0.40
2:I:718:GLY:HA3	2:I:737:LEU:HA	2.02	0.40
2:I:792:LEU:HD22	2:I:799:GLU:H	1.86	0.40
2:I:870:ILE:HD12	2:I:870:ILE:HA	1.96	0.40
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.89	0.40
2:B:4705:VAL:HB	2:B:4778:TRP:CG	2.56	0.40
2:B:864:PRO:HA	2:B:865:PRO:HD3	1.96	0.40
2:E:1154:ASP:O	2:E:1158:ASN:N	2.54	0.40
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	2.02	0.40
2:E:4705:VAL:HB	2:E:4778:TRP:CG	2.56	0.40
2:G:4973:HIS:HB3	2:G:4976:GLU:HB3	2.04	0.40
2:G:626:LEU:HG	2:G:628:GLY:H	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3674:ILE:HG13	2:I:3732:SER:HB3	2.03	0.40
2:I:3959:LYS:O	2:I:3963:ASN:ND2	2.54	0.40
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.86	0.40
2:B:1154:ASP:O	2:B:1158:ASN:N	2.54	0.40
2:B:615:ARG:NH2	2:B:1677:GLY:O	2.55	0.40
2:B:1948:ASP:OD1	2:B:2126:ARG:NH2	2.50	0.40
2:B:583:ILE:HA	2:B:586:ILE:HD12	2.04	0.40
2:B:580:GLU:HG3	2:B:620:LEU:HD22	2.03	0.40
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.55	0.40
2:E:3977:GLN:NE2	2:E:4032:GLU:OE1	2.55	0.40
2:E:4973:HIS:HB3	2:E:4976:GLU:HB3	2.04	0.40
2:E:742:ASP:HA	2:E:760:ASN:HD21	1.87	0.40
2:G:134:ASP:OD1	2:G:134:ASP:N	2.54	0.40
2:G:3765:TYR:HD2	2:G:3769:ARG:HH21	1.69	0.40
2:G:793:LEU:HD22	2:G:821:LEU:HD13	2.04	0.40
2:I:1105:ALA:O	2:I:1189:LEU:N	2.54	0.40
2:I:3662:ILE:HG13	2:I:3662:ILE:H	1.77	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	95 (90%)	10 (10%)	0	100	100
1	F	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	H	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	J	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
2	B	3235/4416 (73%)	2926 (90%)	304 (9%)	5 (0%)	52	86
2	E	3235/4416 (73%)	2924 (90%)	306 (10%)	5 (0%)	52	86
2	G	3235/4416 (73%)	2925 (90%)	305 (9%)	5 (0%)	52	86

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	I	3235/4416 (73%)	2922 (90%)	308 (10%)	5 (0%)	52 86
All	All	13360/18096 (74%)	12077 (90%)	1263 (10%)	20 (0%)	59 90

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	4985	LEU
2	I	4985	LEU
2	E	4985	LEU
2	G	4985	LEU
2	B	1708	ARG
2	B	1932	PRO
2	I	1708	ARG
2	I	1932	PRO
2	E	1708	ARG
2	E	1932	PRO
2	G	1708	ARG
2	G	1932	PRO
2	B	1840	PRO
2	G	1840	PRO
2	I	1840	PRO
2	E	1840	PRO
2	B	4641	PRO
2	I	4641	PRO
2	E	4641	PRO
2	G	4641	PRO

5.3.2 Protein sidechains (i)

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	88/89 (99%)	88 (100%)	0	100 100
2	B	2492/3022 (82%)	2473 (99%)	19 (1%)	86 94
2	E	2492/3022 (82%)	2473 (99%)	19 (1%)	86 94
2	G	2492/3022 (82%)	2473 (99%)	19 (1%)	86 94
2	I	2492/3022 (82%)	2473 (99%)	19 (1%)	86 94
All	All	10320/12444 (83%)	10244 (99%)	76 (1%)	89 94

All (76) 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	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	3663	LEU
2	B	3762	ARG
2	B	3787	LYS
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4839	MET
2	B	4913	ARG
2	B	4959	PHE
2	B	4960	ILE
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	3663	LEU
2	I	3762	ARG
2	I	3787	LYS

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Mol	Chain	Res	Type
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4839	MET
2	I	4913	ARG
2	I	4959	PHE
2	I	4960	ILE
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3663	LEU
2	E	3762	ARG
2	E	3787	LYS
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4839	MET
2	E	4913	ARG
2	E	4959	PHE
2	E	4960	ILE
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
2	G	3663	LEU
2	G	3762	ARG
2	G	3787	LYS
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN

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Mol	Chain	Res	Type
2	G	4839	MET
2	G	4913	ARG
2	G	4959	PHE
2	G	4960	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (154) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	43	ASN
1	F	87	HIS
1	A	43	ASN
1	A	87	HIS
1	H	43	ASN
1	H	87	HIS
1	J	43	ASN
1	J	87	HIS
2	B	57	ASN
2	B	111	HIS
2	B	113	HIS
2	B	273	HIS
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	413	GLN
2	B	479	GLN
2	B	582	HIS
2	B	838	HIS
2	B	1598	GLN
2	B	1640	HIS
2	B	1679	ASN
2	B	1688	HIS
2	B	1691	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	2127	GLN
2	B	3809	ASN
2	B	3830	GLN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN

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Mol	Chain	Res	Type
2	B	3963	ASN
2	B	3976	ASN
2	B	3994	HIS
2	B	4034	ASN
2	B	4054	ASN
2	B	4120	ASN
2	B	4142	ASN
2	B	4946	GLN
2	B	4949	GLN
2	B	5003	HIS
2	I	57	ASN
2	I	111	HIS
2	I	113	HIS
2	I	156	GLN
2	I	273	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	413	GLN
2	I	479	GLN
2	I	582	HIS
2	I	838	HIS
2	I	1598	GLN
2	I	1640	HIS
2	I	1679	ASN
2	I	1688	HIS
2	I	1691	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	1941	ASN
2	I	2127	GLN
2	I	3809	ASN
2	I	3830	GLN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3963	ASN
2	I	3976	ASN
2	I	3994	HIS
2	I	4034	ASN

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Mol	Chain	Res	Type
2	I	4054	ASN
2	I	4120	ASN
2	I	4142	ASN
2	I	4946	GLN
2	I	4949	GLN
2	I	5003	HIS
2	E	57	ASN
2	E	111	HIS
2	E	113	HIS
2	E	156	GLN
2	E	273	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	413	GLN
2	E	479	GLN
2	E	582	HIS
2	E	838	HIS
2	E	1598	GLN
2	E	1640	HIS
2	E	1679	ASN
2	E	1688	HIS
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	1941	ASN
2	E	2127	GLN
2	E	3809	ASN
2	E	3830	GLN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3963	ASN
2	E	3976	ASN
2	E	3994	HIS
2	E	4034	ASN
2	E	4054	ASN
2	E	4120	ASN
2	E	4946	GLN
2	E	4949	GLN

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Mol	Chain	Res	Type
2	E	5003	HIS
2	G	57	ASN
2	G	111	HIS
2	G	113	HIS
2	G	273	HIS
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	413	GLN
2	G	479	GLN
2	G	582	HIS
2	G	838	HIS
2	G	1598	GLN
2	G	1640	HIS
2	G	1679	ASN
2	G	1688	HIS
2	G	1719	HIS
2	G	1775	HIS
2	G	1941	ASN
2	G	2127	GLN
2	G	3809	ASN
2	G	3830	GLN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3963	ASN
2	G	3976	ASN
2	G	3994	HIS
2	G	4034	ASN
2	G	4054	ASN
2	G	4120	ASN
2	G	4946	GLN
2	G	4949	GLN
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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ATP	B	5101	-	26,33,33	0.94	1 (3%)	26,52,52	1.61	1 (3%)
4	CFF	B	5102	-	8,15,15	2.37	3 (37%)	8,23,23	1.24	1 (12%)
3	ATP	E	5101	-	26,33,33	0.93	1 (3%)	26,52,52	1.62	1 (3%)
4	CFF	E	5102	-	8,15,15	2.38	3 (37%)	8,23,23	1.24	1 (12%)
3	ATP	G	5101	-	26,33,33	0.94	1 (3%)	26,52,52	1.62	1 (3%)
4	CFF	G	5102	-	8,15,15	2.37	3 (37%)	8,23,23	1.23	1 (12%)
3	ATP	I	5101	-	26,33,33	0.94	1 (3%)	26,52,52	1.61	1 (3%)
4	CFF	I	5102	-	8,15,15	2.37	3 (37%)	8,23,23	1.25	1 (12%)

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
3	ATP	B	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	B	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	E	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	E	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	G	5101	-	-	0/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CFF	G	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	I	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	0/0/0/0	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5102	CFF	C4-N3	-4.57	1.33	1.39
4	G	5102	CFF	C4-N3	-4.51	1.33	1.39
4	I	5102	CFF	C4-N3	-4.50	1.33	1.39
4	B	5102	CFF	C4-N3	-4.50	1.33	1.39
4	I	5102	CFF	C6-N1	-3.82	1.32	1.38
4	E	5102	CFF	C6-N1	-3.81	1.32	1.38
4	G	5102	CFF	C6-N1	-3.79	1.32	1.38
4	B	5102	CFF	C6-N1	-3.78	1.32	1.38
4	I	5102	CFF	O13-C6	-2.36	1.18	1.24
4	E	5102	CFF	O13-C6	-2.36	1.18	1.24
4	G	5102	CFF	O13-C6	-2.36	1.18	1.24
4	B	5102	CFF	O13-C6	-2.36	1.18	1.24
3	E	5101	ATP	C5-C4	2.87	1.47	1.40
3	G	5101	ATP	C5-C4	2.87	1.47	1.40
3	B	5101	ATP	C5-C4	2.89	1.47	1.40
3	I	5101	ATP	C5-C4	2.89	1.47	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	5101	ATP	N3-C2-N1	-6.41	123.83	128.87
3	E	5101	ATP	N3-C2-N1	-6.37	123.87	128.87
3	I	5101	ATP	N3-C2-N1	-6.35	123.88	128.87
3	B	5101	ATP	N3-C2-N1	-6.35	123.88	128.87
4	G	5102	CFF	C14-N7-C8	-2.54	112.07	125.31
4	B	5102	CFF	C14-N7-C8	-2.53	112.11	125.31
4	I	5102	CFF	C14-N7-C8	-2.53	112.11	125.31
4	E	5102	CFF	C14-N7-C8	-2.52	112.14	125.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	1	0
3	E	5101	ATP	1	0
3	G	5101	ATP	1	0
3	I	5101	ATP	1	0

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	14
2	B	14
2	I	14
2	E	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	72.97
1	I	4345:UNK	C	4540:PHE	N	72.97
1	E	4345:UNK	C	4540:PHE	N	72.97
1	G	4345:UNK	C	4540:PHE	N	72.97
1	B	3613:UNK	C	3639:THR	N	44.25
1	I	3613:UNK	C	3639:THR	N	44.25
1	E	3613:UNK	C	3639:THR	N	44.25
1	G	3613:UNK	C	3639:THR	N	44.25
1	B	4253:GLU	C	4320:UNK	N	27.48
1	I	4253:GLU	C	4320:UNK	N	27.48
1	E	4253:GLU	C	4320:UNK	N	27.48
1	G	4253:GLU	C	4320:UNK	N	27.48
1	B	3163:UNK	C	3170:UNK	N	16.07
1	I	3163:UNK	C	3170:UNK	N	16.07
1	E	3163:UNK	C	3170:UNK	N	16.07
1	G	3163:UNK	C	3170:UNK	N	16.07
1	B	3063:UNK	C	3134:UNK	N	15.01
1	I	3063:UNK	C	3134:UNK	N	15.01
1	E	3063:UNK	C	3134:UNK	N	15.01
1	G	3063:UNK	C	3134:UNK	N	15.01

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3468:UNK	C	3511:UNK	N	14.60
1	I	3468:UNK	C	3511:UNK	N	14.60
1	E	3468:UNK	C	3511:UNK	N	14.60
1	G	3468:UNK	C	3511:UNK	N	14.60
1	B	2703:UNK	C	2734:ASN	N	14.12
1	I	2703:UNK	C	2734:ASN	N	14.12
1	E	2703:UNK	C	2734:ASN	N	14.12
1	G	2703:UNK	C	2734:ASN	N	14.12
1	B	3236:UNK	C	3241:UNK	N	13.51
1	I	3236:UNK	C	3241:UNK	N	13.51
1	E	3236:UNK	C	3241:UNK	N	13.51
1	G	3236:UNK	C	3241:UNK	N	13.51
1	B	1564:UNK	C	1573:MET	N	12.36
1	I	1564:UNK	C	1573:MET	N	12.36
1	E	1564:UNK	C	1573:MET	N	12.36
1	G	1564:UNK	C	1573:MET	N	12.36
1	B	2976:UNK	C	2995:UNK	N	12.31
1	I	2976:UNK	C	2995:UNK	N	12.31
1	E	2976:UNK	C	2995:UNK	N	12.31
1	G	2976:UNK	C	2995:UNK	N	12.31
1	I	3254:UNK	C	3261:UNK	N	8.30
1	B	3254:UNK	C	3261:UNK	N	8.29
1	E	3254:UNK	C	3261:UNK	N	8.29
1	G	3254:UNK	C	3261:UNK	N	8.29
1	B	1297:UNK	C	1430:UNK	N	5.73
1	I	1297:UNK	C	1430:UNK	N	5.73
1	E	1297:UNK	C	1430:UNK	N	5.73
1	G	1297:UNK	C	1430:UNK	N	5.73
1	B	2939:ARG	C	2942:UNK	N	3.51
1	I	2939:ARG	C	2942:UNK	N	3.51
1	E	2939:ARG	C	2942:UNK	N	3.51
1	G	2939:ARG	C	2942:UNK	N	3.51
1	B	2479:LEU	C	2487:UNK	N	3.41
1	I	2479:LEU	C	2487:UNK	N	3.41
1	E	2479:LEU	C	2487:UNK	N	3.41
1	G	2479:LEU	C	2487:UNK	N	3.41