wwPDB EM Map/Model Validation Report (i)

Oct 17, 2016 – 08:05 PM EDT

PDB ID	:	5TAP
EMDB ID:	:	EMD-8381
Title	:	Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, all particles)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-10
Resolution	:	4.40 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

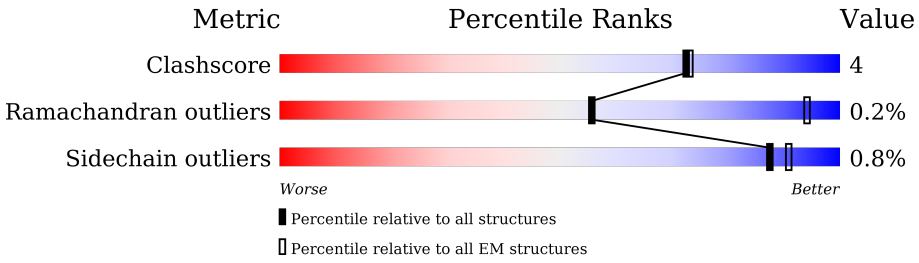
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 4.40 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	85% 14% .
1	F	108	85% 14% .
1	H	108	83% 16% .
1	J	108	84% 15% .
2	B	4416	85% 9% 5%
2	E	4416	85% 9% 5%
2	G	4416	86% 9% 5%
2	I	4416	86% 9% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 121452 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.

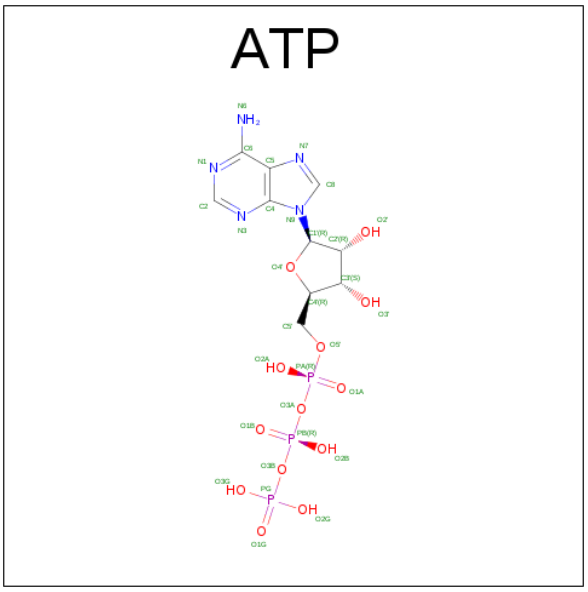
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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.

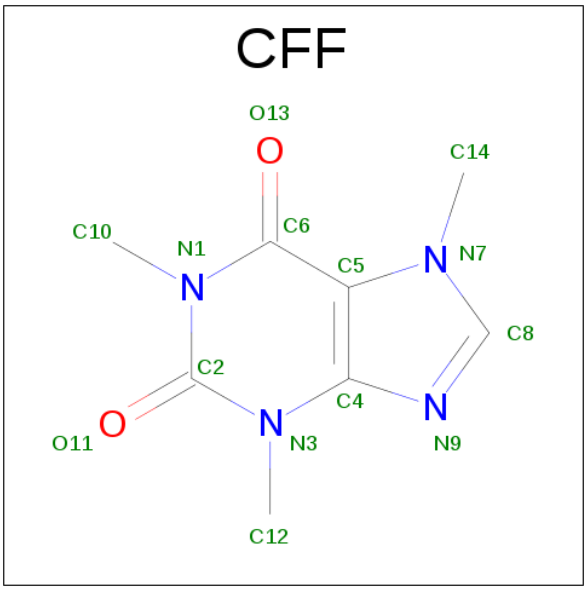
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- 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	E	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	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	E	1	Total	C	N	O	0
			14	8	4	2	
4	I	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).

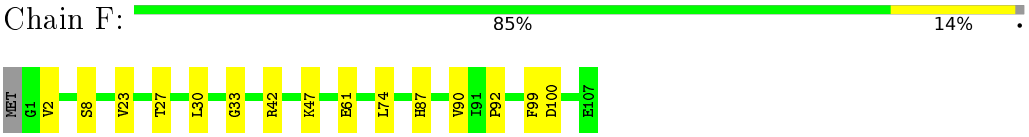
Mol	Chain	Residues	Atoms		AltConf
5	G	1	Total	Zn	0
			1	1	
5	B	1	Total	Zn	0
			1	1	
5	I	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	

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.

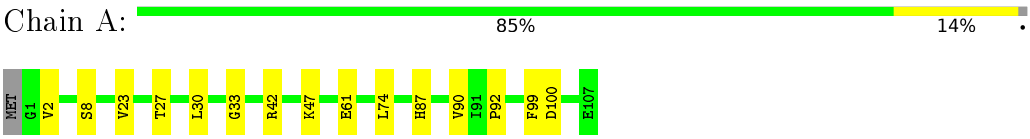
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



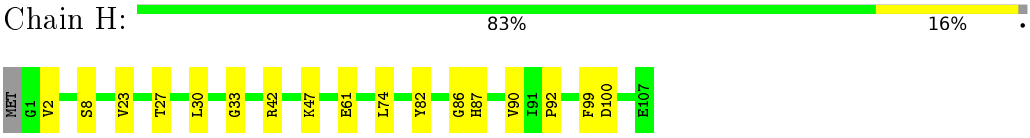
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



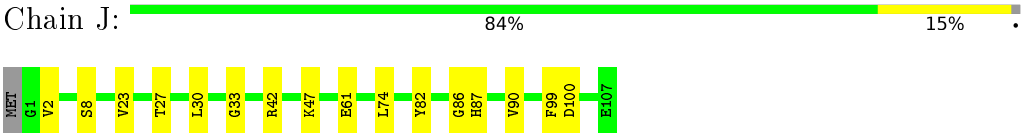
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



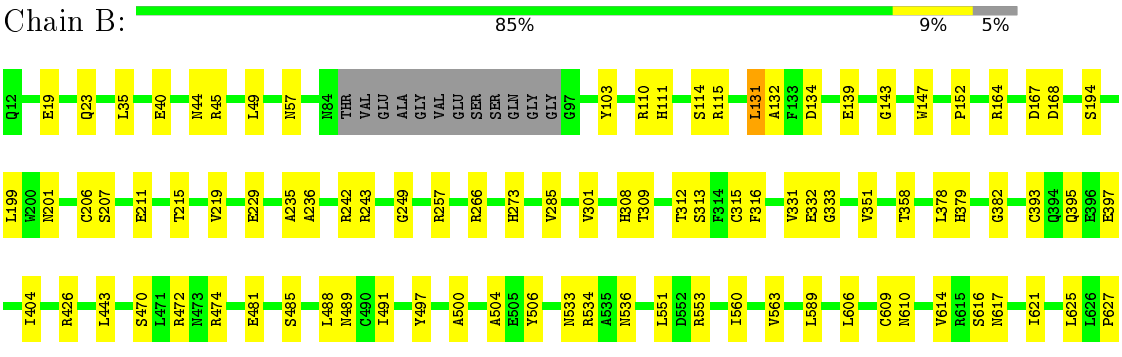
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

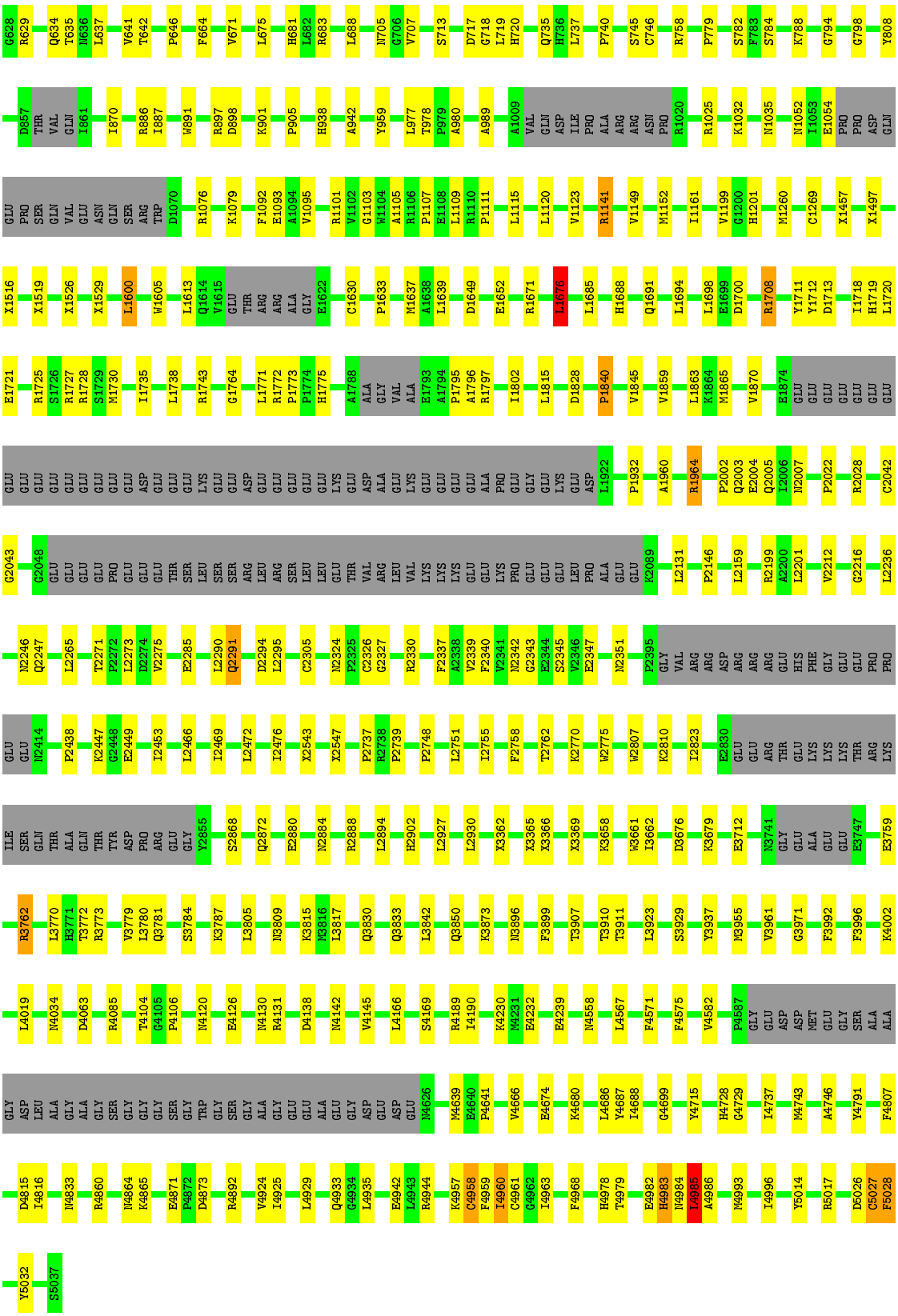
Chain J:



- Molecule 2: Ryanodine receptor 1

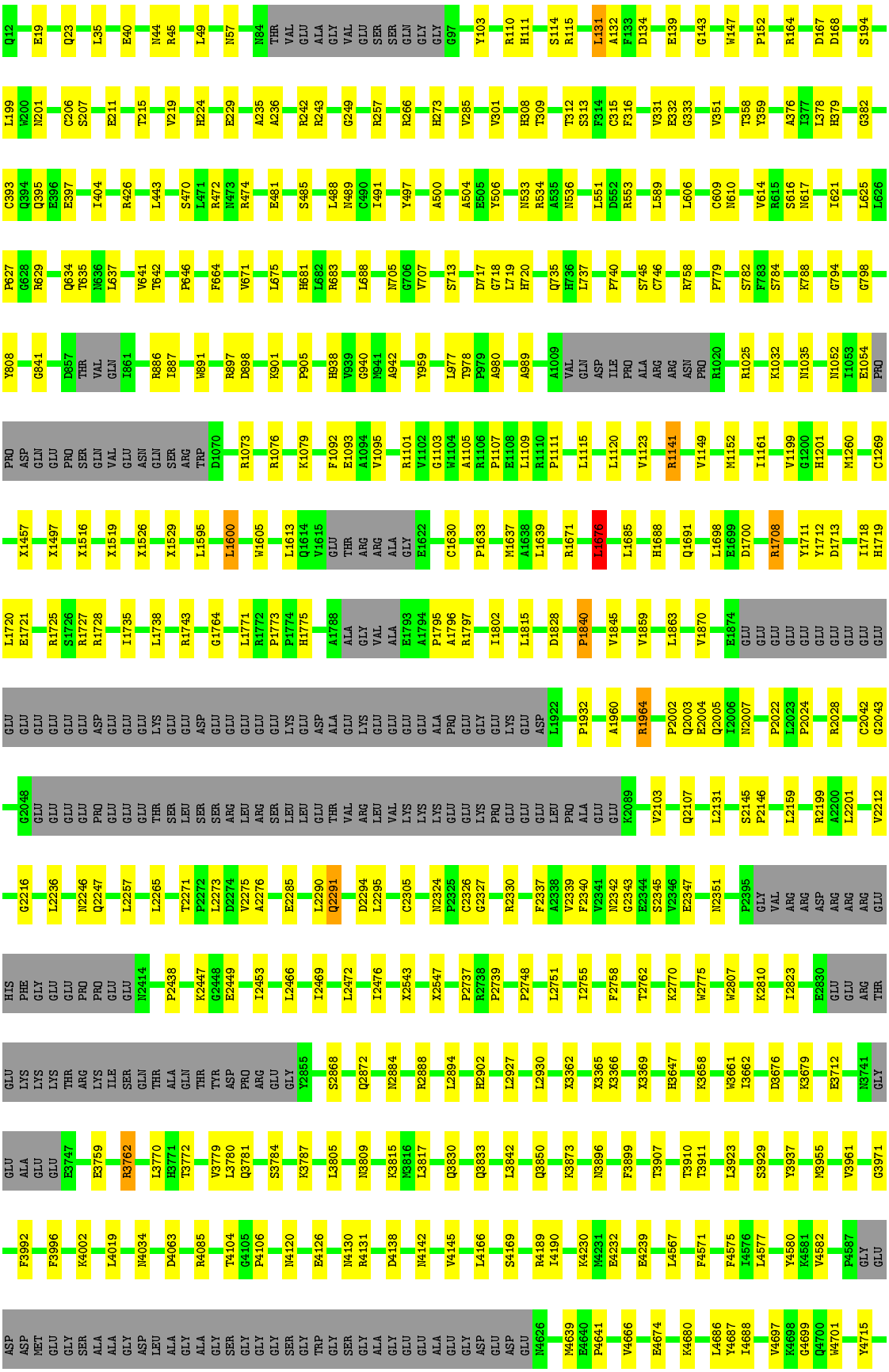
Chain B:

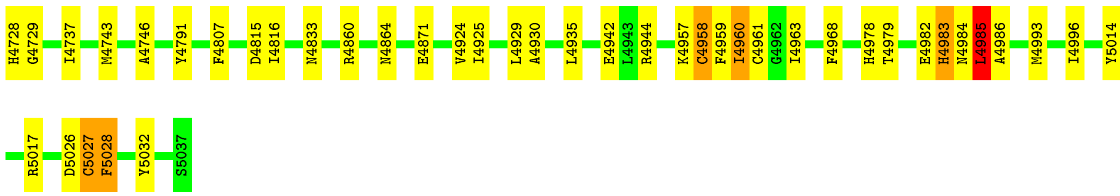




- Molecule 2: Ryanodine receptor 1

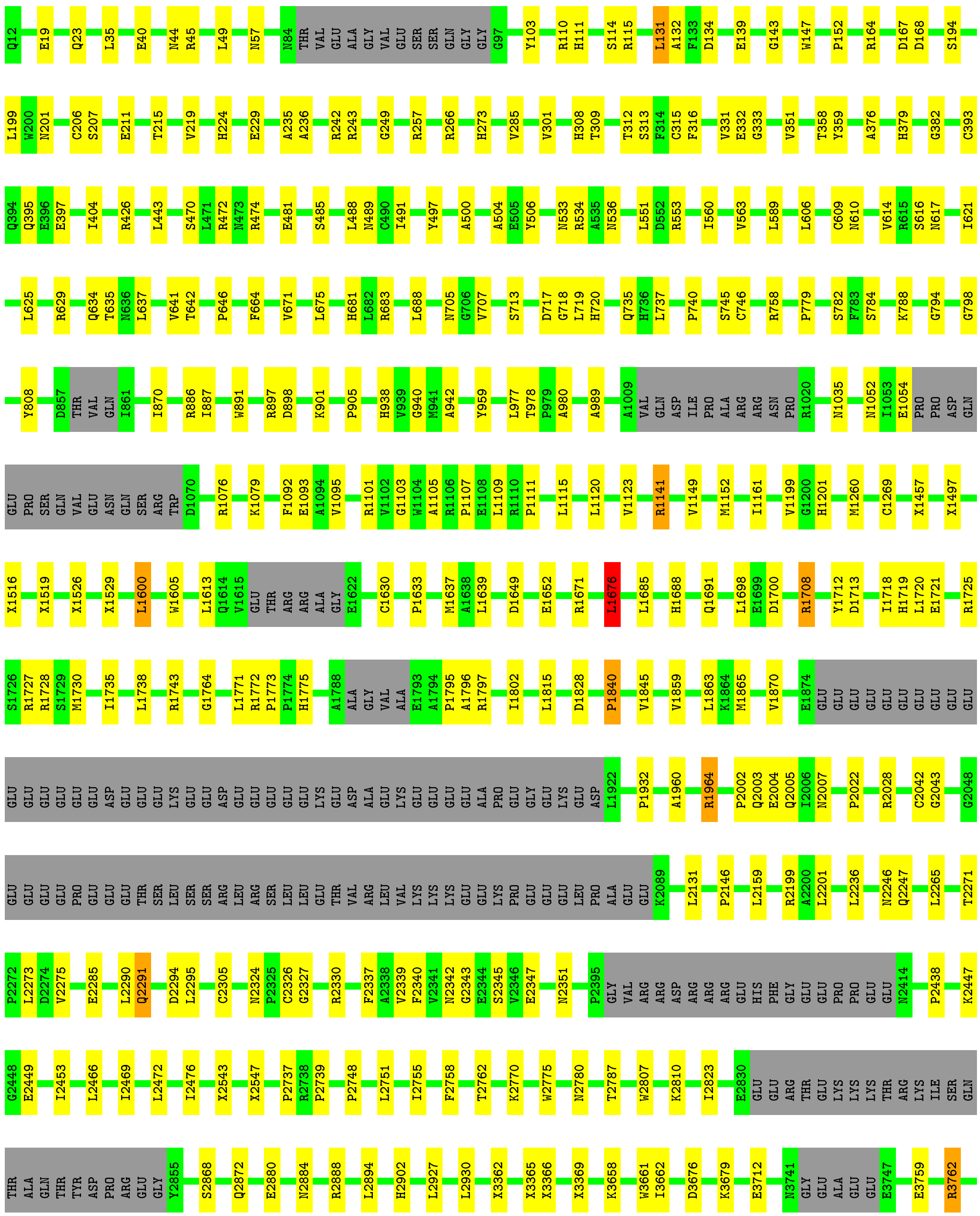
Chain E:

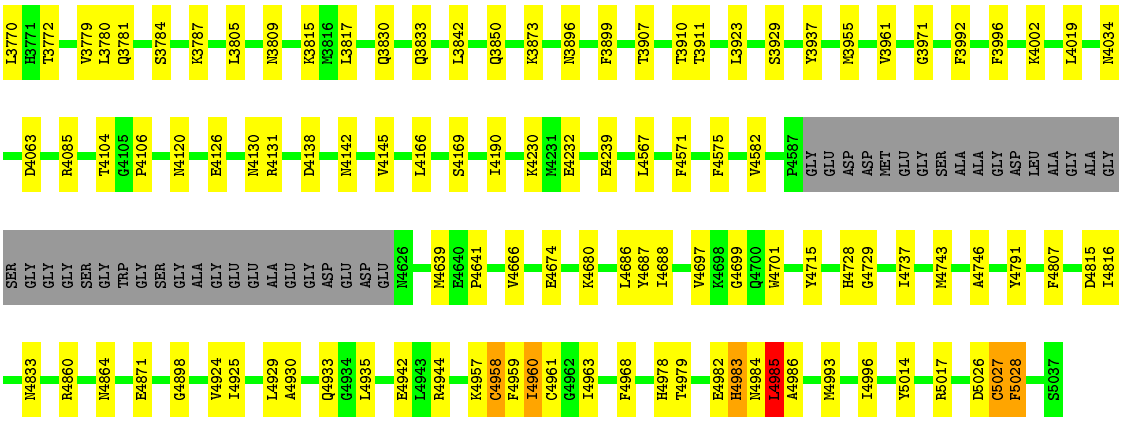




- Molecule 2: Ryanodine receptor 1

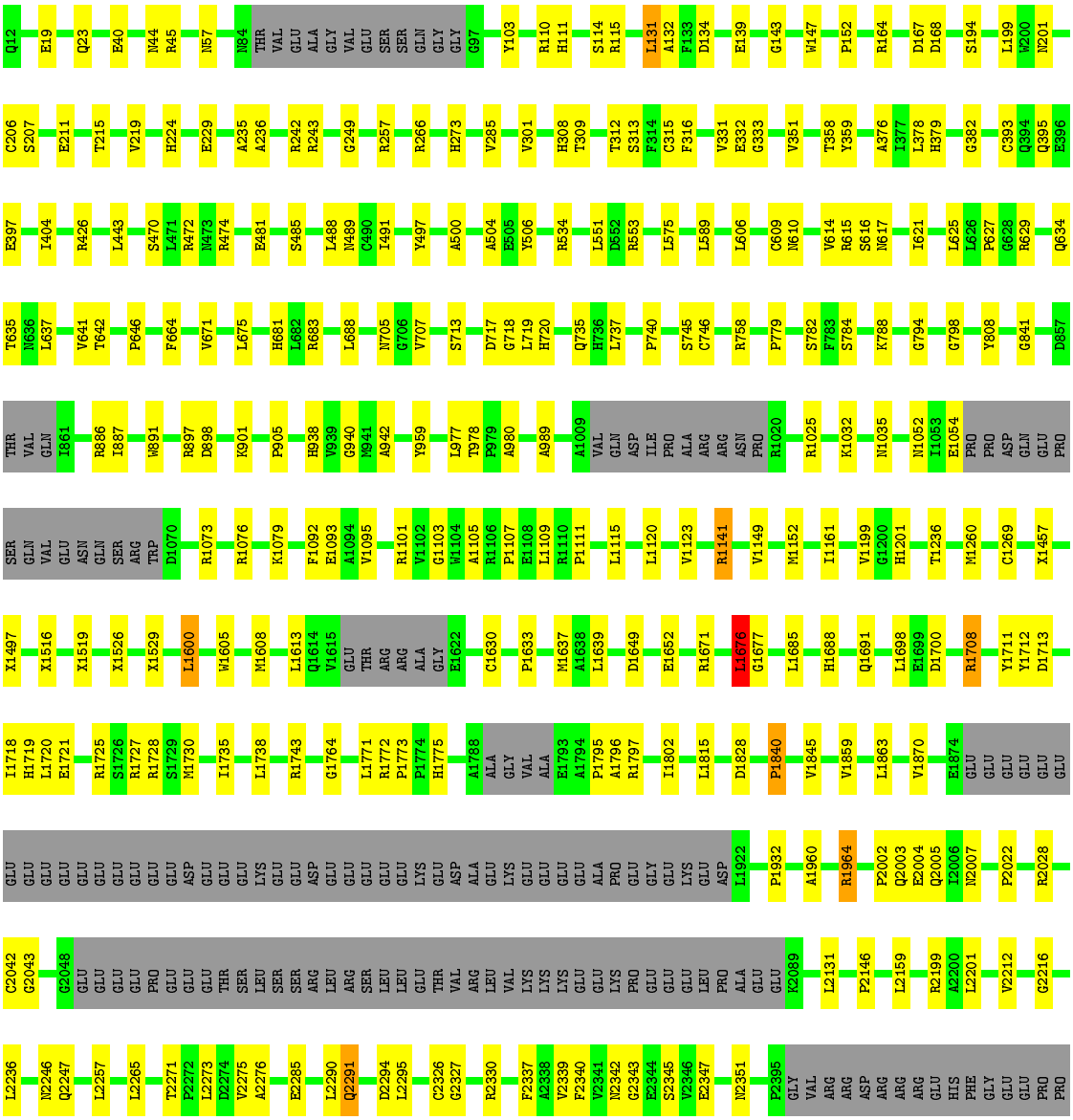
Chain I:

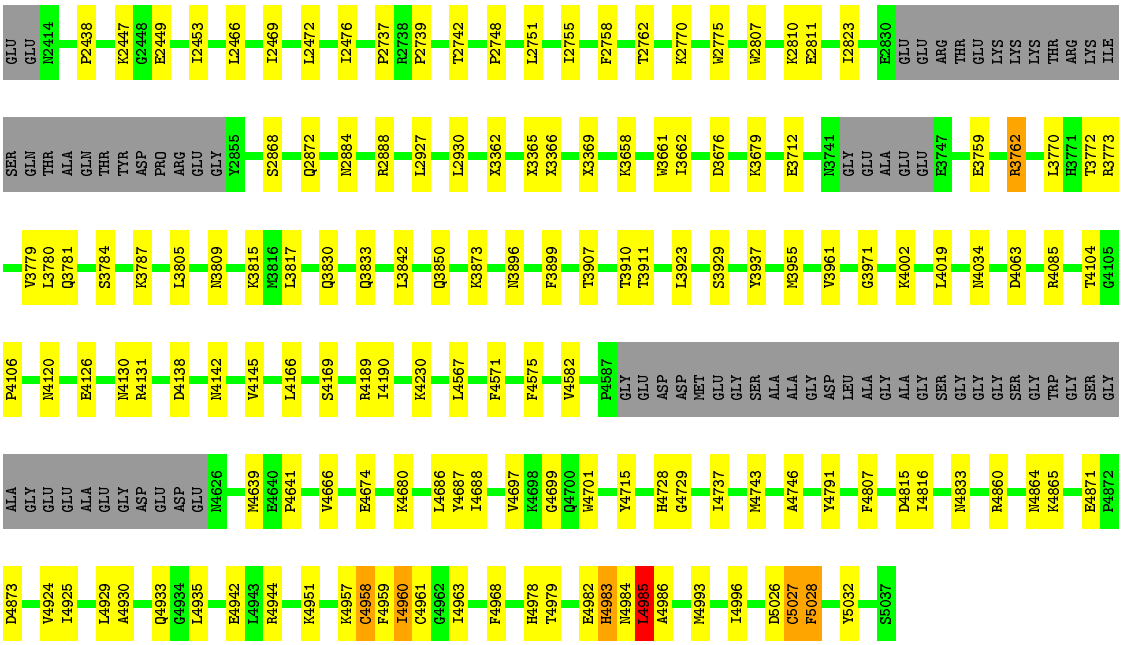





• Molecule 2: Ryanodine receptor 1

Chain G:




GLU GLU N2414 P2438 K2447 G2448 E2449 I2453 L2466 I2469 L2472 I2476 P2737 R2738 P2739 T2742 P2748 L2751 I2755 F2758 T2762 K2770 W2775 W2807 K2810 E2811 I2823 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE
SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 S2868 Q2872 N2884 R2888 L2927 L2930 X3362 X3365 X3366 X3369 K3658 W3661 I3662 D3676 K3679 E3712 N3741 GLY GLU ALA GLU GLU E3747 E3759 R3762 L3770 H3771 T3772 R3773
V3779 L3780 Q3781 S3784 K3787 L3805 N3809 K3815 M3816 L3817 Q3830 Q3833 L3842 Q3850 K3873 N3896 F3899 T3907 T3910 T3911 L3923 S3929 Y3937 M3955 V3961 G3971 K4002 L4019 N4034 D4063 R4085 T4104 G4105
P4106 N4120 E4126 N4130 R4131 D4138 N4142 V4145 L4166 S4169 R4189 I4190 K4230 L4567 F4571 F4575 V4582 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 M4639 E4640 P4641 V4666 E4674 K4680 L4686 Y4687 I4688 V4697 K4698 G4699 Q4700 W4701 Y4715 H4728 G4729 I4737 M4743 A4746 Y4791 F4807 D4815 I4816 N4833 R4860 N4864 K4865 E4871 P4872
D4873 V4924 I4925 L4929 A4930 Q4933 G4934 L4935 E4942 L4943 R4944 K4951 K4957 C4958 F4959 I4960 C4961 G4962 I4963 F4968 H4978 T4979 E4982 H4983 N4984 L4985 A4986 M4993 I4996 D5026 C5027 F5028 Y5032 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	0.32	0/834	0.51	0/1123
1	F	0.32	0/834	0.51	0/1123
1	H	0.32	0/834	0.51	0/1123
1	J	0.32	0/834	0.51	0/1123
2	B	0.31	1/25428 (0.0%)	0.54	9/34534 (0.0%)
2	E	0.31	1/25428 (0.0%)	0.54	9/34534 (0.0%)
2	G	0.31	1/25428 (0.0%)	0.54	9/34534 (0.0%)
2	I	0.31	1/25428 (0.0%)	0.54	9/34534 (0.0%)
All	All	0.31	4/105048 (0.0%)	0.54	36/142628 (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	15
2	E	0	15
2	G	0	15
2	I	0	15
All	All	0	64

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2476	ILE	C-N	5.37	1.44	1.34
2	B	2476	ILE	C-N	5.34	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2476	ILE	C-N	5.33	1.44	1.34
2	G	2476	ILE	C-N	5.30	1.44	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	131	LEU	CA-CB-CG	8.29	134.37	115.30
2	G	131	LEU	CA-CB-CG	8.28	134.35	115.30
2	B	131	LEU	CA-CB-CG	8.27	134.32	115.30
2	E	131	LEU	CA-CB-CG	8.27	134.32	115.30
2	G	1600	LEU	CA-CB-CG	7.05	131.52	115.30
2	I	1600	LEU	CA-CB-CG	7.04	131.49	115.30
2	B	1600	LEU	CA-CB-CG	7.04	131.49	115.30
2	E	1600	LEU	CA-CB-CG	7.03	131.48	115.30
2	I	1676	LEU	CA-CB-CG	6.55	130.37	115.30
2	B	1676	LEU	CA-CB-CG	6.54	130.33	115.30
2	G	1676	LEU	CA-CB-CG	6.52	130.31	115.30
2	E	1676	LEU	CA-CB-CG	6.51	130.28	115.30
2	I	4985	LEU	CA-CB-CG	6.23	129.63	115.30
2	G	4985	LEU	CA-CB-CG	6.23	129.63	115.30
2	B	4985	LEU	CA-CB-CG	6.22	129.60	115.30
2	E	4985	LEU	CA-CB-CG	6.22	129.60	115.30
2	G	977	LEU	CA-CB-CG	5.37	127.64	115.30
2	G	688	LEU	CA-CB-CG	5.36	127.63	115.30
2	B	977	LEU	CA-CB-CG	5.35	127.61	115.30
2	I	977	LEU	CA-CB-CG	5.35	127.61	115.30
2	I	688	LEU	CA-CB-CG	5.35	127.60	115.30
2	E	977	LEU	CA-CB-CG	5.34	127.59	115.30
2	B	688	LEU	CA-CB-CG	5.33	127.57	115.30
2	E	688	LEU	CA-CB-CG	5.33	127.57	115.30
2	E	3770	LEU	CA-CB-CG	5.12	127.07	115.30
2	B	3770	LEU	CA-CB-CG	5.12	127.06	115.30
2	G	3770	LEU	CA-CB-CG	5.11	127.04	115.30
2	I	3770	LEU	CA-CB-CG	5.10	127.03	115.30
2	I	2290	LEU	CA-CB-CG	5.08	126.97	115.30
2	E	2290	LEU	CA-CB-CG	5.07	126.95	115.30
2	B	2290	LEU	CA-CB-CG	5.06	126.95	115.30
2	G	2290	LEU	CA-CB-CG	5.06	126.94	115.30
2	I	4639	MET	C-N-CA	5.05	134.32	121.70
2	G	4639	MET	C-N-CA	5.03	134.27	121.70
2	E	4639	MET	C-N-CA	5.03	134.27	121.70
2	B	4639	MET	C-N-CA	5.03	134.26	121.70

There are no chirality outliers.

All (64) 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	1720	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	2291	GLN	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	1720	LEU	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	2291	GLN	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	1720	LEU	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
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	1720	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	2291	GLN	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 (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	8	0
1	F	818	0	824	8	0
1	H	818	0	824	9	0
1	J	818	0	824	8	0
2	B	29499	0	24749	236	0
2	E	29499	0	24749	235	0
2	G	29499	0	24749	231	0
2	I	29499	0	24749	233	0
3	B	31	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	31	0	12	2	0
3	G	31	0	12	2	0
3	I	31	0	12	2	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	121452	0	102380	949	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 (949) 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:I:4230:LYS:HD2	2:I:4959:PHE:HE1	1.38	0.88
2:E:4230:LYS:HD2	2:E:4959:PHE:HE1	1.38	0.88
2:B:4230:LYS:HD2	2:B:4959:PHE:HE1	1.38	0.87
2:G:4230:LYS:HD2	2:G:4959:PHE:HE1	1.38	0.87
2:B:4983:HIS:H	2:B:4983:HIS:CD2	1.94	0.86
2:G:4983:HIS:H	2:G:4983:HIS:CD2	1.94	0.86
2:I:4983:HIS:CD2	2:I:4983:HIS:H	1.94	0.84
2:B:4230:LYS:CD	2:B:4959:PHE:HE1	1.92	0.83
2:I:4230:LYS:CD	2:I:4959:PHE:HE1	1.92	0.82
2:E:4983:HIS:H	2:E:4983:HIS:CD2	1.94	0.82
2:E:4230:LYS:CD	2:E:4959:PHE:HE1	1.92	0.82
2:B:4230:LYS:HD2	2:B:4959:PHE:CE1	2.15	0.81
2:G:4230:LYS:HD2	2:G:4959:PHE:CE1	2.15	0.81
2:I:4230:LYS:HD2	2:I:4959:PHE:CE1	2.15	0.81
2:G:4230:LYS:CD	2:G:4959:PHE:HE1	1.92	0.81
2:E:4230:LYS:HD2	2:E:4959:PHE:CE1	2.15	0.80
2:G:4983:HIS:H	2:G:4983:HIS:HD2	1.29	0.79
2:B:4983:HIS:H	2:B:4983:HIS:HD2	1.29	0.77
2:I:4983:HIS:HD2	2:I:4983:HIS:H	1.29	0.77
2:E:4983:HIS:H	2:E:4983:HIS:HD2	1.29	0.77
2:B:4968:PHE:CZ	2:B:4978:HIS:CE1	2.77	0.73
2:E:4968:PHE:CZ	2:E:4978:HIS:CE1	2.77	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4968:PHE:CZ	2:G:4978:HIS:CE1	2.77	0.72
2:I:4968:PHE:CZ	2:I:4978:HIS:CE1	2.77	0.72
2:G:4960:ILE:N	2:G:4960:ILE:HD13	2.04	0.72
2:I:4960:ILE:N	2:I:4960:ILE:HD13	2.04	0.71
2:E:4960:ILE:HD13	2:E:4960:ILE:N	2.04	0.71
2:B:4960:ILE:HD13	2:B:4960:ILE:N	2.04	0.71
2:B:4968:PHE:CE2	2:B:4978:HIS:ND1	2.61	0.69
2:E:4968:PHE:CE2	2:E:4978:HIS:ND1	2.61	0.68
2:G:4968:PHE:CE2	2:G:4978:HIS:ND1	2.61	0.68
2:I:4968:PHE:CE2	2:I:4978:HIS:ND1	2.61	0.68
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.76	0.67
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.77	0.67
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.76	0.67
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.76	0.67
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.78	0.66
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.78	0.66
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.61	0.65
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.61	0.65
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.61	0.64
2:G:379:HIS:HD2	2:G:382:GLY:H	1.45	0.64
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.62	0.64
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.78	0.64
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.80	0.64
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.80	0.64
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.61	0.64
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.78	0.64
2:B:4944:ARG:HH22	2:I:4942:GLU:HA	1.63	0.63
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.80	0.63
2:I:379:HIS:HD2	2:I:382:GLY:H	1.45	0.63
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.81	0.63
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.81	0.63
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.80	0.63
2:E:379:HIS:HD2	2:E:382:GLY:H	1.45	0.63
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.81	0.63
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.64	0.63
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.64	0.63
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.81	0.63
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.63	0.63
2:B:379:HIS:HD2	2:B:382:GLY:H	1.45	0.63
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.64	0.62
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.81	0.62
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.81	0.62
2:G:4982:GLU:HB3	2:G:4983:HIS:HD2	1.65	0.62
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.63	0.62
2:E:4982:GLU:HB3	2:E:4983:HIS:HD2	1.65	0.62
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.65	0.62
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.81	0.62
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.33	0.62
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.64	0.61
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.83	0.61
2:B:4982:GLU:HB3	2:B:4983:HIS:HD2	1.65	0.61
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.81	0.61
2:I:4982:GLU:HB3	2:I:4983:HIS:HD2	1.65	0.61
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.65	0.61
2:I:4944:ARG:HH22	2:G:4942:GLU:HA	1.65	0.61
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.82	0.61
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.83	0.61
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.33	0.61
2:E:4961:CYS:HB3	2:E:4983:HIS:HE1	1.66	0.61
2:I:4230:LYS:CG	2:I:4959:PHE:HE1	2.14	0.61
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.33	0.60
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.83	0.60
2:B:4230:LYS:CG	2:B:4959:PHE:HE1	2.14	0.60
2:G:4961:CYS:HB3	2:G:4983:HIS:HE1	1.66	0.60
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.34	0.60
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.33	0.60
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.82	0.60
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.82	0.60
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.83	0.60
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.65	0.60
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.65	0.60
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.82	0.60
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.34	0.60
2:B:4961:CYS:HB3	2:B:4983:HIS:HE1	1.65	0.60
2:E:4230:LYS:CG	2:E:4959:PHE:HE1	2.14	0.60
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.35	0.60
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.83	0.60
2:G:4230:LYS:CG	2:G:4959:PHE:HE1	2.14	0.60
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.83	0.59
2:B:4979:THR:HG22	3:B:5101:ATP:H2	1.67	0.59
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4979:THR:HG22	3:I:5101:ATP:H2	1.67	0.59
2:I:4961:CYS:HB3	2:I:4983:HIS:HE1	1.65	0.59
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.85	0.59
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.83	0.59
2:B:132:ALA:HA	2:B:194:SER:HB2	1.84	0.59
2:E:4942:GLU:HA	2:G:4944:ARG:HH22	1.67	0.59
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.85	0.59
2:E:132:ALA:HA	2:E:194:SER:HB2	1.84	0.59
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.85	0.59
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.85	0.59
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.36	0.59
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.85	0.59
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.85	0.59
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.85	0.59
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.35	0.59
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.36	0.59
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.35	0.59
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.35	0.59
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.36	0.58
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.86	0.58
2:I:4791:TYR:OH	2:I:4815:ASP:O	2.22	0.58
2:I:4190:ILE:HD13	2:I:5026:ASP:CG	2.24	0.58
2:B:4791:TYR:OH	2:B:4815:ASP:O	2.22	0.58
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.37	0.58
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.85	0.58
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.85	0.58
2:G:2131:LEU:HB3	2:G:3662:ILE:HD13	1.85	0.58
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.85	0.58
2:E:2131:LEU:HB3	2:E:3662:ILE:HD13	1.85	0.58
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.37	0.58
2:G:4979:THR:HG22	3:G:5101:ATP:H2	1.67	0.58
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.36	0.58
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.86	0.58
2:B:2131:LEU:HB3	2:B:3662:ILE:HD13	1.85	0.58
2:E:4791:TYR:OH	2:E:4815:ASP:O	2.22	0.58
2:E:4979:THR:HG22	3:E:5101:ATP:H2	1.67	0.58
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.85	0.58
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.37	0.58
2:E:4190:ILE:HD13	2:E:5026:ASP:CG	2.24	0.58
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.34	0.58
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.85	0.57
2:B:4190:ILE:HD13	2:B:5026:ASP:CG	2.24	0.57
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.86	0.57
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.34	0.57
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.86	0.57
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.85	0.57
2:I:2131:LEU:HB3	2:I:3662:ILE:HD13	1.85	0.57
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.69	0.57
2:G:4791:TYR:OH	2:G:4815:ASP:O	2.22	0.57
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.86	0.57
2:G:132:ALA:HA	2:G:194:SER:HB2	1.84	0.57
2:G:4190:ILE:HD13	2:G:5026:ASP:CG	2.24	0.57
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.37	0.57
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.86	0.57
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.69	0.57
2:E:315:CYS:SG	2:E:316:PHE:N	2.78	0.57
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.87	0.57
2:I:132:ALA:HA	2:I:194:SER:HB2	1.84	0.57
2:I:4567:LEU:HD12	2:I:4816:ILE:HD12	1.87	0.57
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.87	0.57
2:B:4567:LEU:HD12	2:B:4816:ILE:HD12	1.87	0.57
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.69	0.57
2:B:315:CYS:SG	2:B:316:PHE:N	2.78	0.57
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.87	0.57
2:E:4968:PHE:CZ	2:E:4978:HIS:ND1	2.73	0.57
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.87	0.57
2:E:4993:MET:HA	2:E:4996:ILE:HD12	1.86	0.56
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.38	0.56
2:I:315:CYS:SG	2:I:316:PHE:N	2.77	0.56
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.86	0.56
2:B:4968:PHE:CZ	2:B:4978:HIS:ND1	2.73	0.56
2:I:4993:MET:HA	2:I:4996:ILE:HD12	1.86	0.56
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.38	0.56
2:E:2347:GLU:O	2:E:2351:ASN:N	2.36	0.56
2:E:4567:LEU:HD12	2:E:4816:ILE:HD12	1.87	0.56
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.70	0.56
2:G:315:CYS:SG	2:G:316:PHE:N	2.78	0.56
2:G:4968:PHE:CZ	2:G:4978:HIS:ND1	2.73	0.56
2:E:23:GLN:HB3	2:E:201:ASN:HB2	1.88	0.56
2:E:609:CYS:SG	2:E:610:ASN:N	2.78	0.56
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4993:MET:HA	2:B:4996:ILE:HD12	1.86	0.56
2:B:609:CYS:SG	2:B:610:ASN:N	2.78	0.56
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.70	0.56
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.38	0.56
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.86	0.56
2:G:4567:LEU:HD12	2:G:4816:ILE:HD12	1.87	0.56
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.86	0.56
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.88	0.56
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.70	0.56
2:B:4190:ILE:CD1	2:B:5026:ASP:OD2	2.54	0.56
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.69	0.56
2:B:23:GLN:HB3	2:B:201:ASN:HB2	1.88	0.56
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.86	0.56
2:G:2347:GLU:O	2:G:2351:ASN:N	2.36	0.56
2:G:23:GLN:HB3	2:G:201:ASN:HB2	1.88	0.56
2:G:4993:MET:HA	2:G:4996:ILE:HD12	1.86	0.56
2:G:609:CYS:SG	2:G:610:ASN:N	2.78	0.56
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.88	0.56
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.88	0.56
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.70	0.56
2:E:470:SER:O	2:E:474:ARG:NE	2.39	0.56
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.38	0.56
2:I:4968:PHE:CZ	2:I:4978:HIS:ND1	2.73	0.56
2:G:470:SER:O	2:G:474:ARG:NE	2.39	0.55
2:I:609:CYS:SG	2:I:610:ASN:N	2.78	0.55
2:E:4968:PHE:CE2	2:E:4978:HIS:CE1	2.95	0.55
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.88	0.55
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.71	0.55
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.88	0.55
2:B:2347:GLU:O	2:B:2351:ASN:N	2.36	0.55
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.88	0.55
2:E:4190:ILE:CD1	2:E:5026:ASP:OD2	2.54	0.55
2:G:683:ARG:NH1	2:G:707:VAL:O	2.39	0.55
2:I:2347:GLU:O	2:I:2351:ASN:N	2.36	0.55
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.95	0.55
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.88	0.55
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.71	0.55
2:I:4190:ILE:CD1	2:I:5026:ASP:OD2	2.54	0.55
2:B:470:SER:O	2:B:474:ARG:NE	2.39	0.55
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.88	0.55
2:I:23:GLN:HB3	2:I:201:ASN:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.71	0.55
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.71	0.55
2:G:4190:ILE:CD1	2:G:5026:ASP:OD2	2.54	0.55
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.88	0.55
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.88	0.55
2:I:683:ARG:NH1	2:I:707:VAL:O	2.39	0.55
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.88	0.55
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.89	0.55
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.88	0.55
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	2.95	0.55
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.89	0.54
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.80	0.54
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.89	0.54
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.88	0.54
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.41	0.54
2:B:683:ARG:NH1	2:B:707:VAL:O	2.39	0.54
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.88	0.54
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.81	0.54
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.88	0.54
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	2.95	0.54
2:E:4190:ILE:CD1	2:E:5026:ASP:CG	2.76	0.54
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.41	0.54
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.88	0.54
2:I:4190:ILE:CD1	2:I:5026:ASP:CG	2.76	0.54
2:B:4190:ILE:CD1	2:B:5026:ASP:CG	2.76	0.54
2:G:4190:ILE:CD1	2:G:5026:ASP:CG	2.76	0.54
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.90	0.54
2:E:331:VAL:HG12	2:E:333:GLY:H	1.73	0.54
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.81	0.54
2:B:111:HIS:HD2	2:B:114:SER:H	1.56	0.54
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.81	0.54
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.90	0.54
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.41	0.54
2:I:470:SER:O	2:I:474:ARG:NE	2.39	0.54
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.90	0.54
2:E:111:HIS:HD2	2:E:114:SER:H	1.56	0.54
2:G:4983:HIS:N	2:G:4983:HIS:CD2	2.70	0.54
2:G:111:HIS:HD2	2:G:114:SER:H	1.56	0.54
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.90	0.54
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.41	0.54
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.26	0.53
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.26	0.53
2:G:794:GLY:H	2:G:798:GLY:HA3	1.73	0.53
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.90	0.53
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.90	0.53
2:I:794:GLY:H	2:I:798:GLY:HA3	1.73	0.53
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.90	0.53
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.90	0.53
2:B:331:VAL:HG12	2:B:333:GLY:H	1.73	0.53
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.91	0.53
2:I:111:HIS:HD2	2:I:114:SER:H	1.56	0.53
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.41	0.53
2:B:794:GLY:H	2:B:798:GLY:HA3	1.73	0.53
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.91	0.53
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.90	0.53
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.90	0.53
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.90	0.53
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.91	0.53
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.90	0.53
2:B:4942:GLU:HA	2:E:4944:ARG:HH22	1.73	0.53
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.91	0.53
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.42	0.53
2:I:313:SER:HB3	2:I:351:VAL:HB	1.91	0.53
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.26	0.53
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.42	0.53
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.90	0.53
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.74	0.53
2:E:794:GLY:H	2:E:798:GLY:HA3	1.74	0.53
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.91	0.53
2:G:331:VAL:HG12	2:G:333:GLY:H	1.73	0.53
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.26	0.53
2:I:331:VAL:HG12	2:I:333:GLY:H	1.73	0.53
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.91	0.52
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.92	0.52
2:B:2868:SER:O	2:B:2872:GLN:N	2.41	0.52
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.90	0.52
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.82	0.52
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.39	0.52
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.75	0.52
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.42	0.52
2:I:1796:ALA:HB1	2:I:1797:ARG:HH21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.90	0.52
2:B:1796:ALA:HB1	2:B:1797:ARG:HH21	1.75	0.52
2:E:313:SER:HB3	2:E:351:VAL:HB	1.91	0.52
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.75	0.52
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.42	0.52
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.92	0.52
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.92	0.52
2:B:313:SER:HB3	2:B:351:VAL:HB	1.91	0.52
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.90	0.52
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.91	0.52
2:E:683:ARG:NH1	2:E:707:VAL:O	2.39	0.52
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.91	0.52
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.92	0.52
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.90	0.52
2:B:978:THR:HB	2:B:980:ALA:H	1.75	0.52
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.91	0.52
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.42	0.52
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.91	0.52
2:I:978:THR:HB	2:I:980:ALA:H	1.75	0.52
2:G:4979:THR:HG22	3:G:5101:ATP:C2	2.45	0.51
2:E:1796:ALA:HB1	2:E:1797:ARG:HH21	1.75	0.51
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.43	0.51
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.43	0.51
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.75	0.51
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.43	0.51
2:B:4979:THR:HG22	3:B:5101:ATP:C2	2.45	0.51
1:F:27:THR:HB	1:F:100:ASP:HB3	1.93	0.51
2:G:313:SER:HB3	2:G:351:VAL:HB	1.91	0.51
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.82	0.51
2:E:485:SER:O	2:E:489:ASN:N	2.39	0.51
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.82	0.51
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.41	0.51
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.41	0.51
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.39	0.51
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.43	0.51
2:G:1796:ALA:HB1	2:G:1797:ARG:HH21	1.75	0.51
2:I:4961:CYS:HB3	2:I:4983:HIS:CE1	2.46	0.51
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.92	0.51
1:A:27:THR:HB	1:A:100:ASP:HB3	1.93	0.51
2:G:978:THR:HB	2:G:980:ALA:H	1.75	0.51
1:J:27:THR:HB	1:J:100:ASP:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.93	0.51
2:B:614:VAL:HG22	2:B:616:SER:H	1.75	0.51
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.82	0.51
2:E:4979:THR:HG22	3:E:5101:ATP:C2	2.45	0.51
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.93	0.51
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.42	0.51
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.43	0.51
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.43	0.51
2:G:614:VAL:HG22	2:G:616:SER:H	1.75	0.51
2:B:4961:CYS:HB3	2:B:4983:HIS:CE1	2.46	0.50
2:G:2342:ASN:N	2:G:2342:ASN:OD1	2.45	0.50
2:I:2758:PHE:O	2:I:2762:THR:N	2.45	0.50
2:E:1457:UNK:N	2:E:1497:UNK:O	2.45	0.50
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.93	0.50
2:B:2342:ASN:N	2:B:2342:ASN:OD1	2.45	0.50
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.43	0.50
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.94	0.50
2:I:4979:THR:HG22	3:I:5101:ATP:C2	2.45	0.50
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.94	0.50
2:E:978:THR:HB	2:E:980:ALA:H	1.75	0.50
2:G:1815:LEU:HD22	2:G:1845:VAL:HG21	1.93	0.50
1:H:27:THR:HB	1:H:100:ASP:HB3	1.93	0.50
2:I:1457:UNK:N	2:I:1497:UNK:O	2.44	0.50
2:I:614:VAL:HG22	2:I:616:SER:H	1.75	0.50
2:E:2868:SER:O	2:E:2872:GLN:N	2.41	0.50
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.45	0.50
2:B:1815:LEU:HD22	2:B:1845:VAL:HG21	1.93	0.50
2:B:211:GLU:OE2	2:B:3907:THR:OG1	2.30	0.50
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.93	0.50
2:G:2758:PHE:O	2:G:2762:THR:N	2.45	0.50
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.94	0.50
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.45	0.50
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.42	0.50
2:E:2758:PHE:O	2:E:2762:THR:N	2.45	0.50
2:E:614:VAL:HG22	2:E:616:SER:H	1.75	0.50
2:G:1457:UNK:N	2:G:1497:UNK:O	2.45	0.50
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.45	0.50
2:G:2868:SER:O	2:G:2872:GLN:N	2.41	0.50
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.93	0.50
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.43	0.49
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:211:GLU:OE2	2:G:3907:THR:OG1	2.30	0.49
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.93	0.49
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.94	0.49
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.43	0.49
2:E:4833:ASN:HB3	2:E:4935:LEU:HD23	1.94	0.49
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.94	0.49
2:B:4230:LYS:CG	2:B:4959:PHE:CE1	2.95	0.49
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.94	0.49
2:E:211:GLU:OE2	2:E:3907:THR:OG1	2.30	0.49
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.94	0.49
2:B:4833:ASN:HB3	2:B:4935:LEU:HD23	1.94	0.49
2:E:1815:LEU:HD22	2:E:1845:VAL:HG21	1.93	0.49
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.45	0.49
2:I:4230:LYS:CG	2:I:4959:PHE:CE1	2.95	0.49
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.94	0.49
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.94	0.49
2:E:629:ARG:HD3	2:E:634:GLN:HG2	1.94	0.49
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.94	0.49
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.95	0.49
2:I:4833:ASN:HB3	2:I:4935:LEU:HD23	1.94	0.49
2:B:1457:UNK:N	2:B:1497:UNK:O	2.45	0.49
2:B:2758:PHE:O	2:B:2762:THR:N	2.45	0.49
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.94	0.49
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.95	0.49
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.95	0.49
2:I:642:THR:HG23	2:I:1613:LEU:HD12	1.95	0.49
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.43	0.49
2:B:642:THR:HG23	2:B:1613:LEU:HD12	1.95	0.49
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.45	0.49
2:E:4230:LYS:CG	2:E:4959:PHE:CE1	2.95	0.49
2:E:4961:CYS:HB3	2:E:4983:HIS:CE1	2.46	0.49
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.95	0.49
2:I:629:ARG:HD3	2:I:634:GLN:HG2	1.94	0.49
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.41	0.49
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.45	0.49
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.43	0.49
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.45	0.49
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.94	0.49
2:G:629:ARG:HD3	2:G:634:GLN:HG2	1.94	0.49
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.94	0.49
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.95	0.49
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.31	0.49
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.46	0.49
2:G:4833:ASN:HB3	2:G:4935:LEU:HD23	1.94	0.49
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.94	0.48
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.95	0.48
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.78	0.48
2:G:3842:LEU:O	2:G:3929:SER:OG	2.31	0.48
2:G:4924:VAL:HG23	2:G:4925:ILE:HG12	1.95	0.48
2:G:4230:LYS:CG	2:G:4959:PHE:CE1	2.95	0.48
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.31	0.48
2:I:2868:SER:O	2:I:2872:GLN:N	2.41	0.48
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.45	0.48
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.94	0.48
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.95	0.48
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.96	0.48
2:I:2342:ASN:N	2:I:2342:ASN:OD1	2.45	0.48
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.95	0.48
2:B:629:ARG:HD3	2:B:634:GLN:HG2	1.94	0.48
2:E:4924:VAL:HG23	2:E:4925:ILE:HG12	1.95	0.48
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.46	0.48
2:I:1815:LEU:HD22	2:I:1845:VAL:HG21	1.93	0.48
2:B:111:HIS:CD2	2:B:114:SER:H	2.32	0.48
2:B:4924:VAL:HG23	2:B:4925:ILE:HG12	1.95	0.48
2:G:642:THR:HG23	2:G:1613:LEU:HD12	1.95	0.48
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.78	0.48
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.43	0.48
2:I:211:GLU:OE2	2:I:3907:THR:OG1	2.30	0.48
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	1.96	0.48
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.46	0.48
2:E:1735:ILE:HG23	2:E:1771:LEU:HD23	1.96	0.48
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.96	0.48
2:G:681:HIS:HB3	2:G:784:SER:HB3	1.96	0.48
2:I:3842:LEU:O	2:I:3929:SER:OG	2.31	0.48
2:I:4925:ILE:HA	2:I:4929:LEU:HD23	1.95	0.48
2:B:3759:GLU:HA	2:B:3762:ARG:HE	1.78	0.48
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.45	0.48
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.49	0.48
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.94	0.48
2:I:3759:GLU:HA	2:I:3762:ARG:HE	1.78	0.48
2:G:111:HIS:CD2	2:G:114:SER:H	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3773:ARG:HG3	2:G:3815:LYS:HZ3	1.79	0.48
2:G:4961:CYS:HB3	2:G:4983:HIS:CE1	2.46	0.48
2:I:4924:VAL:HG23	2:I:4925:ILE:HG12	1.95	0.48
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.31	0.48
2:I:111:HIS:CD2	2:I:114:SER:H	2.32	0.48
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.79	0.48
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.78	0.48
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.79	0.47
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.49	0.47
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.31	0.47
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.94	0.47
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.79	0.47
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.79	0.47
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.78	0.47
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.96	0.47
2:B:681:HIS:HB3	2:B:784:SER:HB3	1.96	0.47
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.49	0.47
2:E:3759:GLU:HA	2:E:3762:ARG:HE	1.78	0.47
2:E:4239:GLU:OE2	2:E:5014:TYR:OH	2.28	0.47
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.46	0.47
2:E:642:THR:HG23	2:E:1613:LEU:HD12	1.95	0.47
2:E:3842:LEU:O	2:E:3929:SER:OG	2.31	0.47
2:G:3759:GLU:HA	2:G:3762:ARG:HE	1.78	0.47
2:G:485:SER:O	2:G:489:ASN:N	2.39	0.47
2:B:3773:ARG:HG3	2:B:3815:LYS:HZ3	1.80	0.47
2:E:111:HIS:CD2	2:E:114:SER:H	2.32	0.47
2:E:681:HIS:HB3	2:E:784:SER:HB3	1.96	0.47
2:G:143:GLY:HA3	2:G:147:TRP:HE1	1.79	0.47
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.79	0.47
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.79	0.47
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.79	0.47
2:G:4925:ILE:HA	2:G:4929:LEU:HD23	1.96	0.47
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.96	0.47
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.96	0.47
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.96	0.47
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.97	0.47
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.79	0.47
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.97	0.47
2:G:898:ASP:HB3	2:G:901:LYS:HB2	1.97	0.47
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.96	0.47
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:681:HIS:HB3	2:I:784:SER:HB3	1.96	0.47
2:E:898:ASP:HB3	2:E:901:LYS:HB2	1.97	0.47
2:G:1730:MET:O	2:G:1772:ARG:NH1	2.47	0.47
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.97	0.47
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.96	0.47
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.97	0.47
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.49	0.47
2:B:3676:ASP:HA	2:B:3679:LYS:HB3	1.97	0.47
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.97	0.47
2:G:1735:ILE:HG23	2:G:1771:LEU:HD23	1.96	0.47
2:I:1735:ILE:HG23	2:I:1771:LEU:HD23	1.96	0.47
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.96	0.47
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.96	0.47
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.79	0.47
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.96	0.47
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.79	0.47
2:I:3676:ASP:HA	2:I:3679:LYS:HB3	1.97	0.47
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.79	0.46
2:B:4925:ILE:HA	2:B:4929:LEU:HD23	1.96	0.46
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.79	0.46
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.97	0.46
2:G:395:GLN:HG3	2:G:397:GLU:H	1.80	0.46
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.79	0.46
2:I:4239:GLU:OE2	2:I:5014:TYR:OH	2.28	0.46
2:B:1738:LEU:HB3	2:B:2146:PRO:HG3	1.97	0.46
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.97	0.46
2:B:3842:LEU:O	2:B:3929:SER:OG	2.31	0.46
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.97	0.46
2:E:395:GLN:HG3	2:E:397:GLU:H	1.80	0.46
2:G:3676:ASP:HA	2:G:3679:LYS:HB3	1.97	0.46
2:I:898:ASP:HB3	2:I:901:LYS:HB2	1.97	0.46
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.97	0.46
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.96	0.46
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.79	0.46
2:G:2327:GLY:HA2	2:G:2330:ARG:HD3	1.97	0.46
2:G:3923:LEU:HD13	2:G:3961:VAL:HG11	1.98	0.46
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.97	0.46
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.98	0.46
2:B:134:ASP:OD1	2:B:134:ASP:N	2.48	0.46
2:E:4925:ILE:HA	2:E:4929:LEU:HD23	1.96	0.46
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.49	0.46
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.49	0.46
2:G:1738:LEU:HB3	2:G:2146:PRO:HG3	1.97	0.46
2:B:404:ILE:HG21	2:B:481:GLU:HG3	1.98	0.46
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.98	0.46
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.96	0.46
2:B:243:ARG:NH1	2:B:301:VAL:O	2.46	0.46
2:B:898:ASP:HB3	2:B:901:LYS:HB2	1.97	0.46
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.96	0.46
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.97	0.46
2:I:2327:GLY:HA2	2:I:2330:ARG:HD3	1.97	0.46
2:B:485:SER:O	2:B:489:ASN:N	2.39	0.46
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.97	0.46
2:G:404:ILE:HG21	2:G:481:GLU:HG3	1.98	0.46
2:E:1738:LEU:HB3	2:E:2146:PRO:HG3	1.97	0.46
2:E:3923:LEU:HD13	2:E:3961:VAL:HG11	1.98	0.46
2:I:1738:LEU:HB3	2:I:2146:PRO:HG3	1.97	0.46
2:E:134:ASP:OD1	2:E:134:ASP:N	2.48	0.46
2:G:4063:ASP:OD1	2:G:4169:SER:OG	2.34	0.46
2:I:1730:MET:O	2:I:1772:ARG:NH1	2.47	0.46
2:I:404:ILE:HG21	2:I:481:GLU:HG3	1.98	0.46
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.49	0.45
2:B:395:GLN:HG3	2:B:397:GLU:H	1.80	0.45
2:G:2466:LEU:HD23	2:G:2469:ILE:HD12	1.98	0.45
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.98	0.45
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.81	0.45
2:I:143:GLY:HA3	2:I:147:TRP:HE1	1.79	0.45
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.97	0.45
2:E:2024:PRO:O	2:E:2028:ARG:NE	2.43	0.45
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.98	0.45
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.81	0.45
2:B:621:ILE:O	2:B:625:LEU:N	2.48	0.45
2:G:134:ASP:OD1	2:G:134:ASP:N	2.48	0.45
2:G:236:ALA:HA	2:G:242:ARG:HD2	1.98	0.45
2:I:395:GLN:HG3	2:I:397:GLU:H	1.80	0.45
2:I:3923:LEU:HD13	2:I:3961:VAL:HG11	1.98	0.45
2:B:2327:GLY:HA2	2:B:2330:ARG:HD3	1.97	0.45
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.98	0.45
2:E:404:ILE:HG21	2:E:481:GLU:HG3	1.98	0.45
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.49	0.45
2:B:1694:LEU:O	2:B:1712:TYR:OH	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:ALA:HA	2:B:242:ARG:HD2	1.98	0.45
2:E:3676:ASP:HA	2:E:3679:LYS:HB3	1.97	0.45
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.39	0.45
2:B:4963:ILE:HD13	2:B:5027:CYS:SG	2.57	0.45
2:E:2327:GLY:HA2	2:E:2330:ARG:HD3	1.97	0.45
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.99	0.45
2:I:2466:LEU:HD23	2:I:2469:ILE:HD12	1.98	0.45
2:I:4963:ILE:HD13	2:I:5027:CYS:SG	2.57	0.45
2:E:940:GLY:O	2:E:1052:ASN:N	2.49	0.45
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.99	0.45
2:I:236:ALA:HA	2:I:242:ARG:HD2	1.98	0.45
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	1.98	0.45
2:B:4983:HIS:N	2:B:4983:HIS:CD2	2.70	0.45
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	1.99	0.45
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	1.99	0.45
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.99	0.45
2:B:4571:PHE:O	2:B:4575:PHE:N	2.50	0.45
2:B:4729:GLY:HA2	2:B:4737:ILE:HG13	1.99	0.45
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	1.99	0.45
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.99	0.45
2:E:4571:PHE:O	2:E:4575:PHE:N	2.50	0.45
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.99	0.45
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.52	0.45
2:B:1516:UNK:N	2:B:1529:UNK:O	2.50	0.45
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.99	0.45
2:E:236:ALA:HA	2:E:242:ARG:HD2	1.98	0.45
2:E:309:THR:O	2:E:313:SER:OG	2.35	0.45
2:E:4963:ILE:HD13	2:E:5027:CYS:SG	2.57	0.45
2:I:4063:ASP:OD1	2:I:4169:SER:OG	2.34	0.45
2:B:4239:GLU:OE2	2:B:5014:TYR:OH	2.28	0.44
2:B:551:LEU:HD11	2:B:589:LEU:HD13	1.99	0.44
2:G:1516:UNK:N	2:G:1529:UNK:O	2.50	0.44
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.99	0.44
2:G:4729:GLY:HA2	2:G:4737:ILE:HG13	1.99	0.44
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.99	0.44
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.51	0.44
2:B:3910:THR:HG23	2:B:3911:THR:HG23	2.00	0.44
2:B:1093:GLU:OE1	2:B:1201:HIS:NE2	2.49	0.44
2:B:500:ALA:HB1	2:B:504:ALA:HB2	2.00	0.44
2:E:164:ARG:N	2:E:167:ASP:OD2	2.51	0.44
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4063:ASP:OD1	2:E:4169:SER:OG	2.34	0.44
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.51	0.44
2:I:1093:GLU:OE1	2:I:1201:HIS:NE2	2.49	0.44
2:I:1863:LEU:HB3	2:I:1870:VAL:HG21	2.00	0.44
2:G:3365:UNK:O	2:G:3369:UNK:N	2.51	0.44
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.99	0.44
2:G:4963:ILE:HD13	2:G:5027:CYS:SG	2.57	0.44
2:I:4142:ASN:HA	2:I:4145:VAL:HG12	2.00	0.44
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.81	0.44
2:E:3910:THR:HG23	2:E:3911:THR:HG23	2.00	0.44
2:E:500:ALA:HB1	2:E:504:ALA:HB2	2.00	0.44
2:G:1863:LEU:HB3	2:G:1870:VAL:HG21	2.00	0.44
2:G:309:THR:O	2:G:313:SER:OG	2.35	0.44
2:G:4142:ASN:HA	2:G:4145:VAL:HG12	2.00	0.44
2:I:164:ARG:N	2:I:167:ASP:OD2	2.51	0.44
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.98	0.44
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	1.99	0.44
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.52	0.44
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	1.99	0.44
2:G:164:ARG:N	2:G:167:ASP:OD2	2.51	0.44
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	1.99	0.44
2:I:134:ASP:OD1	2:I:134:ASP:N	2.49	0.44
2:I:1516:UNK:N	2:I:1529:UNK:O	2.50	0.44
2:I:2447:LYS:HG3	2:I:2449:GLU:H	1.83	0.44
2:I:266:ARG:NH1	2:I:332:GLU:OE2	2.51	0.44
2:I:309:THR:O	2:I:313:SER:OG	2.35	0.44
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.81	0.44
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.98	0.44
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.99	0.44
2:E:1516:UNK:N	2:E:1529:UNK:O	2.50	0.44
2:E:2159:LEU:HD22	2:E:2201:LEU:HD23	1.99	0.44
2:E:551:LEU:HD11	2:E:589:LEU:HD13	1.99	0.44
2:G:2447:LYS:HG3	2:G:2449:GLU:H	1.83	0.44
2:B:4142:ASN:HA	2:B:4145:VAL:HG12	2.00	0.44
2:B:897:ARG:HB2	2:B:905:PRO:HG3	2.00	0.44
2:E:2236:LEU:HD23	2:E:2275:VAL:HG21	2.00	0.44
2:E:621:ILE:O	2:E:625:LEU:N	2.48	0.44
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	2.00	0.44
2:G:2236:LEU:HD23	2:G:2275:VAL:HG21	2.00	0.44
2:G:5028:PHE:O	2:G:5028:PHE:CG	2.70	0.44
2:B:2159:LEU:HD22	2:B:2201:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3365:UNK:O	2:E:3369:UNK:N	2.51	0.44
2:G:897:ARG:HB2	2:G:905:PRO:HG3	2.00	0.44
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	2.00	0.44
2:I:2159:LEU:HD22	2:I:2201:LEU:HD23	1.99	0.44
2:I:224:HIS:N	2:I:229:GLU:O	2.46	0.44
2:I:3365:UNK:O	2:I:3369:UNK:N	2.51	0.44
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.99	0.44
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.83	0.43
2:E:4729:GLY:HA2	2:E:4737:ILE:HG13	1.99	0.43
2:E:4983:HIS:N	2:E:4983:HIS:CD2	2.70	0.43
2:G:500:ALA:HB1	2:G:504:ALA:HB2	2.00	0.43
2:G:497:TYR:HB3	2:G:500:ALA:HB2	2.00	0.43
2:G:887:ILE:HG21	2:G:959:TYR:HA	2.00	0.43
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.50	0.43
2:I:5028:PHE:O	2:I:5028:PHE:CG	2.70	0.43
2:I:551:LEU:HD11	2:I:589:LEU:HD13	1.99	0.43
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	1.99	0.43
2:B:2447:LYS:HG3	2:B:2449:GLU:H	1.83	0.43
2:B:2466:LEU:HD23	2:B:2469:ILE:HD12	1.98	0.43
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.84	0.43
2:E:1863:LEU:HB3	2:E:1870:VAL:HG21	2.00	0.43
2:E:4142:ASN:HA	2:E:4145:VAL:HG12	2.00	0.43
2:E:887:ILE:HG21	2:E:959:TYR:HA	2.00	0.43
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.84	0.43
2:G:266:ARG:NH1	2:G:332:GLU:OE2	2.51	0.43
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.52	0.43
2:I:500:ALA:HB1	2:I:504:ALA:HB2	2.00	0.43
2:B:3365:UNK:O	2:B:3369:UNK:N	2.51	0.43
2:B:4063:ASP:OD1	2:B:4169:SER:OG	2.34	0.43
2:E:497:TYR:HB3	2:E:500:ALA:HB2	2.00	0.43
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	2.00	0.43
2:E:2466:LEU:HD23	2:E:2469:ILE:HD12	1.98	0.43
2:E:4697:VAL:O	2:E:4701:TRP:N	2.50	0.43
2:G:4571:PHE:O	2:G:4575:PHE:N	2.50	0.43
2:G:621:ILE:O	2:G:625:LEU:N	2.48	0.43
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	1.99	0.43
2:B:309:THR:O	2:B:313:SER:OG	2.35	0.43
2:B:4933:GLN:HG2	2:I:4930:ALA:HB2	2.00	0.43
2:B:5028:PHE:CG	2:B:5028:PHE:O	2.70	0.43
2:E:243:ARG:NH1	2:E:301:VAL:O	2.46	0.43
2:E:266:ARG:NH1	2:E:332:GLU:OE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:897:ARG:HB2	2:E:905:PRO:HG3	2.00	0.43
2:G:551:LEU:HD11	2:G:589:LEU:HD13	1.99	0.43
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.52	0.43
2:I:897:ARG:HB2	2:I:905:PRO:HG3	2.00	0.43
2:B:497:TYR:HB3	2:B:500:ALA:HB2	2.00	0.43
2:E:5028:PHE:CG	2:E:5028:PHE:O	2.70	0.43
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.00	0.43
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.84	0.43
2:I:887:ILE:HG21	2:I:959:TYR:HA	2.00	0.43
1:J:23:VAL:HG22	1:J:47:LYS:HG2	2.01	0.43
1:A:23:VAL:HG22	1:A:47:LYS:HG2	2.01	0.43
2:B:2236:LEU:HD23	2:B:2275:VAL:HG21	2.00	0.43
2:B:4984:ASN:C	2:B:4986:ALA:H	2.22	0.43
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.50	0.43
2:I:4960:ILE:N	2:I:4960:ILE:CD1	2.73	0.43
2:I:4984:ASN:C	2:I:4986:ALA:H	2.22	0.43
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.00	0.43
2:G:4982:GLU:HB3	2:G:4983:HIS:H	1.67	0.43
2:B:4892:ARG:NH2	2:I:4898:GLY:O	2.52	0.43
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.41	0.43
2:E:2447:LYS:HG3	2:E:2449:GLU:H	1.83	0.43
2:I:4571:PHE:O	2:I:4575:PHE:N	2.50	0.43
2:B:1863:LEU:HB3	2:B:1870:VAL:HG21	2.00	0.43
2:B:887:ILE:HG21	2:B:959:TYR:HA	2.00	0.43
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	2.00	0.43
2:E:4138:ASP:N	2:E:4138:ASP:OD1	2.52	0.43
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	2.01	0.43
2:I:235:ALA:HA	2:I:257:ARG:HD3	2.01	0.43
2:I:497:TYR:HB3	2:I:500:ALA:HB2	2.00	0.43
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	2.00	0.42
2:E:2103:VAL:O	2:E:2107:GLN:N	2.46	0.42
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.51	0.42
2:B:266:ARG:NH1	2:B:332:GLU:OE2	2.51	0.42
1:F:30:LEU:HD23	1:F:33:GLY:HA3	2.01	0.42
1:F:23:VAL:HG22	1:F:47:LYS:HG2	2.01	0.42
2:I:4729:GLY:HA2	2:I:4737:ILE:HG13	1.99	0.42
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.52	0.42
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.02	0.42
2:E:4982:GLU:HB3	2:E:4983:HIS:H	1.67	0.42
2:E:4984:ASN:C	2:E:4986:ALA:H	2.22	0.42
1:H:30:LEU:HD23	1:H:33:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2236:LEU:HD23	2:I:2275:VAL:HG21	2.00	0.42
2:I:4688:ILE:HG21	2:I:4728:HIS:HB3	2.01	0.42
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.52	0.42
2:B:164:ARG:N	2:B:167:ASP:OD2	2.51	0.42
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.00	0.42
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.50	0.42
2:G:224:HIS:N	2:G:229:GLU:O	2.46	0.42
2:G:243:ARG:NH1	2:G:301:VAL:O	2.46	0.42
2:I:485:SER:O	2:I:489:ASN:N	2.39	0.42
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.50	0.42
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.52	0.42
2:G:2159:LEU:HD22	2:G:2201:LEU:HD23	1.99	0.42
2:G:4138:ASP:N	2:G:4138:ASP:OD1	2.52	0.42
2:B:1730:MET:O	2:B:1772:ARG:NH1	2.47	0.42
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.02	0.42
2:G:235:ALA:HA	2:G:257:ARG:HD3	2.01	0.42
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	2.01	0.42
2:G:4984:ASN:C	2:G:4986:ALA:H	2.22	0.42
2:B:4558:ASN:N	2:B:4558:ASN:OD1	2.51	0.42
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.53	0.42
2:I:4190:ILE:HD13	2:I:5026:ASP:OD2	2.19	0.42
1:A:30:LEU:HD23	1:A:33:GLY:HA3	2.01	0.42
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.53	0.42
1:H:23:VAL:HG22	1:H:47:LYS:HG2	2.01	0.42
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.51	0.42
2:B:3992:PHE:O	2:B:3996:PHE:N	2.42	0.42
2:B:4688:ILE:HG21	2:B:4728:HIS:HB3	2.01	0.42
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	2.01	0.42
2:G:3781:GLN:HA	2:G:3784:SER:HB3	2.02	0.42
1:J:30:LEU:HD23	1:J:33:GLY:HA3	2.01	0.42
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.53	0.42
2:I:621:ILE:O	2:I:625:LEU:N	2.48	0.42
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	2.02	0.41
2:B:206:CYS:SG	2:B:207:SER:N	2.93	0.41
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	2.02	0.41
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	2.02	0.41
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	2.02	0.41
2:B:4230:LYS:CD	2:B:4959:PHE:CE1	2.83	0.41
2:E:3781:GLN:HA	2:E:3784:SER:HB3	2.02	0.41
2:E:4189:ARG:NH1	2:E:5032:TYR:OH	2.53	0.41
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1093:GLU:OE1	2:G:1201:HIS:NE2	2.49	0.41
2:G:2212:VAL:O	2:G:2216:GLY:N	2.45	0.41
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.53	0.41
2:G:358:THR:HG21	2:G:382:GLY:HA2	2.02	0.41
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	2.02	0.41
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.53	0.41
2:I:940:GLY:O	2:I:1052:ASN:N	2.49	0.41
2:B:4958:CYS:SG	2:B:4958:CYS:O	2.79	0.41
2:E:3362:UNK:O	2:E:3366:UNK:N	2.53	0.41
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.94	0.41
2:I:3362:UNK:O	2:I:3366:UNK:N	2.53	0.41
2:E:1141:ARG:HD2	2:E:1141:ARG:H	1.86	0.41
2:E:215:THR:HG22	2:E:273:HIS:HA	2.03	0.41
2:E:359:TYR:HA	2:E:376:ALA:HA	2.02	0.41
2:E:4958:CYS:SG	2:E:4958:CYS:O	2.79	0.41
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.41	0.41
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.86	0.41
2:B:215:THR:HG22	2:B:273:HIS:HA	2.03	0.41
2:B:35:LEU:HD13	2:B:49:LEU:HD13	2.03	0.41
2:E:1101:ARG:HH21	2:E:1115:LEU:HB3	1.86	0.41
2:E:206:CYS:SG	2:E:207:SER:N	2.93	0.41
2:G:615:ARG:NH2	2:G:1677:GLY:O	2.47	0.41
2:G:1671:ARG:NH2	2:G:1713:ASP:HB3	2.36	0.41
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	2.03	0.41
2:I:870:ILE:HD12	2:I:870:ILE:HA	1.92	0.41
2:B:1671:ARG:NH2	2:B:1713:ASP:HB3	2.36	0.41
2:B:3362:UNK:O	2:B:3366:UNK:N	2.53	0.41
2:B:4189:ARG:NH1	2:B:5032:TYR:OH	2.53	0.41
2:E:1595:LEU:HD23	2:E:1595:LEU:HA	1.96	0.41
2:G:206:CYS:SG	2:G:207:SER:N	2.93	0.41
2:G:2265:LEU:O	2:G:2330:ARG:NH1	2.54	0.41
2:G:2339:VAL:HG12	2:G:2345:SER:H	1.86	0.41
2:G:3362:UNK:O	2:G:3366:UNK:N	2.53	0.41
2:I:358:THR:HG21	2:I:382:GLY:HA2	2.02	0.41
2:I:4138:ASP:N	2:I:4138:ASP:OD1	2.52	0.41
2:I:707:VAL:HG23	2:I:713:SER:HB2	2.03	0.41
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	2.02	0.41
2:E:358:THR:HG21	2:E:382:GLY:HA2	2.02	0.41
2:E:35:LEU:HD13	2:E:49:LEU:HD13	2.03	0.41
2:G:378:LEU:HA	2:G:378:LEU:HD23	1.88	0.41
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	2.02	0.41
2:I:215:THR:HG22	2:I:273:HIS:HA	2.03	0.41
2:I:4983:HIS:CD2	2:I:4983:HIS:N	2.70	0.41
2:I:35:LEU:HD13	2:I:49:LEU:HD13	2.03	0.41
2:B:168:ASP:HB3	2:B:199:LEU:HD22	2.02	0.41
2:B:2339:VAL:HG12	2:B:2345:SER:H	1.85	0.41
2:B:4865:LYS:HB2	2:B:4873:ASP:HB3	2.03	0.41
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.53	0.41
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.53	0.41
2:G:1141:ARG:HD2	2:G:1141:ARG:H	1.86	0.41
2:G:359:TYR:HA	2:G:376:ALA:HA	2.02	0.41
2:G:938:HIS:HB2	2:G:1054:GLU:HB2	2.03	0.41
2:G:940:GLY:O	2:G:1052:ASN:N	2.49	0.41
2:I:243:ARG:NH1	2:I:301:VAL:O	2.46	0.41
2:B:1708:ARG:HG2	2:B:1711:TYR:CE2	2.56	0.41
2:B:235:ALA:HA	2:B:257:ARG:HD3	2.01	0.41
2:B:938:HIS:HB2	2:B:1054:GLU:HB2	2.03	0.41
2:E:2265:LEU:O	2:E:2330:ARG:NH1	2.54	0.41
2:E:235:ALA:HA	2:E:257:ARG:HD3	2.01	0.41
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	2.02	0.41
2:G:2742:THR:OG1	2:G:2811:GLU:OE1	2.35	0.41
2:G:4951:LYS:HB3	2:G:4951:LYS:HE2	1.96	0.41
2:G:707:VAL:HG23	2:G:713:SER:HB2	2.03	0.41
2:I:1671:ARG:NH2	2:I:1713:ASP:HB3	2.36	0.41
2:I:168:ASP:HB3	2:I:199:LEU:HD22	2.02	0.41
2:I:359:TYR:HA	2:I:376:ALA:HA	2.02	0.41
2:I:4958:CYS:O	2:I:4958:CYS:SG	2.79	0.41
2:B:3781:GLN:HA	2:B:3784:SER:HB3	2.02	0.41
2:E:224:HIS:N	2:E:229:GLU:O	2.46	0.41
2:E:2339:VAL:HG12	2:E:2345:SER:H	1.86	0.41
2:G:1708:ARG:HG2	2:G:1711:TYR:CE2	2.56	0.41
2:I:1101:ARG:HH21	2:I:1115:LEU:HB3	1.86	0.41
2:I:2543:UNK:O	2:I:2547:UNK:N	2.54	0.41
2:I:4982:GLU:N	2:I:4982:GLU:OE1	2.54	0.41
1:J:82:TYR:O	1:J:86:GLY:N	2.54	0.41
2:B:2305:CYS:O	2:B:2324:ASN:ND2	2.54	0.41
2:B:378:LEU:HD23	2:B:378:LEU:HA	1.88	0.41
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.94	0.41
2:E:1093:GLU:OE1	2:E:1201:HIS:NE2	2.49	0.41
2:E:168:ASP:HB3	2:E:199:LEU:HD22	2.03	0.41
2:E:2543:UNK:O	2:E:2547:UNK:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.86	0.41
2:G:1101:ARG:HH21	2:G:1115:LEU:HB3	1.86	0.41
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	2.03	0.41
2:G:4697:VAL:O	2:G:4701:TRP:N	2.50	0.41
2:G:4958:CYS:O	2:G:4958:CYS:SG	2.79	0.41
2:I:2880:GLU:O	2:I:2884:ASN:N	2.53	0.41
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.41	0.41
2:B:358:THR:HG21	2:B:382:GLY:HA2	2.02	0.40
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	2.03	0.40
2:B:4968:PHE:CZ	2:B:4978:HIS:HE1	2.37	0.40
2:B:4982:GLU:N	2:B:4982:GLU:OE1	2.54	0.40
2:B:707:VAL:HG23	2:B:713:SER:HB2	2.03	0.40
2:E:2894:LEU:HD11	2:E:2902:HIS:HB2	2.04	0.40
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	2.03	0.40
2:G:215:THR:HG22	2:G:273:HIS:HA	2.03	0.40
2:I:4933:GLN:HG2	2:G:4930:ALA:HB2	2.03	0.40
2:G:575:LEU:HD22	2:G:609:CYS:HB3	2.03	0.40
2:I:206:CYS:SG	2:I:207:SER:N	2.93	0.40
2:I:4982:GLU:HB3	2:I:4983:HIS:H	1.67	0.40
2:I:938:HIS:HB2	2:I:1054:GLU:HB2	2.03	0.40
2:B:1101:ARG:HH21	2:B:1115:LEU:HB3	1.86	0.40
2:B:1865:MET:SD	2:B:1865:MET:N	2.95	0.40
2:B:4138:ASP:N	2:B:4138:ASP:OD1	2.52	0.40
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	2.02	0.40
2:E:4930:ALA:HB2	2:G:4933:GLN:HG2	2.03	0.40
2:G:168:ASP:HB3	2:G:199:LEU:HD22	2.02	0.40
1:H:92:PRO:HD3	2:G:627:PRO:HB2	2.02	0.40
1:H:82:TYR:O	1:H:86:GLY:N	2.54	0.40
2:I:1865:MET:SD	2:I:1865:MET:N	2.94	0.40
2:I:2894:LEU:HD11	2:I:2902:HIS:HB2	2.04	0.40
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	2.03	0.40
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.86	0.40
2:B:870:ILE:HA	2:B:870:ILE:HD12	1.92	0.40
2:E:1708:ARG:HG2	2:E:1711:TYR:CE2	2.56	0.40
2:E:1671:ARG:NH2	2:E:1713:ASP:HB3	2.36	0.40
2:E:378:LEU:HD23	2:E:378:LEU:HA	1.88	0.40
2:E:3992:PHE:O	2:E:3996:PHE:N	2.42	0.40
2:E:4982:GLU:N	2:E:4982:GLU:OE1	2.54	0.40
2:E:938:HIS:HB2	2:E:1054:GLU:HB2	2.03	0.40
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.79	0.40
2:G:4865:LYS:HB2	2:G:4873:ASP:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	2.04	0.40
2:I:2265:LEU:O	2:I:2330:ARG:NH1	2.54	0.40
2:I:2339:VAL:HG12	2:I:2345:SER:H	1.86	0.40
2:I:3781:GLN:HA	2:I:3784:SER:HB3	2.02	0.40
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.94	0.40
2:I:4697:VAL:O	2:I:4701:TRP:N	2.50	0.40
2:I:560:ILE:HA	2:I:563:VAL:HG12	2.04	0.40
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	2.03	0.40
2:B:2543:UNK:O	2:B:2547:UNK:N	2.54	0.40
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	2.02	0.40
2:B:560:ILE:HA	2:B:563:VAL:HG12	2.04	0.40
2:E:2212:VAL:O	2:E:2216:GLY:N	2.45	0.40
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	2.04	0.40
2:G:4189:ARG:NH1	2:G:5032:TYR:OH	2.53	0.40
2:I:3992:PHE:O	2:I:3996:PHE:N	2.42	0.40
2:B:2212:VAL:O	2:B:2216:GLY:N	2.45	0.40
2:B:2265:LEU:O	2:B:2330:ARG:NH1	2.54	0.40
2:B:2880:GLU:O	2:B:2884:ASN:N	2.53	0.40
2:B:2894:LEU:HD11	2:B:2902:HIS:HB2	2.04	0.40
2:E:2305:CYS:O	2:E:2324:ASN:ND2	2.55	0.40
2:E:2145:SER:HB2	2:E:3647:HIS:CE1	2.57	0.40
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	2.03	0.40
2:E:707:VAL:HG23	2:E:713:SER:HB2	2.03	0.40
2:I:2305:CYS:O	2:I:2324:ASN:ND2	2.54	0.40
2:I:2780:ASN:O	2:I:2787:THR:OG1	2.31	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%)	96 (91%)	9 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	H	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	J	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	B	3235/4416 (73%)	2906 (90%)	323 (10%)	6 (0%)	52	86
2	E	3235/4416 (73%)	2908 (90%)	321 (10%)	6 (0%)	52	86
2	G	3235/4416 (73%)	2906 (90%)	323 (10%)	6 (0%)	52	86
2	I	3235/4416 (73%)	2906 (90%)	323 (10%)	6 (0%)	52	86
All	All	13360/18096 (74%)	12010 (90%)	1326 (10%)	24 (0%)	56	86

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5028	PHE
2	E	5028	PHE
2	I	5028	PHE
2	G	5028	PHE
2	B	1708	ARG
2	B	4985	LEU
2	E	1708	ARG
2	E	4985	LEU
2	I	1708	ARG
2	I	4985	LEU
2	G	1708	ARG
2	G	4985	LEU
2	B	1840	PRO
2	E	1840	PRO
2	I	1840	PRO
2	G	1840	PRO
2	B	4641	PRO
2	E	4641	PRO
2	I	4641	PRO
2	G	4641	PRO
2	B	1932	PRO
2	E	1932	PRO
2	I	1932	PRO
2	G	1932	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
1	J	88/89 (99%)	88 (100%)	0	100 100
2	B	2493/3022 (82%)	2472 (99%)	21 (1%)	86 93
2	E	2493/3022 (82%)	2472 (99%)	21 (1%)	86 93
2	G	2493/3022 (82%)	2472 (99%)	21 (1%)	86 93
2	I	2493/3022 (82%)	2472 (99%)	21 (1%)	86 93
All	All	10324/12444 (83%)	10240 (99%)	84 (1%)	87 93

All (84) 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	3762	ARG
2	B	3787	LYS
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4131	ARG
2	B	4166	LEU
2	B	4957	LYS
2	B	4958	CYS
2	B	4960	ILE

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Mol	Chain	Res	Type
2	B	4983	HIS
2	B	5027	CYS
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	3762	ARG
2	E	3787	LYS
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4131	ARG
2	E	4166	LEU
2	E	4957	LYS
2	E	4958	CYS
2	E	4960	ILE
2	E	4983	HIS
2	E	5027	CYS
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	3762	ARG
2	I	3787	LYS
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4131	ARG
2	I	4166	LEU
2	I	4957	LYS
2	I	4958	CYS
2	I	4960	ILE

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Mol	Chain	Res	Type
2	I	4983	HIS
2	I	5027	CYS
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	3762	ARG
2	G	3787	LYS
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4131	ARG
2	G	4166	LEU
2	G	4957	LYS
2	G	4958	CYS
2	G	4960	ILE
2	G	4983	HIS
2	G	5027	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) 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	224	HIS
2	B	273	HIS
2	B	379	HIS
2	B	383	HIS
2	B	582	HIS

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Mol	Chain	Res	Type
2	B	1041	GLN
2	B	1598	GLN
2	B	1688	HIS
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	2005	GLN
2	B	2041	HIS
2	B	3809	ASN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	4034	ASN
2	B	4120	ASN
2	B	4806	ASN
2	B	4973	HIS
2	B	4983	HIS
2	E	57	ASN
2	E	111	HIS
2	E	224	HIS
2	E	273	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	582	HIS
2	E	1041	GLN
2	E	1598	GLN
2	E	1688	HIS
2	E	1691	GLN
2	E	1693	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	2005	GLN
2	E	2041	HIS
2	E	3781	GLN
2	E	3809	ASN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN

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Mol	Chain	Res	Type
2	E	4034	ASN
2	E	4120	ASN
2	E	4806	ASN
2	E	4973	HIS
2	E	4983	HIS
2	I	57	ASN
2	I	111	HIS
2	I	224	HIS
2	I	273	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	582	HIS
2	I	1041	GLN
2	I	1598	GLN
2	I	1688	HIS
2	I	1691	GLN
2	I	1693	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	2005	GLN
2	I	2041	HIS
2	I	2884	ASN
2	I	3809	ASN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	4034	ASN
2	I	4120	ASN
2	I	4806	ASN
2	I	4973	HIS
2	I	4983	HIS
2	G	57	ASN
2	G	111	HIS
2	G	224	HIS
2	G	273	HIS
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	582	HIS
2	G	1041	GLN

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Mol	Chain	Res	Type
2	G	1598	GLN
2	G	1688	HIS
2	G	1691	GLN
2	G	1693	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	2005	GLN
2	G	2041	HIS
2	G	3781	GLN
2	G	3809	ASN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	4034	ASN
2	G	4120	ASN
2	G	4806	ASN
2	G	4973	HIS
2	G	4983	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	0.91	1 (3%)	26,52,52	1.71	3 (11%)
4	CFF	B	5102	-	8,15,15	2.52	3 (37%)	8,23,23	1.30	1 (12%)
3	ATP	E	5101	-	26,33,33	0.91	1 (3%)	26,52,52	1.72	3 (11%)
4	CFF	E	5102	-	8,15,15	2.52	3 (37%)	8,23,23	1.30	1 (12%)
3	ATP	G	5101	-	26,33,33	0.91	1 (3%)	26,52,52	1.72	3 (11%)
4	CFF	G	5102	-	8,15,15	2.51	3 (37%)	8,23,23	1.30	1 (12%)
3	ATP	I	5101	-	26,33,33	0.91	1 (3%)	26,52,52	1.71	3 (11%)
4	CFF	I	5102	-	8,15,15	2.53	3 (37%)	8,23,23	1.29	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
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	-4.87	1.33	1.39
4	I	5102	CFF	C4-N3	-4.84	1.33	1.39
4	B	5102	CFF	C4-N3	-4.84	1.33	1.39
4	G	5102	CFF	C4-N3	-4.81	1.33	1.39
4	I	5102	CFF	C6-N1	-4.07	1.32	1.38
4	G	5102	CFF	C6-N1	-4.02	1.32	1.38
4	B	5102	CFF	C6-N1	-4.02	1.32	1.38
4	E	5102	CFF	C6-N1	-4.01	1.32	1.38
4	G	5102	CFF	O13-C6	-2.41	1.18	1.24
4	I	5102	CFF	O13-C6	-2.40	1.18	1.24
4	B	5102	CFF	O13-C6	-2.40	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5102	CFF	O13-C6	-2.37	1.18	1.24
3	I	5101	ATP	C5-C4	2.56	1.46	1.40
3	B	5101	ATP	C5-C4	2.58	1.46	1.40
3	G	5101	ATP	C5-C4	2.58	1.46	1.40
3	E	5101	ATP	C5-C4	2.62	1.46	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	5101	ATP	N3-C2-N1	-6.72	123.60	128.87
3	E	5101	ATP	N3-C2-N1	-6.68	123.62	128.87
3	B	5101	ATP	N3-C2-N1	-6.65	123.64	128.87
3	I	5101	ATP	N3-C2-N1	-6.60	123.69	128.87
4	I	5102	CFF	C14-N7-C8	-2.53	112.09	125.31
4	B	5102	CFF	C14-N7-C8	-2.53	112.09	125.31
4	E	5102	CFF	C14-N7-C8	-2.53	112.11	125.31
4	G	5102	CFF	C14-N7-C8	-2.52	112.14	125.31
3	E	5101	ATP	O3G-PG-O2G	2.08	115.07	107.44
3	I	5101	ATP	O4'-C1'-N9	2.08	112.03	108.11
3	B	5101	ATP	O3G-PG-O2G	2.08	115.09	107.44
3	B	5101	ATP	O4'-C1'-N9	2.08	112.04	108.11
3	G	5101	ATP	O3G-PG-O2G	2.09	115.10	107.44
3	E	5101	ATP	O4'-C1'-N9	2.09	112.05	108.11
3	I	5101	ATP	O3G-PG-O2G	2.09	115.12	107.44
3	G	5101	ATP	O4'-C1'-N9	2.10	112.06	108.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	2	0
3	E	5101	ATP	2	0
3	G	5101	ATP	2	0
3	I	5101	ATP	2	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	74.00
1	E	4345:UNK	C	4540:PHE	N	74.00
1	I	4345:UNK	C	4540:PHE	N	74.00
1	G	4345:UNK	C	4540:PHE	N	74.00
1	B	3613:UNK	C	3639:THR	N	43.80
1	E	3613:UNK	C	3639:THR	N	43.80
1	I	3613:UNK	C	3639:THR	N	43.80
1	G	3613:UNK	C	3639:THR	N	43.80
1	B	4253:GLU	C	4320:UNK	N	26.28
1	E	4253:GLU	C	4320:UNK	N	26.28
1	I	4253:GLU	C	4320:UNK	N	26.28
1	G	4253:GLU	C	4320:UNK	N	26.28
1	G	3163:UNK	C	3170:UNK	N	16.13
1	B	3163:UNK	C	3170:UNK	N	16.12
1	E	3163:UNK	C	3170:UNK	N	16.12
1	I	3163:UNK	C	3170:UNK	N	16.12
1	B	3063:UNK	C	3134:UNK	N	15.30
1	E	3063:UNK	C	3134:UNK	N	15.30
1	I	3063:UNK	C	3134:UNK	N	15.30
1	G	3063:UNK	C	3134:UNK	N	15.30
1	B	3468:UNK	C	3511:UNK	N	14.89
1	E	3468:UNK	C	3511:UNK	N	14.89
1	I	3468:UNK	C	3511:UNK	N	14.89
1	G	3468:UNK	C	3511:UNK	N	14.89
1	B	2703:UNK	C	2734:ASN	N	13.90
1	E	2703:UNK	C	2734:ASN	N	13.90
1	I	2703:UNK	C	2734:ASN	N	13.90
1	G	2703:UNK	C	2734:ASN	N	13.90
1	B	3236:UNK	C	3241:UNK	N	13.63
1	E	3236:UNK	C	3241:UNK	N	13.63
1	I	3236:UNK	C	3241:UNK	N	13.63
1	G	3236:UNK	C	3241:UNK	N	13.63

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	2976:UNK	C	2995:UNK	N	12.77
1	E	2976:UNK	C	2995:UNK	N	12.77
1	I	2976:UNK	C	2995:UNK	N	12.77
1	G	2976:UNK	C	2995:UNK	N	12.77
1	B	1564:UNK	C	1573:MET	N	12.33
1	E	1564:UNK	C	1573:MET	N	12.33
1	I	1564:UNK	C	1573:MET	N	12.33
1	G	1564:UNK	C	1573:MET	N	12.33
1	B	3254:UNK	C	3261:UNK	N	8.26
1	E	3254:UNK	C	3261:UNK	N	8.26
1	I	3254:UNK	C	3261:UNK	N	8.26
1	G	3254:UNK	C	3261:UNK	N	8.26
1	E	1297:UNK	C	1430:UNK	N	6.06
1	G	1297:UNK	C	1430:UNK	N	6.06
1	B	1297:UNK	C	1430:UNK	N	6.05
1	I	1297:UNK	C	1430:UNK	N	6.05
1	B	2939:ARG	C	2942:UNK	N	3.63
1	E	2939:ARG	C	2942:UNK	N	3.63
1	I	2939:ARG	C	2942:UNK	N	3.63
1	G	2939:ARG	C	2942:UNK	N	3.63
1	B	2479:LEU	C	2487:UNK	N	3.24
1	E	2479:LEU	C	2487:UNK	N	3.24
1	I	2479:LEU	C	2487:UNK	N	3.24
1	G	2479:LEU	C	2487:UNK	N	3.24