wwPDB EM Map/Model Validation Report (i)

Oct 17, 2016 – 07:39 PM EDT

PDB ID	:	5TAV
EMDB ID:	:	EMD-8386
Title	:	Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, class 4)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-10
Resolution	:	4.80 Å(reported)

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

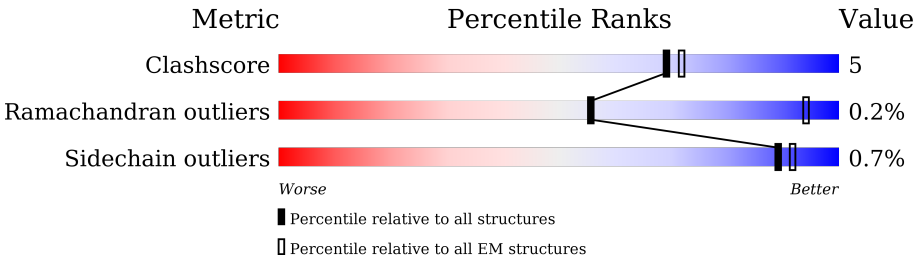
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 4.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	108	92% 7% .
1	F	108	91% 8% .
1	H	108	92% 7% .
1	J	108	93% 6% .
2	B	4416	84% 10% 5%
2	E	4416	84% 10% 5%
2	G	4416	85% 10% 5%
2	I	4416	84% 10% 5%

2 Entry composition

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.

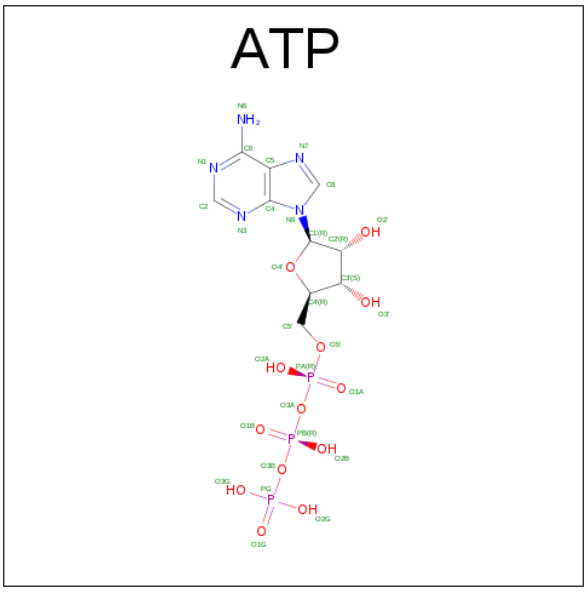
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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.

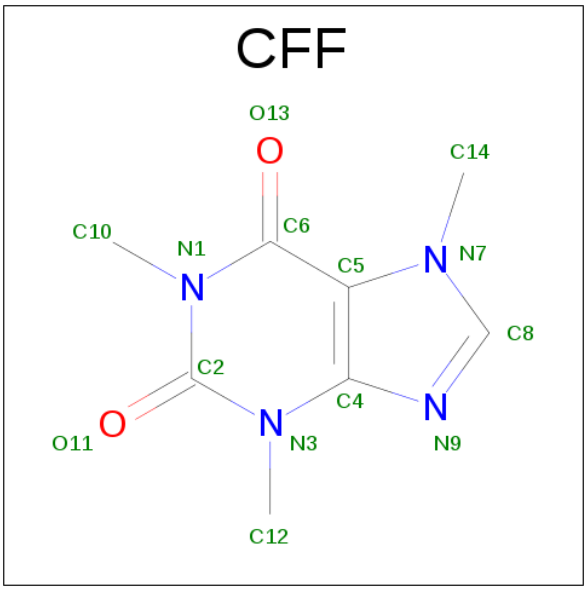
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- 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).

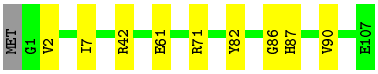
Mol	Chain	Residues	Atoms		AltConf
5	G	1	Total	Zn	0
			1	1	
5	B	1	Total	Zn	0
			1	1	
5	I	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	

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

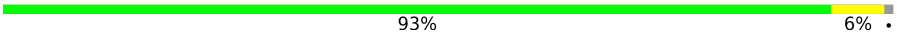
Chain A:

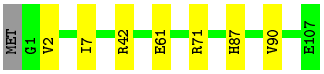
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:

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

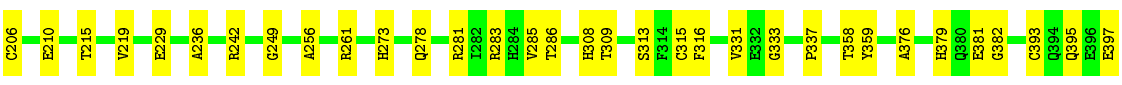
Chain J:

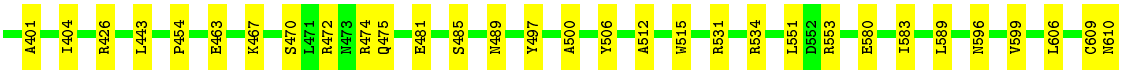


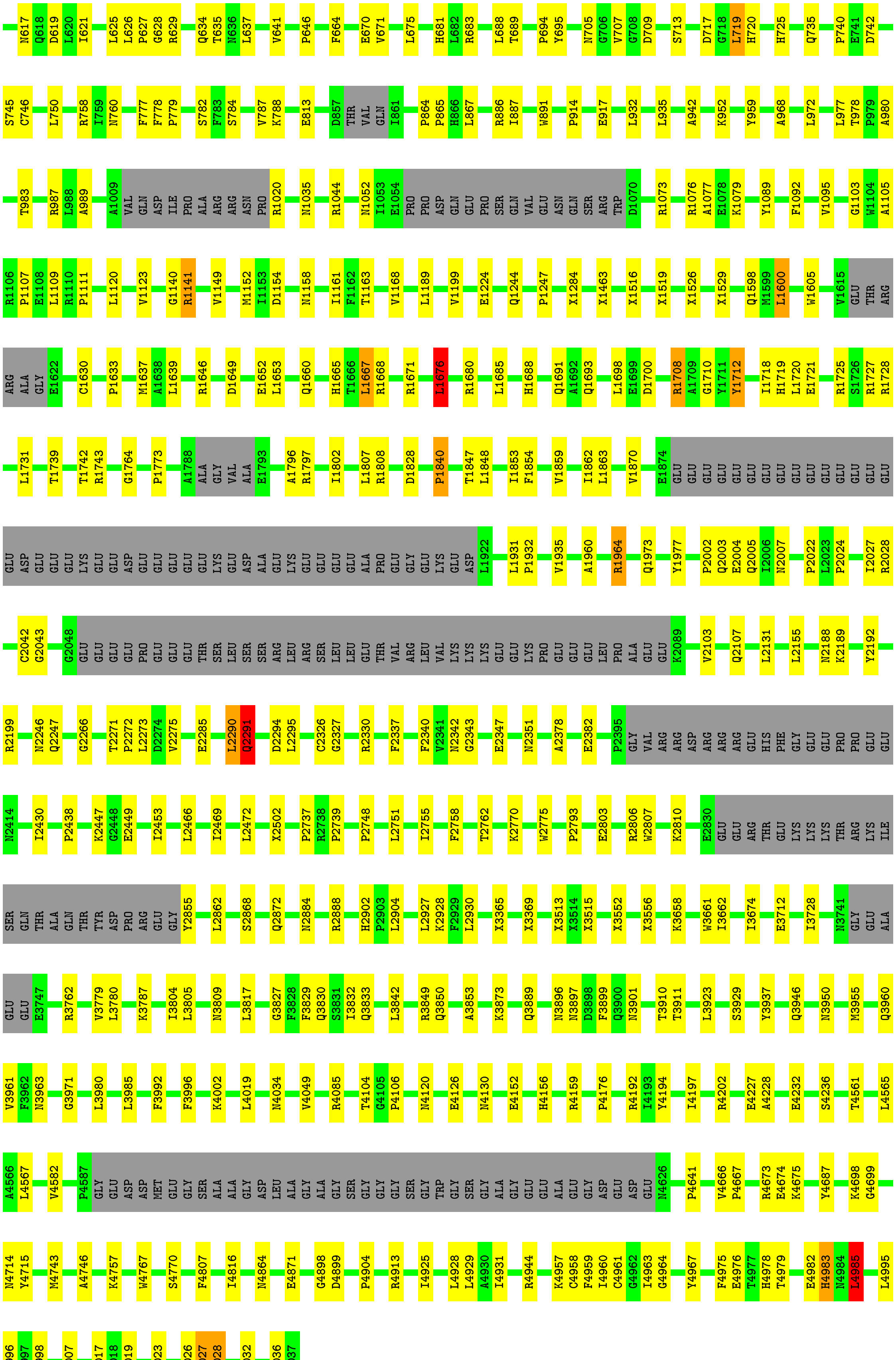


- Molecule 2: Ryanodine receptor 1

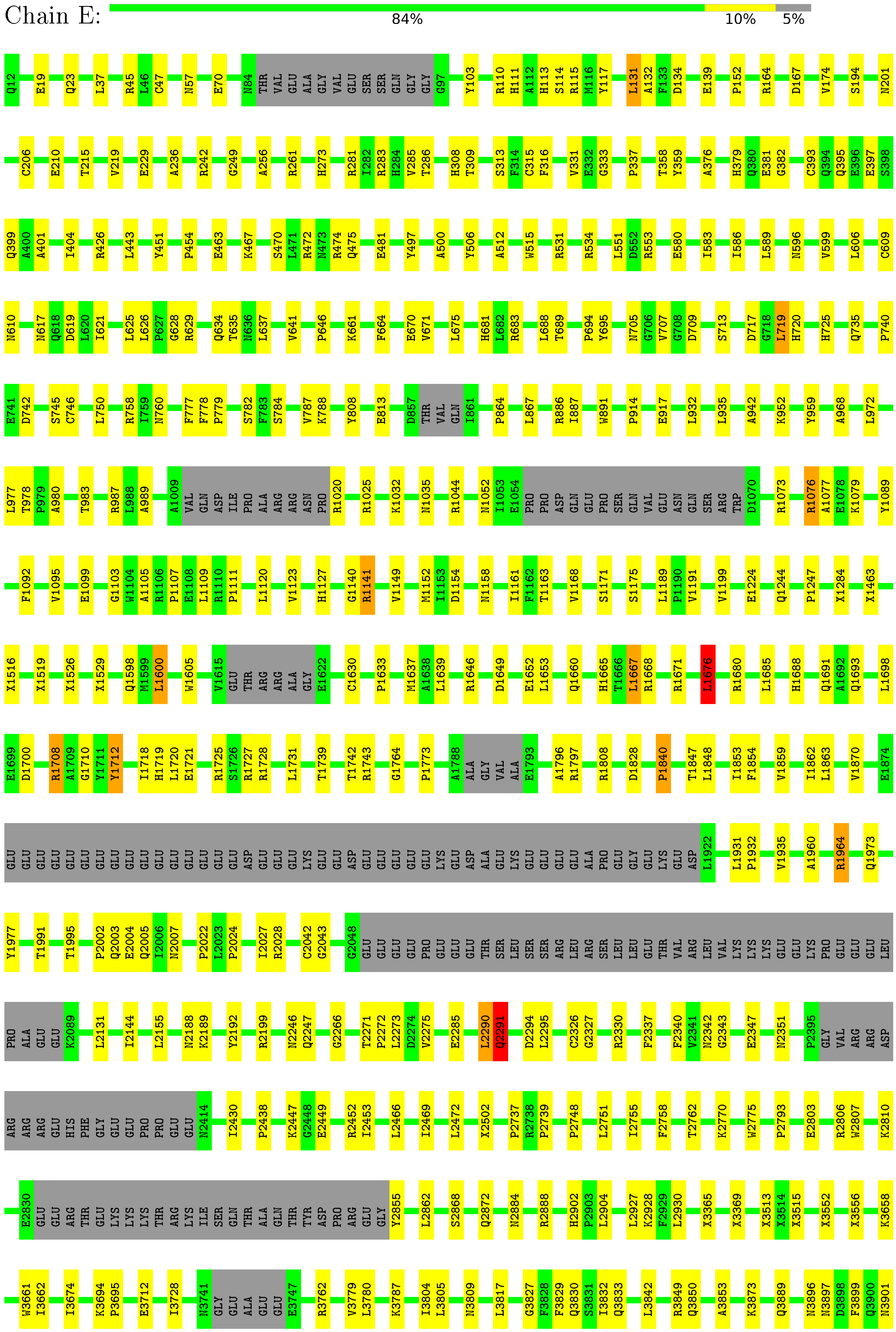
Chain B:

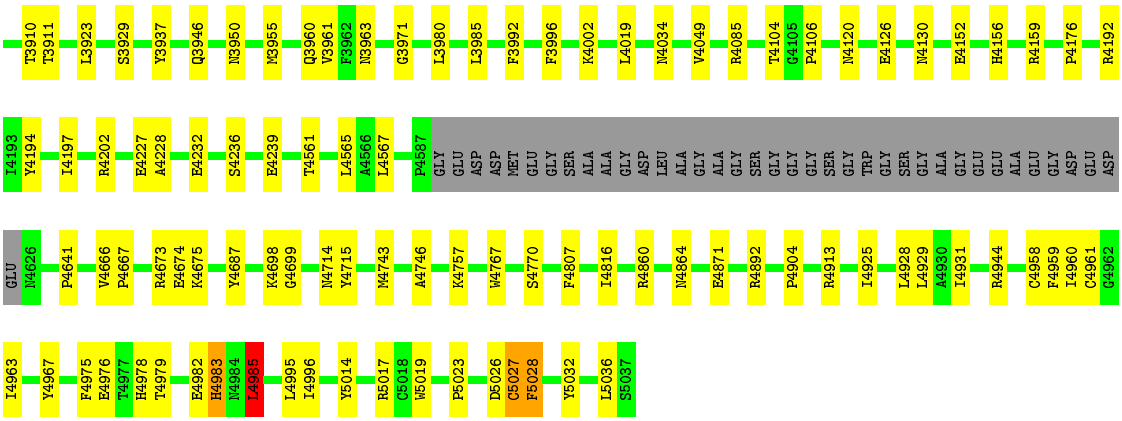





N617 Q618 D619 L620 I621 L625 L626 P627 G628 R629 Q634 T635 N636 L637 V641 P646 F664 E670 V671 L675 H681 L682 R683 L688 T689 P694 Y695 N705 G706 V707 G708 D709 S713 D717 G718 L719 H720 H725 Q735 P740 E741 D742
S745 C746 L750 R758 I759 N760 F777 F778 P779 S782 F783 S784 V787 K788 E813 D857 THR VAL GLN I861 P864 P865 H866 L867 R886 I887 W891 P914 E917 L932 L935 A942 K952 Y959 A968 L972 L977 T978 P979 A980
T983 R987 L988 A989 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 N1035 R1044 N1052 I1053 E1054 PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1073 R1076 A1077 E1078 K1079 Y1089 F1092 V1095 G1103 W1104 A1105
R1106 P1107 E1108 L1109 R1110 P1111 L1120 V1123 G1140 R1141 V1149 M1152 I1153 D1154 N1158 I1161 F1162 T1163 V1168 L1189 V1199 E1224 Q1244 P1247 K1284 K1463 X1516 X1519 X1526 X1529 Q1598 M1599 L1600 W1605 V1615 GLU THR ARG
ARG ALA GLY E1622 C1630 P1633 M1637 A1638 L1639 R1646 D1649 E1652 L1653 Q1660 H1665 T1666 L1667 R1668 R1671 L1676 R1680 L1685 H1688 Q1691 A1692 Q1693 L1698 E1699 D1700 R1708 A1709 G1710 Y1711 Y1712 I1718 H1719 L1720 E1721 R1725 S1726 R1727 R1728
L1731 T1739 T1742 R1743 G1764 P1773 A1788 ALA GLY VAL ALA E1793 A1796 R1797 I1802 L1807 R1808 D1828 P1840 T1847 L1848 I1853 F1854 V1859 I1862 L1863 V1870 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU
GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 L1931 P1932 V1935 A1960 R1964 Q1973 Y1977 P2002 Q2003 E2004 Q2005 I2006 N2007 P2022 L2023 P2024 I2027 R2028
C2042 G2043 G2048 GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU K2089 V2103 Q2107 L2131 L2155 N2188 K2189 Y2192
R2199 N2246 Q2247 G2266 T2271 P2272 L2273 D2274 V2275 E2285 L2290 Q2291 D2294 L2295 C2326 G2327 R2330 F2337 F2340 V2341 N2342 G2343 E2347 N2351 A2378 E2382 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU
N2414 I2430 P2438 K2447 G2448 E2449 I2453 L2466 I2469 L2472 X2502 P2737 R2738 P2739 P2748 L2751 I2755 F2758 T2762 K2770 W2775 P2793 E2803 R2806 W2807 K2810 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 L2862 S2868 Q2872 N2884 R2888 H2902 P2903 L2904 L2927 K2928 F2929 L2930 X3365 X3369 X3513 X3514 X3515 X3552 X3556 K3658 W3661 I3662 I3674 E3712 I3728 N3741 GLY GLU ALA
GLU GLU E3747 R3762 V3779 L3780 K3787 I3804 L3805 N3809 L3817 G3827 F3828 F3829 Q3830 S3831 I3832 Q3833 L3842 R3849 Q3850 A3853 K3873 Q3889 N3896 N3897 D3898 F3899 Q3900 N3901 T3910 T3911 L3923 S3929 Y3937 Q3946 N3950 M3955 Q3960
V3961 F3962 N3963 G3971 L3980 L3985 F3992 F3996 K4002 L4019 N4034 V4049 R4085 T4104 G4105 P4106 N4120 E4126 N4130 E4152 H4156 R4159 P4176 R4192 I4193 Y4194 I4197 R4202 E4227 A4228 E4232 S4236 T4561 L4565
A4566 L4567 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 ASP GLU N4626 P4641 V4666 P4667 R4673 E4674 K4675 Y4687 K4698 G4699
N4714 Y4715 M4743 A4746 K4757 W4767 S4770 F4807 I4816 N4864 E4871 G4898 D4899 P4904 R4913 I4925 L4928 L4929 A4930 I4931 R4944 K4957 C4958 F4959 I4960 C4961 G4962 I4963 G4964 Y4967 F4975 E4976 T4977 H4978 T4979 E4982 H4983 N4984 L4985 L4995
I4996 N4997 K4998 E5007 R5017 C5018 W5019 P5023 D5026 C5027 F5028 Y5032 L5036 S5037

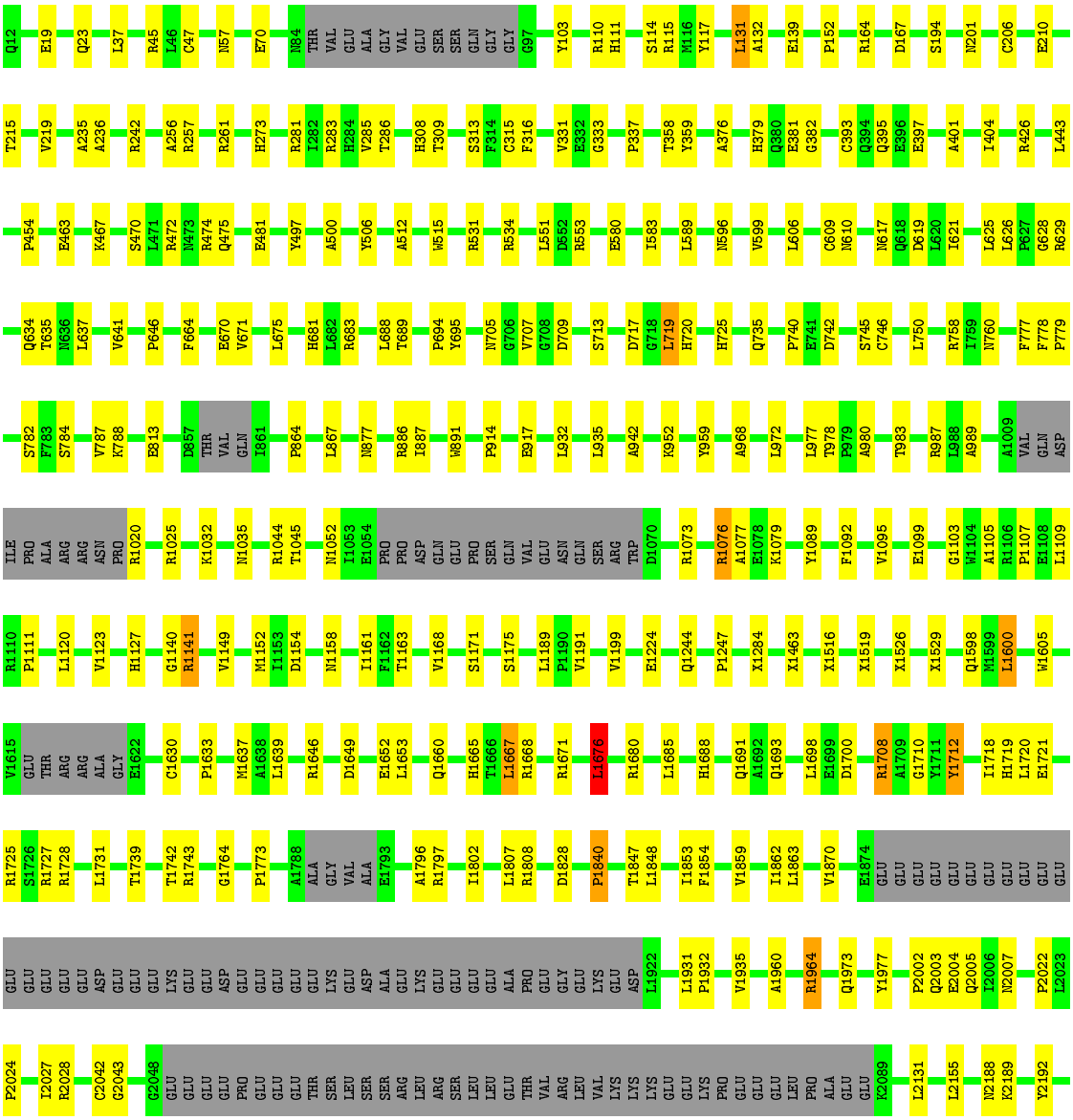
- Molecule 2: Ryanodine receptor 1

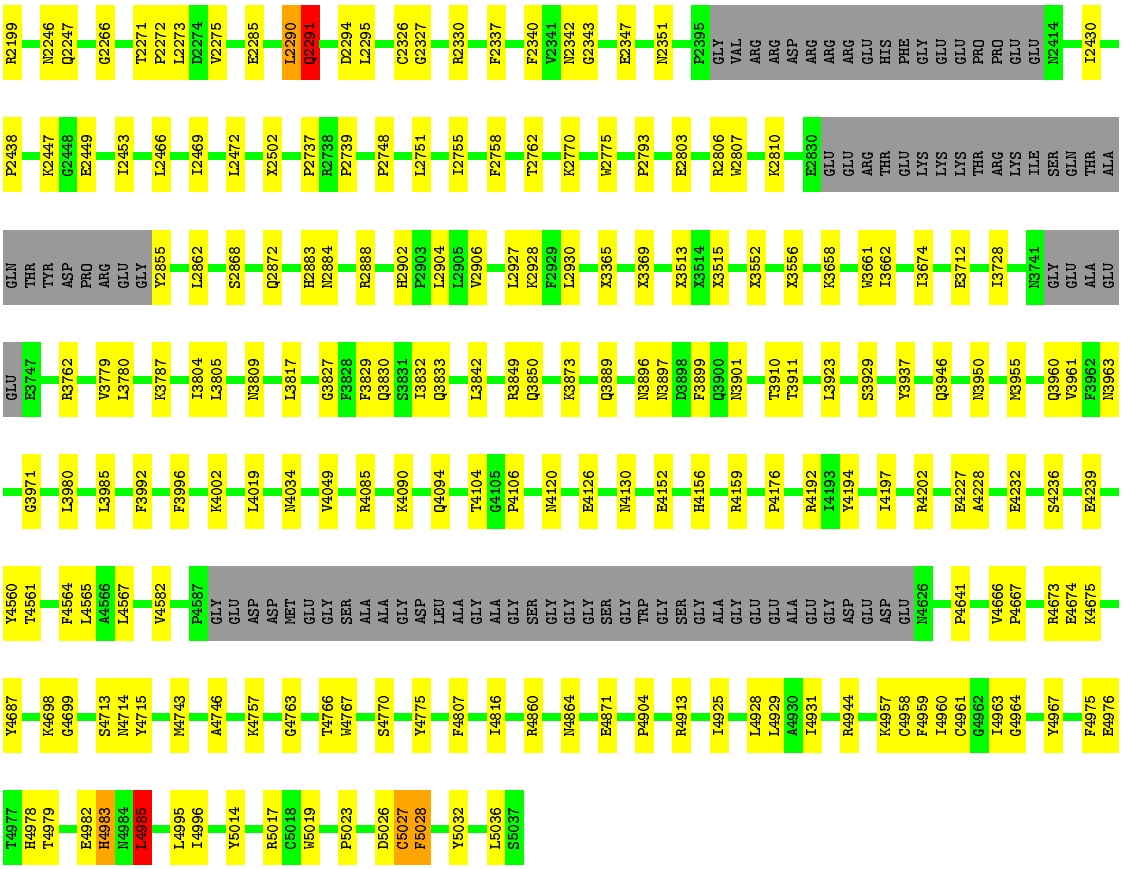




• Molecule 2: Ryanodine receptor 1

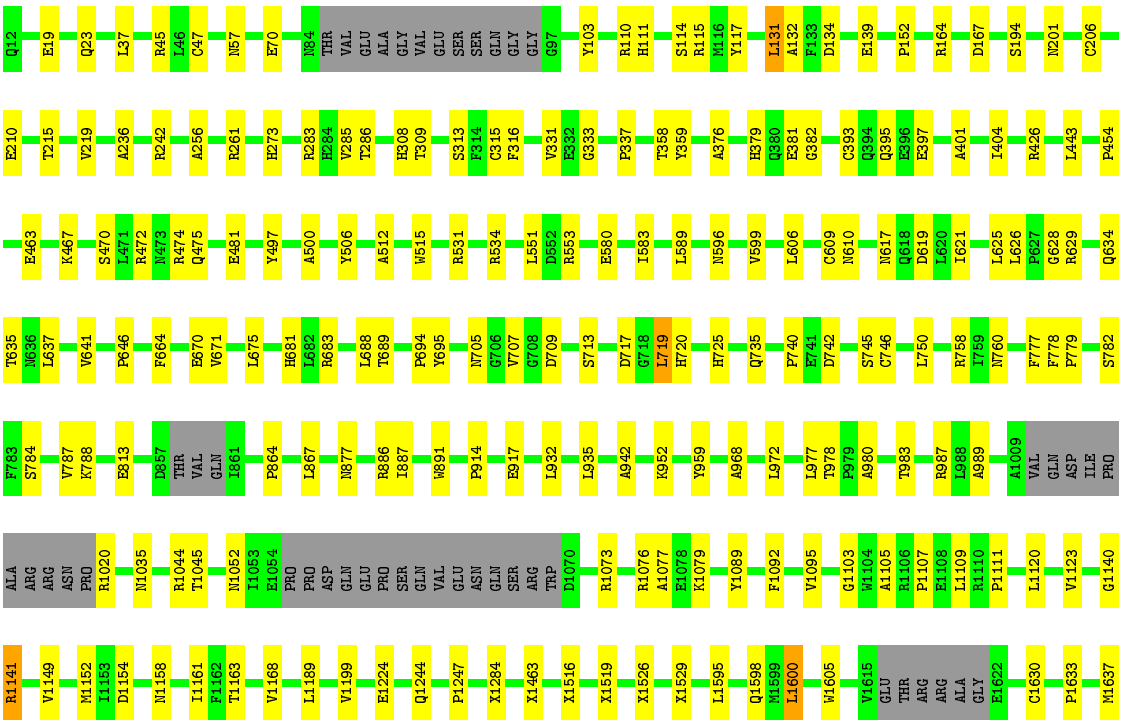
Chain I:

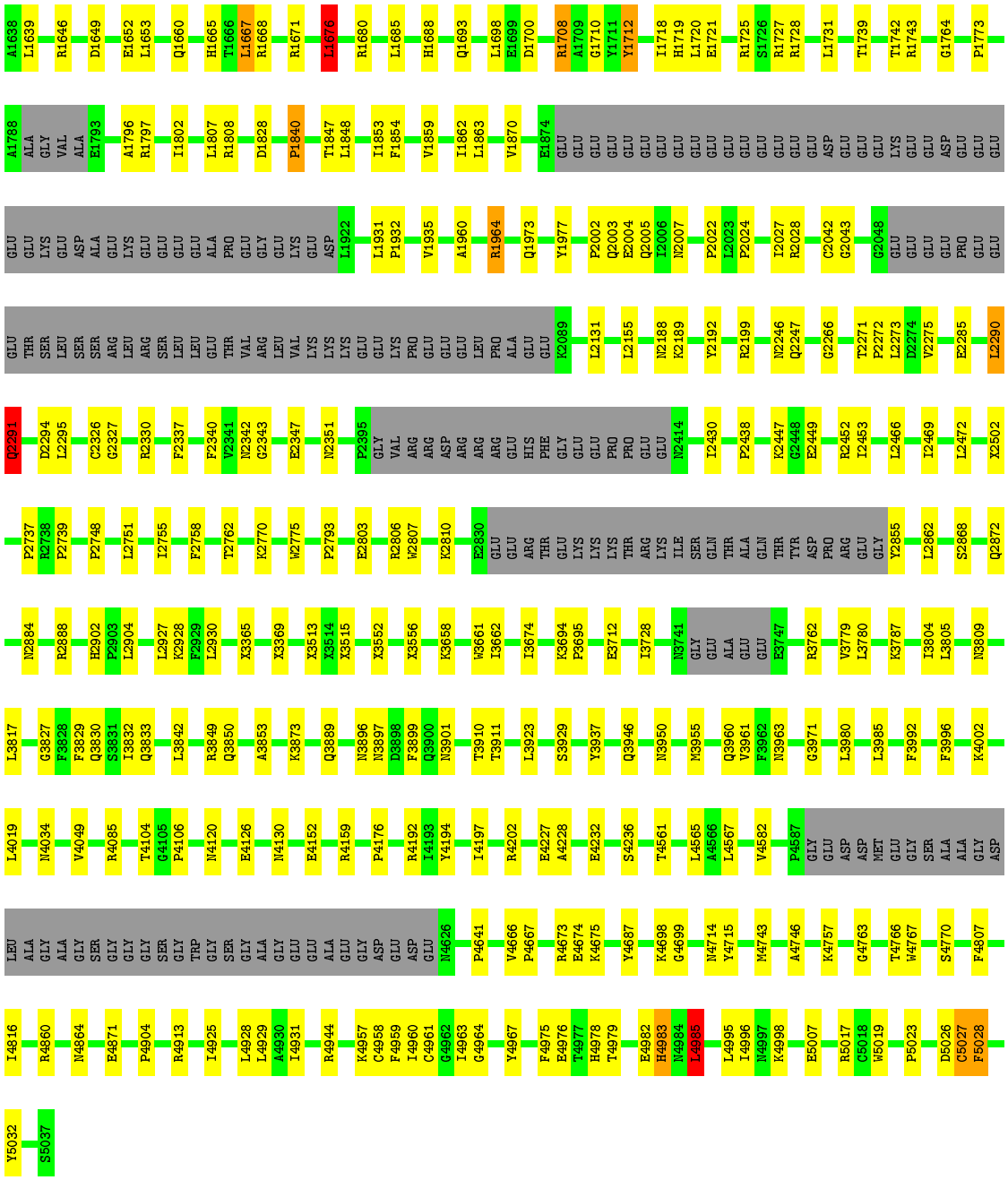




• Molecule 2: Ryanodine receptor 1

Chain G:





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	0.29	0/834	0.52	0/1123
1	F	0.29	0/834	0.52	0/1123
1	H	0.29	0/834	0.52	0/1123
1	J	0.29	0/834	0.52	0/1123
2	B	0.29	0/25428	0.54	10/34534 (0.0%)
2	E	0.29	0/25428	0.54	10/34534 (0.0%)
2	G	0.29	0/25428	0.54	10/34534 (0.0%)
2	I	0.29	0/25428	0.54	10/34534 (0.0%)
All	All	0.29	0/105048	0.54	40/142628 (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
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 (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	131	LEU	CA-CB-CG	8.42	134.66	115.30
2	B	131	LEU	CA-CB-CG	8.41	134.65	115.30
2	E	131	LEU	CA-CB-CG	8.41	134.63	115.30
2	I	131	LEU	CA-CB-CG	8.39	134.60	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1600	LEU	CA-CB-CG	6.97	131.33	115.30
2	G	1600	LEU	CA-CB-CG	6.96	131.31	115.30
2	E	1600	LEU	CA-CB-CG	6.96	131.31	115.30
2	I	1600	LEU	CA-CB-CG	6.96	131.30	115.30
2	E	4985	LEU	CA-CB-CG	6.75	130.83	115.30
2	B	4985	LEU	CA-CB-CG	6.74	130.79	115.30
2	I	4985	LEU	CA-CB-CG	6.73	130.79	115.30
2	G	4985	LEU	CA-CB-CG	6.73	130.78	115.30
2	G	1676	LEU	CA-CB-CG	6.73	130.77	115.30
2	E	1676	LEU	CA-CB-CG	6.72	130.76	115.30
2	I	1676	LEU	CA-CB-CG	6.71	130.75	115.30
2	B	1676	LEU	CA-CB-CG	6.71	130.74	115.30
2	E	1140	GLY	C-N-CA	5.96	136.60	121.70
2	I	1140	GLY	C-N-CA	5.96	136.59	121.70
2	B	1140	GLY	C-N-CA	5.95	136.57	121.70
2	G	1140	GLY	C-N-CA	5.94	136.55	121.70
2	G	2290	LEU	CA-CB-CG	5.83	128.70	115.30
2	B	2290	LEU	CA-CB-CG	5.82	128.69	115.30
2	I	2290	LEU	CA-CB-CG	5.81	128.67	115.30
2	E	2290	LEU	CA-CB-CG	5.80	128.65	115.30
2	E	688	LEU	CA-CB-CG	5.55	128.07	115.30
2	B	688	LEU	CA-CB-CG	5.53	128.03	115.30
2	G	688	LEU	CA-CB-CG	5.53	128.02	115.30
2	I	688	LEU	CA-CB-CG	5.52	127.99	115.30
2	G	719	LEU	CA-CB-CG	5.35	127.60	115.30
2	B	719	LEU	CA-CB-CG	5.34	127.58	115.30
2	I	719	LEU	CA-CB-CG	5.34	127.57	115.30
2	E	719	LEU	CA-CB-CG	5.33	127.56	115.30
2	G	977	LEU	CA-CB-CG	5.08	126.98	115.30
2	B	977	LEU	CA-CB-CG	5.08	126.97	115.30
2	G	1667	LEU	CA-CB-CG	5.06	126.94	115.30
2	E	977	LEU	CA-CB-CG	5.06	126.94	115.30
2	I	977	LEU	CA-CB-CG	5.06	126.94	115.30
2	E	1667	LEU	CA-CB-CG	5.05	126.92	115.30
2	B	1667	LEU	CA-CB-CG	5.05	126.91	115.30
2	I	1667	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	B	1676	LEU	Peptide
2	B	1712	TYR	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	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	694	PRO	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1712	TYR	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	3971	GLY	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	694	PRO	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1712	TYR	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	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	4807	PHE	Peptide
2	G	694	PRO	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1712	TYR	Peptide
2	I	1828	ASP	Peptide

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Mol	Chain	Res	Type	Group
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	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	694	PRO	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	5	0
1	F	818	0	824	5	0
1	H	818	0	824	4	0
1	J	818	0	824	4	0
2	B	29499	0	24746	252	0
2	E	29499	0	24746	258	0
2	G	29499	0	24746	248	0
2	I	29499	0	24746	255	0
3	B	31	0	12	0	0
3	E	31	0	12	0	0
3	G	31	0	12	0	0
3	I	31	0	12	0	0
4	B	14	0	10	1	0
4	E	14	0	10	1	0
4	G	14	0	10	1	0
4	I	14	0	10	1	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	102368	1020	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 5.

All (1020) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:5028:PHE:HE1	2:G:5032:TYR:CD2	1.87	0.93
2:I:5028:PHE:HE1	2:I:5032:TYR:CD2	1.87	0.93
2:B:5028:PHE:HE1	2:B:5032:TYR:CD2	1.87	0.92
2:E:5028:PHE:HE1	2:E:5032:TYR:CD2	1.87	0.92
2:G:5028:PHE:CE1	2:G:5032:TYR:CD2	2.58	0.92
2:I:5028:PHE:CE1	2:I:5032:TYR:CD2	2.58	0.92
2:B:5028:PHE:CE1	2:B:5032:TYR:CD2	2.58	0.92
2:E:5028:PHE:CE1	2:E:5032:TYR:CD2	2.58	0.91
2:G:5028:PHE:HE1	2:G:5032:TYR:CE2	1.99	0.81
2:E:5028:PHE:HE1	2:E:5032:TYR:CE2	1.99	0.80
2:G:5028:PHE:CE1	2:G:5032:TYR:HD2	1.99	0.79
2:I:5028:PHE:HE1	2:I:5032:TYR:CE2	1.99	0.79
2:B:5028:PHE:HE1	2:B:5032:TYR:CE2	1.99	0.79
2:E:4978:HIS:HA	2:E:4982:GLU:HB2	1.63	0.79
2:G:4978:HIS:HA	2:G:4982:GLU:HB2	1.63	0.79
2:I:5028:PHE:CE1	2:I:5032:TYR:HD2	1.99	0.79
2:I:4978:HIS:HA	2:I:4982:GLU:HB2	1.63	0.78
2:B:4978:HIS:HA	2:B:4982:GLU:HB2	1.64	0.78
2:E:5028:PHE:CE1	2:E:5032:TYR:HD2	2.00	0.77
2:B:5028:PHE:CE1	2:B:5032:TYR:HD2	2.00	0.76
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.74	0.70
2:E:379:HIS:HD2	2:E:382:GLY:H	1.41	0.69
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.74	0.69
2:I:4904:PRO:HB3	2:I:4913:ARG:HD3	1.75	0.69
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.74	0.69
2:I:379:HIS:HD2	2:I:382:GLY:H	1.41	0.69
2:G:4904:PRO:HB3	2:G:4913:ARG:HD3	1.75	0.69
2:E:4904:PRO:HB3	2:E:4913:ARG:HD3	1.75	0.68
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.74	0.68
2:B:4904:PRO:HB3	2:B:4913:ARG:HD3	1.75	0.68
2:G:379:HIS:HD2	2:G:382:GLY:H	1.41	0.68
2:B:379:HIS:HD2	2:B:382:GLY:H	1.41	0.68
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.59	0.68
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.59	0.68
2:I:4975:PHE:O	2:I:4979:THR:HG23	1.95	0.67
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.78	0.66
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.77	0.66
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.59	0.66
2:B:4975:PHE:O	2:B:4979:THR:HG23	1.95	0.66
2:G:4975:PHE:O	2:G:4979:THR:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.78	0.66
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.78	0.66
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.78	0.66
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.78	0.66
2:E:4975:PHE:O	2:E:4979:THR:HG23	1.95	0.65
2:E:4983:HIS:H	2:E:4983:HIS:CD2	2.13	0.65
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.78	0.65
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.13	0.65
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.59	0.65
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.78	0.65
2:B:4983:HIS:H	2:B:4983:HIS:CD2	2.13	0.64
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.78	0.64
2:G:4983:HIS:H	2:G:4983:HIS:CD2	2.13	0.64
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.62	0.64
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.31	0.64
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.62	0.64
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.63	0.63
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.31	0.63
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.31	0.63
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.31	0.63
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.63	0.62
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.64	0.62
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.82	0.62
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.64	0.62
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.82	0.61
2:B:2266:GLY:O	2:B:2330:ARG:NH2	2.33	0.61
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.64	0.61
2:I:4192:ARG:HD2	2:I:5028:PHE:CD2	2.35	0.61
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.82	0.61
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.82	0.61
2:G:2266:GLY:O	2:G:2330:ARG:NH2	2.33	0.61
2:B:4192:ARG:HD2	2:B:5028:PHE:CD2	2.35	0.61
2:E:4192:ARG:HD2	2:E:5028:PHE:CD2	2.35	0.61
2:I:2266:GLY:O	2:I:2330:ARG:NH2	2.33	0.61
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.64	0.60
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.83	0.60
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.82	0.60
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.83	0.60
2:G:4192:ARG:HD2	2:G:5028:PHE:CD2	2.35	0.60
2:E:2266:GLY:O	2:E:2330:ARG:NH2	2.33	0.60
2:G:683:ARG:NH1	2:G:707:VAL:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.67	0.60
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.82	0.60
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.82	0.59
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.82	0.59
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.83	0.59
2:B:683:ARG:NH1	2:B:707:VAL:O	2.35	0.59
2:G:609:CYS:SG	2:G:610:ASN:N	2.76	0.59
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.84	0.59
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.85	0.59
2:B:5028:PHE:CE1	2:B:5032:TYR:CE2	2.88	0.59
2:E:609:CYS:SG	2:E:610:ASN:N	2.76	0.59
2:E:683:ARG:NH1	2:E:707:VAL:O	2.35	0.59
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.67	0.59
2:B:609:CYS:SG	2:B:610:ASN:N	2.76	0.59
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.85	0.59
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.85	0.59
2:I:609:CYS:SG	2:I:610:ASN:N	2.76	0.59
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.36	0.58
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.85	0.58
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.85	0.58
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.84	0.58
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.85	0.58
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.85	0.58
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.85	0.58
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.37	0.58
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.85	0.58
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.67	0.58
2:G:331:VAL:HG12	2:G:333:GLY:H	1.68	0.58
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.85	0.58
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.85	0.58
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.83	0.58
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.86	0.58
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.84	0.58
2:I:331:VAL:HG12	2:I:333:GLY:H	1.68	0.58
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.85	0.58
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.85	0.58
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.86	0.58
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.36	0.58
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.85	0.58
2:B:331:VAL:HG12	2:B:333:GLY:H	1.68	0.58
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.85	0.58
2:I:683:ARG:NH1	2:I:707:VAL:O	2.35	0.57
2:I:315:CYS:SG	2:I:316:PHE:N	2.77	0.57
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.86	0.57
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.37	0.57
2:E:315:CYS:SG	2:E:316:PHE:N	2.77	0.57
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.37	0.57
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.86	0.57
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.87	0.57
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.86	0.57
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.38	0.57
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.37	0.57
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.37	0.57
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.86	0.57
2:E:331:VAL:HG12	2:E:333:GLY:H	1.68	0.57
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.38	0.57
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.37	0.57
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.38	0.57
2:G:315:CYS:SG	2:G:316:PHE:N	2.77	0.57
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.86	0.57
2:B:315:CYS:SG	2:B:316:PHE:N	2.77	0.57
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.38	0.57
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.85	0.57
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.85	0.57
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.86	0.57
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.37	0.57
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.38	0.57
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.67	0.57
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.86	0.57
2:B:132:ALA:HA	2:B:194:SER:HB2	1.86	0.57
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.37	0.57
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.86	0.57
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.38	0.57
2:I:359:TYR:HA	2:I:376:ALA:HA	1.86	0.57
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.38	0.57
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.39	0.56
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.87	0.56
2:E:4983:HIS:N	2:E:4983:HIS:CD2	2.73	0.56
2:G:4983:HIS:N	2:G:4983:HIS:CD2	2.73	0.56
2:G:132:ALA:HA	2:G:194:SER:HB2	1.86	0.56
2:B:4983:HIS:N	2:B:4983:HIS:CD2	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.37	0.56
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.39	0.56
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.87	0.56
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.87	0.56
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.86	0.56
2:B:359:TYR:HA	2:B:376:ALA:HA	1.87	0.56
2:E:132:ALA:HA	2:E:194:SER:HB2	1.86	0.56
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.38	0.56
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.37	0.56
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.39	0.56
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.71	0.56
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.88	0.56
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.86	0.56
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.87	0.56
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.71	0.56
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.38	0.56
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.39	0.56
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.86	0.56
2:G:359:TYR:HA	2:G:376:ALA:HA	1.86	0.56
2:E:111:HIS:HD2	2:E:114:SER:H	1.54	0.56
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.87	0.56
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.88	0.56
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.38	0.56
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.37	0.56
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.39	0.56
2:I:132:ALA:HA	2:I:194:SER:HB2	1.86	0.56
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.39	0.56
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.37	0.55
2:B:111:HIS:HD2	2:B:114:SER:H	1.54	0.55
2:E:359:TYR:HA	2:E:376:ALA:HA	1.86	0.55
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.88	0.55
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.89	0.55
2:E:23:GLN:HB3	2:E:201:ASN:HB2	1.89	0.55
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.89	0.55
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.40	0.55
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.39	0.55
2:G:111:HIS:HD2	2:G:114:SER:H	1.54	0.55
2:G:4567:LEU:HD12	2:G:4816:ILE:HD12	1.89	0.55
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.40	0.55
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.87	0.55
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.39	0.55
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.79	0.55
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.79	0.55
2:I:4567:LEU:HD12	2:I:4816:ILE:HD12	1.89	0.55
2:B:23:GLN:HB3	2:B:201:ASN:HB2	1.89	0.54
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.79	0.54
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.90	0.54
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.71	0.54
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.88	0.54
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.90	0.54
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.90	0.54
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.89	0.54
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.37	0.54
2:I:2868:SER:O	2:I:2872:GLN:N	2.38	0.54
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.39	0.54
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.71	0.54
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.88	0.54
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.39	0.54
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.89	0.54
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.40	0.54
2:G:23:GLN:HB3	2:G:201:ASN:HB2	1.89	0.54
2:I:111:HIS:HD2	2:I:114:SER:H	1.54	0.54
2:I:23:GLN:HB3	2:I:201:ASN:HB2	1.89	0.54
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.89	0.54
2:E:470:SER:O	2:E:474:ARG:NE	2.39	0.54
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.90	0.54
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.89	0.54
2:E:4567:LEU:HD12	2:E:4816:ILE:HD12	1.89	0.54
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.90	0.54
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.39	0.54
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.41	0.54
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.89	0.54
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.90	0.54
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.90	0.54
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.90	0.54
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.41	0.54
2:E:5028:PHE:CE1	2:E:5032:TYR:CE2	2.88	0.54
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.89	0.54
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.90	0.54
2:B:4567:LEU:HD12	2:B:4816:ILE:HD12	1.89	0.53
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.90	0.53
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.42	0.53
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.42	0.53
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.40	0.53
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.73	0.53
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.42	0.53
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.73	0.53
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.42	0.53
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.42	0.53
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.90	0.53
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.90	0.53
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.39	0.53
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.90	0.53
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.42	0.53
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.41	0.53
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.42	0.53
2:I:3897:ASN:O	2:I:3901:ASN:ND2	2.42	0.53
2:I:4983:HIS:N	2:I:4983:HIS:CD2	2.73	0.53
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.38	0.53
2:G:470:SER:O	2:G:474:ARG:NE	2.39	0.53
2:E:3897:ASN:O	2:E:3901:ASN:ND2	2.42	0.53
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.90	0.53
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.27	0.52
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.27	0.52
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.73	0.52
2:B:3897:ASN:O	2:B:3901:ASN:ND2	2.42	0.52
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.41	0.52
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.90	0.52
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.38	0.52
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.91	0.52
2:E:689:THR:H	2:E:778:PHE:HE2	1.58	0.52
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.42	0.52
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.90	0.52
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.40	0.52
2:B:689:THR:H	2:B:778:PHE:HE2	1.58	0.52
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.73	0.52
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.91	0.52
2:G:3842:LEU:O	2:G:3929:SER:OG	2.26	0.52
2:G:3897:ASN:O	2:G:3901:ASN:ND2	2.42	0.52
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.91	0.52
2:I:5028:PHE:CE1	2:I:5032:TYR:CE2	2.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.42	0.52
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.42	0.52
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.92	0.52
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.90	0.52
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.90	0.52
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.92	0.52
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.92	0.52
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.91	0.52
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.92	0.52
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.42	0.52
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.91	0.52
2:B:3842:LEU:O	2:B:3929:SER:OG	2.26	0.51
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.91	0.51
2:G:1516:UNK:N	2:G:1529:UNK:O	2.43	0.51
2:G:5028:PHE:CE1	2:G:5032:TYR:CE2	2.88	0.51
2:I:689:THR:H	2:I:778:PHE:HE2	1.58	0.51
2:B:1516:UNK:N	2:B:1529:UNK:O	2.43	0.51
2:E:1516:UNK:N	2:E:1529:UNK:O	2.43	0.51
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.91	0.51
2:E:3842:LEU:O	2:E:3929:SER:OG	2.27	0.51
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.92	0.51
2:B:470:SER:O	2:B:474:ARG:NE	2.39	0.51
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.90	0.51
2:E:2868:SER:O	2:E:2872:GLN:N	2.38	0.51
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.92	0.51
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.92	0.51
2:G:689:THR:H	2:G:778:PHE:HE2	1.58	0.51
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.44	0.51
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.91	0.51
2:I:4236:SER:OG	2:I:4675:LYS:NZ	2.41	0.51
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.27	0.51
2:B:978:THR:HB	2:B:980:ALA:H	1.75	0.51
2:G:2342:ASN:N	2:G:2342:ASN:OD1	2.44	0.51
2:I:3842:LEU:O	2:I:3929:SER:OG	2.27	0.51
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.27	0.51
2:E:813:GLU:OE2	2:E:1020:ARG:N	2.44	0.51
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.40	0.51
2:G:978:THR:HB	2:G:980:ALA:H	1.75	0.51
2:I:1516:UNK:N	2:I:1529:UNK:O	2.43	0.51
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.40	0.51
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4958:CYS:SG	2:I:4961:CYS:N	2.84	0.51
2:B:2342:ASN:N	2:B:2342:ASN:OD1	2.44	0.51
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.76	0.51
2:B:4958:CYS:SG	2:B:4961:CYS:N	2.84	0.51
2:B:670:GLU:HG3	2:B:787:VAL:HG13	1.93	0.51
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.76	0.51
2:I:626:LEU:HG	2:I:628:GLY:H	1.76	0.51
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.44	0.51
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.93	0.51
2:E:978:THR:HB	2:E:980:ALA:H	1.75	0.51
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.93	0.51
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.93	0.51
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.93	0.51
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.93	0.50
2:G:813:GLU:OE2	2:G:1020:ARG:N	2.44	0.50
2:I:813:GLU:OE2	2:I:1020:ARG:N	2.44	0.50
2:B:813:GLU:OE2	2:B:1020:ARG:N	2.44	0.50
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.44	0.50
2:E:4236:SER:OG	2:E:4675:LYS:NZ	2.41	0.50
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.91	0.50
2:G:626:LEU:HG	2:G:628:GLY:H	1.76	0.50
2:E:3804:ILE:O	2:E:3809:ASN:ND2	2.45	0.50
2:E:395:GLN:HG3	2:E:397:GLU:H	1.77	0.50
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.93	0.50
2:E:670:GLU:HG3	2:E:787:VAL:HG13	1.93	0.50
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.76	0.50
2:I:3992:PHE:O	2:I:3996:PHE:N	2.40	0.50
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.93	0.50
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.76	0.50
2:E:626:LEU:HG	2:E:628:GLY:H	1.76	0.50
2:I:629:ARG:HD3	2:I:634:GLN:HG2	1.94	0.50
2:I:978:THR:HB	2:I:980:ALA:H	1.75	0.50
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.93	0.50
2:G:454:PRO:HG2	2:G:531:ARG:HH12	1.77	0.50
2:B:629:ARG:HD3	2:B:634:GLN:HG2	1.94	0.50
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.93	0.50
2:B:3804:ILE:O	2:B:3809:ASN:ND2	2.45	0.50
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.93	0.50
2:E:4176:PRO:O	2:E:4202:ARG:NH2	2.45	0.50
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.44	0.50
2:G:670:GLU:HG3	2:G:787:VAL:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4236:SER:OG	2:B:4675:LYS:NZ	2.41	0.50
2:G:111:HIS:CD2	2:G:114:SER:H	2.30	0.50
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.45	0.50
2:I:2342:ASN:N	2:I:2342:ASN:OD1	2.44	0.50
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.93	0.49
2:B:626:LEU:HG	2:B:628:GLY:H	1.76	0.49
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.45	0.49
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.93	0.49
2:E:621:ILE:O	2:E:625:LEU:N	2.45	0.49
2:I:111:HIS:CD2	2:I:114:SER:H	2.30	0.49
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.94	0.49
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.77	0.49
2:G:395:GLN:HG3	2:G:397:GLU:H	1.77	0.49
2:I:395:GLN:HG3	2:I:397:GLU:H	1.77	0.49
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.93	0.49
2:G:621:ILE:O	2:G:625:LEU:N	2.45	0.49
2:I:3804:ILE:O	2:I:3809:ASN:ND2	2.45	0.49
2:B:395:GLN:HG3	2:B:397:GLU:H	1.77	0.49
2:G:3804:ILE:O	2:G:3809:ASN:ND2	2.45	0.49
2:I:3827:GLY:HA2	2:I:3830:GLN:HE21	1.78	0.49
2:I:470:SER:O	2:I:474:ARG:NE	2.39	0.49
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.79	0.49
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.44	0.49
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.93	0.49
2:G:4958:CYS:SG	2:G:4961:CYS:N	2.84	0.49
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.45	0.49
2:I:670:GLU:HG3	2:I:787:VAL:HG13	1.93	0.49
2:E:1796:ALA:HB1	2:E:1797:ARG:HH21	1.78	0.49
2:E:358:THR:HG21	2:E:382:GLY:HA2	1.95	0.49
2:G:629:ARG:HD3	2:G:634:GLN:HG2	1.94	0.49
2:E:629:ARG:HD3	2:E:634:GLN:HG2	1.94	0.49
2:I:1796:ALA:HB1	2:I:1797:ARG:HH21	1.78	0.49
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.45	0.49
2:B:4228:ALA:O	2:B:4232:GLU:N	2.46	0.49
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.95	0.49
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.95	0.49
2:I:621:ILE:O	2:I:625:LEU:N	2.45	0.49
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.46	0.49
2:B:404:ILE:HG21	2:B:481:GLU:HG3	1.95	0.49
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.45	0.49
2:G:3827:GLY:HA2	2:G:3830:GLN:HE21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:358:THR:HG21	2:I:382:GLY:HA2	1.95	0.49
2:I:1863:LEU:HB3	2:I:1870:VAL:HG21	1.95	0.49
2:I:2347:GLU:O	2:I:2351:ASN:N	2.39	0.49
2:I:4228:ALA:O	2:I:4232:GLU:N	2.46	0.49
2:E:454:PRO:HG2	2:E:531:ARG:HH12	1.77	0.48
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	1.95	0.48
2:G:358:THR:HG21	2:G:382:GLY:HA2	1.95	0.48
2:I:4976:GLU:HA	2:I:4979:THR:HG23	1.95	0.48
2:B:111:HIS:CD2	2:B:114:SER:H	2.30	0.48
2:B:4176:PRO:O	2:B:4202:ARG:NH2	2.45	0.48
2:B:4976:GLU:HA	2:B:4979:THR:HG23	1.95	0.48
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.95	0.48
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.46	0.48
2:E:4958:CYS:SG	2:E:4961:CYS:N	2.84	0.48
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.46	0.48
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.95	0.48
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	1.95	0.48
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.46	0.48
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.95	0.48
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	1.95	0.48
2:I:404:ILE:HG21	2:I:481:GLU:HG3	1.95	0.48
2:B:358:THR:HG21	2:B:382:GLY:HA2	1.95	0.48
2:G:1863:LEU:HB3	2:G:1870:VAL:HG21	1.95	0.48
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.46	0.48
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	1.95	0.48
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.93	0.48
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.78	0.48
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.78	0.48
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.96	0.48
2:E:111:HIS:CD2	2:E:114:SER:H	2.30	0.48
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	1.95	0.48
2:E:3980:LEU:HD22	2:E:3985:LEU:HD22	1.96	0.48
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.46	0.48
2:G:37:LEU:HD11	2:G:47:CYS:HB3	1.96	0.48
2:G:404:ILE:HG21	2:G:481:GLU:HG3	1.95	0.48
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.95	0.48
2:B:454:PRO:HG2	2:B:531:ARG:HH12	1.77	0.48
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.46	0.48
2:E:4228:ALA:O	2:E:4232:GLU:N	2.46	0.48
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.96	0.48
2:G:2347:GLU:O	2:G:2351:ASN:N	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4713:SER:HG	2:I:4775:TYR:HH	1.59	0.48
2:B:3827:GLY:HA2	2:B:3830:GLN:HE21	1.78	0.48
2:B:3980:LEU:HD22	2:B:3985:LEU:HD22	1.96	0.48
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.45	0.48
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.49	0.48
2:G:2868:SER:O	2:G:2872:GLN:N	2.38	0.48
2:G:4176:PRO:O	2:G:4202:ARG:NH2	2.45	0.48
2:G:4228:ALA:O	2:G:4232:GLU:N	2.46	0.48
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.96	0.48
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.95	0.48
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.47	0.48
2:B:1796:ALA:HB1	2:B:1797:ARG:HH21	1.78	0.48
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.96	0.48
2:I:37:LEU:HD11	2:I:47:CYS:HB3	1.96	0.48
2:I:4963:ILE:HG21	2:I:4967:TYR:HD2	1.79	0.48
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.96	0.48
2:B:1863:LEU:HB3	2:B:1870:VAL:HG21	1.95	0.48
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	1.95	0.48
2:G:3980:LEU:HD22	2:G:3985:LEU:HD22	1.96	0.48
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.45	0.48
2:I:4176:PRO:O	2:I:4202:ARG:NH2	2.45	0.48
2:E:4976:GLU:HA	2:E:4979:THR:HG23	1.95	0.48
2:I:3980:LEU:HD22	2:I:3985:LEU:HD22	1.96	0.48
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	1.95	0.47
2:E:4963:ILE:HG21	2:E:4967:TYR:HD2	1.79	0.47
2:G:1796:ALA:HB1	2:G:1797:ARG:HH21	1.78	0.47
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.47	0.47
2:B:742:ASP:HA	2:B:760:ASN:HD21	1.79	0.47
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.96	0.47
2:E:3827:GLY:HA2	2:E:3830:GLN:HE21	1.78	0.47
2:E:404:ILE:HG21	2:E:481:GLU:HG3	1.95	0.47
2:G:1720:LEU:HD12	2:G:1847:THR:HG23	1.97	0.47
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	1.95	0.47
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.95	0.47
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.33	0.47
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.33	0.47
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.96	0.47
2:G:4976:GLU:HA	2:G:4979:THR:HG23	1.95	0.47
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.96	0.47
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.49	0.47
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:742:ASP:HA	2:I:760:ASN:HD21	1.79	0.47
2:E:1863:LEU:HB3	2:E:1870:VAL:HG21	1.95	0.47
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.78	0.47
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.79	0.47
2:G:4192:ARG:HD2	2:G:5028:PHE:CE2	2.50	0.47
2:I:1720:LEU:HD12	2:I:1847:THR:HG23	1.96	0.47
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.46	0.47
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.96	0.47
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.49	0.47
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	1.97	0.47
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.47	0.47
2:B:2868:SER:O	2:B:2872:GLN:N	2.38	0.47
2:B:3992:PHE:O	2:B:3996:PHE:N	2.40	0.47
2:B:4898:GLY:O	2:E:4892:ARG:NH2	2.47	0.47
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.79	0.47
2:E:5023:PRO:HB3	2:E:5026:ASP:O	2.14	0.47
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.47	0.47
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.33	0.47
2:G:5023:PRO:HB3	2:G:5026:ASP:O	2.15	0.47
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.33	0.47
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.49	0.47
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	1.97	0.47
2:B:4192:ARG:HD2	2:B:5028:PHE:CE2	2.50	0.47
2:B:4963:ILE:HG21	2:B:4967:TYR:HD2	1.79	0.47
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.78	0.47
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.96	0.47
2:G:4963:ILE:HG21	2:G:4967:TYR:HD2	1.79	0.47
2:B:1720:LEU:HD12	2:B:1847:THR:HG23	1.97	0.47
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.96	0.47
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.47	0.47
2:E:750:LEU:HD21	2:E:777:PHE:HE2	1.80	0.47
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.97	0.47
2:E:1720:LEU:HD12	2:E:1847:THR:HG23	1.96	0.47
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	1.97	0.47
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.96	0.47
2:B:750:LEU:HD21	2:B:777:PHE:HE2	1.80	0.47
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.47	0.47
2:E:742:ASP:HA	2:E:760:ASN:HD21	1.79	0.47
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.97	0.47
2:B:5023:PRO:HB3	2:B:5026:ASP:O	2.15	0.47
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4192:ARG:HD2	2:E:5028:PHE:CE2	2.50	0.47
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.96	0.47
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.80	0.47
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.96	0.47
2:I:750:LEU:HD21	2:I:777:PHE:HE2	1.80	0.47
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.47	0.46
2:E:70:GLU:HG3	2:E:117:TYR:HE1	1.80	0.46
2:G:742:ASP:HA	2:G:760:ASN:HD21	1.79	0.46
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	1.97	0.46
2:I:5023:PRO:HB3	2:I:5026:ASP:O	2.15	0.46
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.81	0.46
2:B:472:ARG:HA	2:B:475:GLN:HB2	1.98	0.46
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.96	0.46
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.97	0.46
2:E:37:LEU:HD11	2:E:47:CYS:HB3	1.96	0.46
2:E:3889:GLN:HE22	2:E:3963:ASN:HB3	1.79	0.46
2:G:70:GLU:HG3	2:G:117:TYR:HE1	1.80	0.46
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.47	0.46
2:E:4561:THR:O	2:E:4565:LEU:N	2.46	0.46
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.41	0.46
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.81	0.46
2:B:37:LEU:HD11	2:B:47:CYS:HB3	1.96	0.46
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.98	0.46
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.96	0.46
2:E:2758:PHE:O	2:E:2762:THR:N	2.49	0.46
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	1.98	0.46
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.81	0.46
2:I:3889:GLN:HE22	2:I:3963:ASN:HB3	1.79	0.46
2:I:4192:ARG:HD2	2:I:5028:PHE:CE2	2.50	0.46
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.81	0.46
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.79	0.46
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.97	0.46
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.81	0.46
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.81	0.46
2:B:621:ILE:O	2:B:625:LEU:N	2.45	0.46
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.81	0.46
2:I:4561:THR:O	2:I:4565:LEU:N	2.46	0.46
2:I:512:ALA:HA	2:I:515:TRP:HB2	1.98	0.46
2:E:472:ARG:HA	2:E:475:GLN:HB2	1.98	0.46
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.98	0.46
2:I:70:GLU:HG3	2:I:117:TYR:HE1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.97	0.46
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	1.98	0.46
2:B:1973:GLN:O	2:B:1977:TYR:N	2.48	0.46
2:B:379:HIS:CD2	2:B:381:GLU:H	2.34	0.46
2:G:1973:GLN:O	2:G:1977:TYR:N	2.48	0.46
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.98	0.46
2:G:750:LEU:HD21	2:G:777:PHE:HE2	1.80	0.46
2:I:472:ARG:HA	2:I:475:GLN:HB2	1.98	0.46
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.81	0.46
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.97	0.46
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.98	0.46
2:B:3889:GLN:HE22	2:B:3963:ASN:HB3	1.79	0.46
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.97	0.46
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.81	0.46
2:E:236:ALA:HA	2:E:242:ARG:HD2	1.98	0.46
2:E:379:HIS:CD2	2:E:381:GLU:H	2.34	0.46
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.81	0.46
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.98	0.45
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.80	0.45
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.81	0.45
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.81	0.45
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.96	0.45
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.98	0.45
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.49	0.45
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.49	0.45
2:G:3365:UNK:O	2:G:3369:UNK:N	2.50	0.45
2:G:4236:SER:OG	2:G:4675:LYS:NZ	2.41	0.45
2:G:512:ALA:HA	2:G:515:TRP:HB2	1.98	0.45
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.97	0.45
2:B:70:GLU:HG3	2:B:117:TYR:HE1	1.80	0.45
2:B:236:ALA:HA	2:B:242:ARG:HD2	1.99	0.45
2:E:3992:PHE:O	2:E:3996:PHE:N	2.40	0.45
2:I:4928:LEU:HA	2:I:4931:ILE:HD12	1.98	0.45
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.98	0.45
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.99	0.45
2:E:1973:GLN:O	2:E:1977:TYR:N	2.48	0.45
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.97	0.45
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.97	0.45
2:G:379:HIS:CD2	2:G:381:GLU:H	2.34	0.45
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.98	0.45
2:B:4928:LEU:HA	2:B:4931:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.99	0.45
2:E:914:PRO:HD2	2:E:917:GLU:HB2	1.98	0.45
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	1.98	0.45
2:G:472:ARG:HA	2:G:475:GLN:HB2	1.98	0.45
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.99	0.45
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.99	0.45
2:B:4561:THR:O	2:B:4565:LEU:N	2.46	0.45
2:E:932:LEU:HA	2:E:935:LEU:HD12	1.98	0.45
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.99	0.45
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.98	0.45
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.49	0.45
2:B:2758:PHE:O	2:B:2762:THR:N	2.49	0.45
2:B:3365:UNK:O	2:B:3369:UNK:N	2.50	0.45
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.99	0.45
2:E:512:ALA:HA	2:E:515:TRP:HB2	1.98	0.45
2:I:236:ALA:HA	2:I:242:ARG:HD2	1.99	0.45
2:B:932:LEU:HA	2:B:935:LEU:HD12	1.98	0.45
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.98	0.45
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.98	0.45
2:E:4963:ILE:HD13	2:E:5027:CYS:SG	2.57	0.45
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.81	0.45
2:G:4928:LEU:HA	2:G:4931:ILE:HD12	1.98	0.45
2:I:379:HIS:CD2	2:I:381:GLU:H	2.34	0.45
2:I:4232:GLU:OE1	2:I:5019:TRP:NE1	2.50	0.45
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	1.98	0.45
2:E:4959:PHE:CG	2:E:4959:PHE:O	2.70	0.45
2:G:215:THR:HG22	2:G:273:HIS:HA	1.99	0.45
2:G:4963:ILE:HD13	2:G:5027:CYS:SG	2.57	0.45
2:I:256:ALA:HB1	2:I:286:THR:HG21	1.99	0.45
2:I:5028:PHE:O	2:I:5028:PHE:CD1	2.70	0.45
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.81	0.45
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.99	0.45
2:B:914:PRO:HD2	2:B:917:GLU:HB2	1.98	0.45
2:E:4928:LEU:HA	2:E:4931:ILE:HD12	1.98	0.45
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.81	0.45
2:E:681:HIS:HB3	2:E:784:SER:HB3	1.99	0.45
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.99	0.45
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.49	0.45
2:G:4959:PHE:CG	2:G:4959:PHE:O	2.70	0.45
2:I:1171:SER:OG	2:I:1175:SER:N	2.45	0.45
2:I:4959:PHE:O	2:I:4959:PHE:CD1	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4963:ILE:HD13	2:B:5027:CYS:SG	2.57	0.44
2:B:5028:PHE:CG	2:B:5028:PHE:O	2.70	0.44
2:B:512:ALA:HA	2:B:515:TRP:HB2	1.98	0.44
2:E:1099:GLU:OE2	2:E:1127:HIS:ND1	2.34	0.44
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.50	0.44
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.98	0.44
2:G:5028:PHE:O	2:G:5028:PHE:CD1	2.70	0.44
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.99	0.44
2:G:914:PRO:HD2	2:G:917:GLU:HB2	1.98	0.44
2:I:4963:ILE:HD13	2:I:5027:CYS:SG	2.57	0.44
2:I:914:PRO:HD2	2:I:917:GLU:HB2	1.98	0.44
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.98	0.44
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.50	0.44
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.82	0.44
2:E:3365:UNK:O	2:E:3369:UNK:N	2.50	0.44
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.99	0.44
2:G:236:ALA:HA	2:G:242:ARG:HD2	1.99	0.44
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.99	0.44
2:I:3365:UNK:O	2:I:3369:UNK:N	2.50	0.44
2:I:5028:PHE:O	2:I:5028:PHE:CG	2.70	0.44
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.83	0.44
2:B:2347:GLU:O	2:B:2351:ASN:N	2.39	0.44
2:E:4959:PHE:CD1	2:E:4959:PHE:O	2.70	0.44
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.98	0.44
2:G:5028:PHE:O	2:G:5028:PHE:CG	2.70	0.44
2:G:551:LEU:HD21	2:G:589:LEU:HD13	2.00	0.44
2:I:1973:GLN:O	2:I:1977:TYR:N	2.48	0.44
2:B:4959:PHE:CG	2:B:4959:PHE:O	2.70	0.44
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.99	0.44
2:E:1163:THR:HA	2:E:1168:VAL:HA	1.99	0.44
2:E:3762:ARG:NH2	2:E:4757:LYS:O	2.51	0.44
2:E:580:GLU:HG2	2:E:583:ILE:HD11	2.00	0.44
2:G:3762:ARG:NH2	2:G:4757:LYS:O	2.51	0.44
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.50	0.44
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.91	0.44
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.45	0.44
2:I:932:LEU:HA	2:I:935:LEU:HD12	1.98	0.44
2:B:4232:GLU:OE1	2:B:5019:TRP:NE1	2.50	0.44
2:B:551:LEU:HD21	2:B:589:LEU:HD13	2.00	0.44
2:B:983:THR:O	2:B:987:ARG:N	2.50	0.44
2:E:983:THR:O	2:E:987:ARG:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4232:GLU:OE1	2:G:5019:TRP:NE1	2.50	0.44
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	2.00	0.44
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.99	0.44
2:I:551:LEU:HD21	2:I:589:LEU:HD13	2.00	0.44
2:B:164:ARG:N	2:B:167:ASP:OD2	2.51	0.44
2:B:3762:ARG:NH2	2:B:4757:LYS:O	2.51	0.44
2:B:485:SER:O	2:B:489:ASN:N	2.42	0.44
2:B:4959:PHE:CD1	2:B:4959:PHE:O	2.70	0.44
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.91	0.44
2:E:215:THR:HG22	2:E:273:HIS:HA	1.99	0.44
2:E:3674:ILE:HD11	2:E:3728:ILE:HG22	1.99	0.44
2:I:1739:THR:H	2:I:1742:THR:HB	1.83	0.44
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	1.99	0.44
2:B:2447:LYS:HG3	2:B:2449:GLU:H	1.83	0.44
2:B:4998:LYS:NZ	2:B:5007:GLU:OE1	2.46	0.44
2:B:5028:PHE:CD1	2:B:5028:PHE:O	2.70	0.44
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.50	0.44
2:E:5028:PHE:CG	2:E:5028:PHE:O	2.70	0.44
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	2.00	0.44
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	1.99	0.44
2:G:4959:PHE:CD1	2:G:4959:PHE:O	2.70	0.44
2:G:932:LEU:HA	2:G:935:LEU:HD12	1.98	0.44
2:I:215:THR:HG22	2:I:273:HIS:HA	1.99	0.44
2:I:4959:PHE:CG	2:I:4959:PHE:O	2.70	0.44
2:B:1163:THR:HA	2:B:1168:VAL:HA	1.99	0.44
2:B:864:PRO:HD2	2:B:867:LEU:HD12	2.00	0.44
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.99	0.44
2:E:551:LEU:HD21	2:E:589:LEU:HD13	2.00	0.44
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.99	0.44
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.82	0.44
2:E:5028:PHE:O	2:E:5028:PHE:CD1	2.70	0.44
2:G:1163:THR:HA	2:G:1168:VAL:HA	1.99	0.44
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.50	0.44
2:G:256:ALA:HB1	2:G:286:THR:HG21	1.99	0.44
2:G:4561:THR:O	2:G:4565:LEU:N	2.46	0.44
2:I:164:ARG:N	2:I:167:ASP:OD2	2.51	0.44
2:I:2447:LYS:HG3	2:I:2449:GLU:H	1.83	0.44
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.91	0.43
2:E:1739:THR:H	2:E:1742:THR:HB	1.83	0.43
2:E:256:ALA:HB1	2:E:286:THR:HG21	1.99	0.43
2:E:4232:GLU:OE1	2:E:5019:TRP:NE1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.99	0.43
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	2.00	0.43
2:I:1163:THR:HA	2:I:1168:VAL:HA	1.99	0.43
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	2.00	0.43
2:I:3762:ARG:NH2	2:I:4757:LYS:O	2.51	0.43
2:B:1154:ASP:O	2:B:1158:ASN:N	2.51	0.43
2:B:1739:THR:H	2:B:1742:THR:HB	1.83	0.43
2:B:256:ALA:HB1	2:B:286:THR:HG21	1.99	0.43
2:G:681:HIS:HB3	2:G:784:SER:HB3	1.99	0.43
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.99	0.43
2:I:681:HIS:HB3	2:I:784:SER:HB3	1.99	0.43
2:B:2466:LEU:HD23	2:B:2469:ILE:HD12	2.00	0.43
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.99	0.43
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	2.00	0.43
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	1.99	0.43
2:G:164:ARG:N	2:G:167:ASP:OD2	2.51	0.43
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.83	0.43
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.91	0.43
2:G:864:PRO:HD2	2:G:867:LEU:HD12	2.00	0.43
2:I:1154:ASP:O	2:I:1158:ASN:N	2.51	0.43
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.52	0.43
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.99	0.43
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.84	0.43
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	2.00	0.43
2:G:2447:LYS:HG3	2:G:2449:GLU:H	1.83	0.43
2:I:2466:LEU:HD23	2:I:2469:ILE:HD12	2.00	0.43
2:E:2447:LYS:HG3	2:E:2449:GLU:H	1.83	0.43
2:G:3992:PHE:O	2:G:3996:PHE:N	2.40	0.43
2:I:1284:UNK:HA	2:I:1463:UNK:HA	2.00	0.43
2:B:215:THR:HG22	2:B:273:HIS:HA	1.99	0.43
2:B:4899:ASP:OD1	2:E:4892:ARG:NH2	2.50	0.43
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	2.00	0.43
2:E:2347:GLU:O	2:E:2351:ASN:N	2.39	0.43
2:E:864:PRO:HD2	2:E:867:LEU:HD12	2.00	0.43
2:G:4767:TRP:HE3	2:G:4770:SER:HB2	1.83	0.43
2:B:1284:UNK:HA	2:B:1463:UNK:HA	2.00	0.43
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	2.00	0.43
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.84	0.43
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	2.00	0.43
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	1.99	0.43
2:B:681:HIS:HB3	2:B:784:SER:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:164:ARG:N	2:E:167:ASP:OD2	2.51	0.43
2:E:2290:LEU:HB3	2:E:3849:ARG:HH12	1.84	0.43
2:G:1154:ASP:O	2:G:1158:ASN:N	2.51	0.43
2:G:1739:THR:H	2:G:1742:THR:HB	1.83	0.43
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	1.99	0.43
2:G:3923:LEU:HD13	2:G:3961:VAL:HG11	2.00	0.43
2:B:1728:ARG:HA	2:B:1731:LEU:HB2	2.01	0.43
2:E:1284:UNK:HA	2:E:1463:UNK:HA	2.00	0.43
2:E:3923:LEU:HD13	2:E:3961:VAL:HG11	2.00	0.43
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.84	0.43
2:G:983:THR:O	2:G:987:ARG:N	2.49	0.43
2:I:1728:ARG:HA	2:I:1731:LEU:HB2	2.01	0.43
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.84	0.43
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.99	0.43
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.99	0.43
2:E:4925:ILE:HA	2:E:4929:LEU:HD23	2.01	0.43
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	2.00	0.43
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.84	0.43
2:G:4925:ILE:HA	2:G:4929:LEU:HD23	2.01	0.43
2:I:401:ALA:HA	2:I:404:ILE:HD12	2.01	0.43
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.84	0.43
2:I:983:THR:O	2:I:987:ARG:N	2.50	0.43
2:E:1154:ASP:O	2:E:1158:ASN:N	2.51	0.43
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	2.01	0.43
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	2.01	0.43
2:E:4767:TRP:HE3	2:E:4770:SER:HB2	1.83	0.43
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	2.01	0.43
2:G:2466:LEU:HD23	2:G:2469:ILE:HD12	2.00	0.43
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.99	0.43
2:I:1808:ARG:HD2	2:I:1854:PHE:HA	2.01	0.43
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	2.00	0.43
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	2.01	0.43
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	2.00	0.42
2:E:2466:LEU:HD23	2:E:2469:ILE:HD12	2.00	0.42
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	2.01	0.42
2:G:309:THR:O	2:G:313:SER:OG	2.37	0.42
2:I:1859:VAL:HA	2:I:1862:ILE:HG12	2.01	0.42
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	2.00	0.42
2:B:4767:TRP:HE3	2:B:4770:SER:HB2	1.83	0.42
2:B:4925:ILE:HA	2:B:4929:LEU:HD23	2.01	0.42
2:E:1808:ARG:HD2	2:E:1854:PHE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:401:ALA:HA	2:E:404:ILE:HD12	2.01	0.42
2:G:1244:GLN:OE1	2:G:1646:ARG:NH1	2.53	0.42
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	2.01	0.42
2:I:1244:GLN:OE1	2:I:1646:ARG:NH1	2.53	0.42
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	2.00	0.42
2:I:4767:TRP:HE3	2:I:4770:SER:HB2	1.83	0.42
2:I:864:PRO:HD2	2:I:867:LEU:HD12	2.00	0.42
2:B:1244:GLN:OE1	2:B:1646:ARG:NH1	2.53	0.42
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.52	0.42
2:G:2290:LEU:HB3	2:G:3849:ARG:HH12	1.84	0.42
1:H:82:TYR:O	1:H:86:GLY:N	2.52	0.42
2:B:2793:PRO:HG3	2:B:2855:TYR:CZ	2.55	0.42
2:B:2290:LEU:HB3	2:B:3849:ARG:HH12	1.84	0.42
2:E:1991:THR:O	2:E:1995:THR:OG1	2.32	0.42
2:G:695:TYR:OH	2:G:1073:ARG:NH1	2.51	0.42
2:I:2758:PHE:O	2:I:2762:THR:N	2.49	0.42
2:I:3513:UNK:O	2:I:3515:UNK:N	2.53	0.42
2:I:4560:TYR:O	2:I:4564:PHE:N	2.49	0.42
2:I:4925:ILE:HA	2:I:4929:LEU:HD23	2.01	0.42
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	2.01	0.42
2:B:1808:ARG:HD2	2:B:1854:PHE:HA	2.02	0.42
2:B:278:GLN:N	2:B:315:CYS:SG	2.92	0.42
2:B:401:ALA:HA	2:B:404:ILE:HD12	2.00	0.42
2:E:1105:ALA:N	2:E:1189:LEU:O	2.53	0.42
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.52	0.42
2:G:1105:ALA:N	2:G:1189:LEU:O	2.53	0.42
2:I:309:THR:O	2:I:313:SER:OG	2.37	0.42
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.84	0.42
2:E:309:THR:O	2:E:313:SER:OG	2.37	0.42
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	2.02	0.42
1:F:82:TYR:O	1:F:86:GLY:N	2.53	0.42
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.44	0.42
2:I:1099:GLU:OE2	2:I:1127:HIS:ND1	2.34	0.42
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	2.01	0.42
2:I:2290:LEU:HB3	2:I:3849:ARG:HH12	1.84	0.42
2:I:2793:PRO:HG3	2:I:2855:TYR:CZ	2.55	0.42
2:I:2902:HIS:CE1	2:I:2904:LEU:HB2	2.55	0.42
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.93	0.42
2:I:3923:LEU:HD13	2:I:3961:VAL:HG11	2.00	0.42
2:B:1105:ALA:N	2:B:1189:LEU:O	2.53	0.42
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.51	0.42
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.93	0.42
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	2.02	0.42
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.51	0.42
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	2.02	0.42
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.93	0.42
2:E:709:ASP:HB3	2:E:725:HIS:CE1	2.55	0.42
2:G:1595:LEU:HD23	2:G:1595:LEU:HA	1.95	0.42
2:G:1808:ARG:HD2	2:G:1854:PHE:HA	2.01	0.42
2:E:174:VAL:O	2:G:2452:ARG:NH1	2.52	0.42
2:I:4239:GLU:OE2	2:I:5014:TYR:OH	2.32	0.42
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	2.02	0.42
2:E:3513:UNK:O	2:E:3515:UNK:N	2.53	0.42
2:G:1141:ARG:HD2	2:G:1141:ARG:H	1.85	0.42
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.85	0.42
2:B:3829:PHE:HA	2:B:3832:ILE:HD12	2.02	0.42
2:B:709:ASP:HB3	2:B:725:HIS:CE1	2.55	0.42
2:E:2902:HIS:CE1	2:E:2904:LEU:HB2	2.55	0.42
2:G:1728:ARG:HA	2:G:1731:LEU:HB2	2.01	0.42
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	2.01	0.41
2:B:2902:HIS:CE1	2:B:2904:LEU:HB2	2.55	0.41
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	2.01	0.41
2:E:635:THR:HG23	2:E:1693:GLN:HE22	1.85	0.41
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	2.01	0.41
2:E:2793:PRO:HG3	2:E:2855:TYR:CZ	2.55	0.41
2:G:2793:PRO:HG3	2:G:2855:TYR:CZ	2.55	0.41
2:G:3513:UNK:O	2:G:3515:UNK:N	2.53	0.41
2:I:1089:TYR:N	2:I:1224:GLU:O	2.53	0.41
2:I:1247:PRO:HA	2:I:1598:GLN:HA	2.02	0.41
2:I:3829:PHE:HA	2:I:3832:ILE:HD12	2.02	0.41
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	2.02	0.41
2:B:1859:VAL:HA	2:B:1862:ILE:HG12	2.01	0.41
2:E:1089:TYR:N	2:E:1224:GLU:O	2.53	0.41
2:E:1244:GLN:OE1	2:E:1646:ARG:NH1	2.53	0.41
2:E:3694:LYS:HA	2:E:3695:PRO:HD3	1.93	0.41
2:E:4197:ILE:HG21	2:E:4202:ARG:HH21	1.85	0.41
2:E:451:TYR:O	2:E:474:ARG:NH1	2.48	0.41
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.84	0.41
2:E:4928:LEU:HD13	2:E:4931:ILE:HD12	2.02	0.41
2:G:1802:ILE:HG21	2:G:1807:LEU:HD22	2.02	0.41
2:G:1859:VAL:HA	2:G:1862:ILE:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2:VAL:HG21	1:H:61:GLU:HB2	2.02	0.41
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	2.01	0.41
2:I:2883:HIS:NE2	2:I:2906:VAL:O	2.50	0.41
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.85	0.41
1:J:2:VAL:HG21	1:J:61:GLU:HB2	2.02	0.41
2:B:309:THR:O	2:B:313:SER:OG	2.37	0.41
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	2.02	0.41
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.85	0.41
2:E:1247:PRO:HA	2:E:1598:GLN:HA	2.02	0.41
2:E:1728:ARG:HA	2:E:1731:LEU:HB2	2.01	0.41
2:G:1284:UNK:HA	2:G:1463:UNK:HA	2.00	0.41
2:G:2902:HIS:CE1	2:G:2904:LEU:HB2	2.55	0.41
2:I:1077:ALA:HB3	2:I:1189:LEU:HD11	2.03	0.41
2:I:4197:ILE:HG21	2:I:4202:ARG:HH21	1.85	0.41
2:B:1247:PRO:HA	2:B:1598:GLN:HA	2.02	0.41
2:B:261:ARG:HB3	2:B:283:ARG:HB3	2.02	0.41
2:B:4957:LYS:HG2	2:B:4964:GLY:HA2	2.03	0.41
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.93	0.41
2:G:401:ALA:HA	2:G:404:ILE:HD12	2.01	0.41
2:E:4239:GLU:OE2	2:E:5014:TYR:OH	2.32	0.41
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	2.01	0.41
2:E:4978:HIS:CA	2:E:4982:GLU:HB2	2.43	0.41
2:G:1077:ALA:HB3	2:G:1189:LEU:HD11	2.03	0.41
2:G:1089:TYR:N	2:G:1224:GLU:O	2.54	0.41
2:G:4197:ILE:HG21	2:G:4202:ARG:HH21	1.85	0.41
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.54	0.41
2:I:2272:PRO:HA	2:I:2275:VAL:HG12	2.03	0.41
2:I:261:ARG:HB3	2:I:283:ARG:HB3	2.02	0.41
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.29	0.41
2:I:596:ASN:HB3	2:I:599:VAL:HG22	2.02	0.41
2:B:3513:UNK:O	2:B:3515:UNK:N	2.53	0.41
2:B:3552:UNK:O	2:B:3556:UNK:N	2.54	0.41
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.56	0.41
2:E:1077:ALA:HB3	2:E:1189:LEU:HD11	2.03	0.41
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	2.03	0.41
2:G:2758:PHE:O	2:G:2762:THR:N	2.49	0.41
2:G:709:ASP:HB3	2:G:725:HIS:CE1	2.55	0.41
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.56	0.41
2:I:4996:ILE:HD12	4:I:5102:CFF:H123	2.03	0.41
1:A:2:VAL:HG21	1:A:61:GLU:HB2	2.02	0.41
2:B:1077:ALA:HB3	2:B:1189:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:864:PRO:HA	2:B:865:PRO:HD3	1.96	0.41
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.44	0.41
2:E:1141:ARG:HD2	2:E:1141:ARG:H	1.85	0.41
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	2.02	0.41
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.56	0.41
2:G:4996:ILE:HD12	4:G:5102:CFF:H123	2.03	0.41
2:G:4998:LYS:NZ	2:G:5007:GLU:OE1	2.46	0.41
2:I:3552:UNK:O	2:I:3556:UNK:N	2.54	0.41
2:I:709:ASP:HB3	2:I:725:HIS:CE1	2.55	0.41
1:A:92:PRO:HD3	2:B:627:PRO:HB2	2.02	0.41
2:B:4197:ILE:HG21	2:B:4202:ARG:HH21	1.85	0.41
2:E:1171:SER:OG	2:E:1175:SER:N	2.45	0.41
2:E:3552:UNK:O	2:E:3556:UNK:N	2.54	0.41
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.84	0.41
2:G:134:ASP:OD1	2:G:134:ASP:N	2.53	0.41
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	2.03	0.41
2:G:3552:UNK:O	2:G:3556:UNK:N	2.54	0.41
2:G:635:THR:HG23	2:G:1693:GLN:HE22	1.85	0.41
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.85	0.41
2:I:4928:LEU:HD13	2:I:4931:ILE:HD12	2.03	0.41
2:B:134:ASP:OD1	2:B:134:ASP:N	2.53	0.41
2:B:2378:ALA:O	2:B:2382:GLU:N	2.54	0.41
2:E:596:ASN:HB3	2:E:599:VAL:HG22	2.02	0.41
2:G:1247:PRO:HA	2:G:1598:GLN:HA	2.02	0.41
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.29	0.41
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	2.03	0.41
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.54	0.41
2:E:2272:PRO:HA	2:E:2275:VAL:HG12	2.03	0.41
2:G:2272:PRO:HA	2:G:2275:VAL:HG12	2.03	0.41
2:I:1802:ILE:HG21	2:I:1807:LEU:HD22	2.02	0.41
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	2.03	0.41
2:B:1089:TYR:N	2:B:1224:GLU:O	2.54	0.41
2:B:2103:VAL:O	2:B:2107:GLN:N	2.46	0.41
2:B:635:THR:HG23	2:B:1693:GLN:HE22	1.85	0.41
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	2.03	0.41
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.56	0.41
1:F:2:VAL:HG21	1:F:61:GLU:HB2	2.02	0.41
2:G:3658:LYS:HA	2:G:3661:TRP:CE2	2.56	0.41
2:G:4928:LEU:HD13	2:G:4931:ILE:HD12	2.03	0.41
2:I:1105:ALA:N	2:I:1189:LEU:O	2.53	0.41
2:B:1802:ILE:HG21	2:B:1807:LEU:HD22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4156:HIS:CE1	2:E:5036:LEU:HD11	2.56	0.40
2:E:583:ILE:HA	2:E:586:ILE:HD12	2.03	0.40
2:G:3694:LYS:HA	2:G:3695:PRO:HD3	1.93	0.40
2:I:1076:ARG:HB3	2:I:1191:VAL:HG23	2.03	0.40
2:I:235:ALA:HA	2:I:257:ARG:HD3	2.03	0.40
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.54	0.40
2:I:4957:LYS:HG2	2:I:4964:GLY:HA2	2.03	0.40
2:I:683:ARG:HG2	2:I:717:ASP:HB3	2.04	0.40
2:B:596:ASN:HB3	2:B:599:VAL:HG22	2.02	0.40
2:E:134:ASP:N	2:E:134:ASP:OD1	2.53	0.40
2:E:3829:PHE:HA	2:E:3832:ILE:HD12	2.02	0.40
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.51	0.40
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.86	0.40
2:G:3829:PHE:HA	2:G:3832:ILE:HD12	2.02	0.40
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.84	0.40
2:G:596:ASN:HB3	2:G:599:VAL:HG22	2.02	0.40
2:I:635:THR:HG23	2:I:1693:GLN:HE22	1.85	0.40
2:I:4090:LYS:O	2:I:4094:GLN:N	2.53	0.40
2:I:4156:HIS:CE1	2:I:5036:LEU:HD11	2.56	0.40
2:B:2272:PRO:HA	2:B:2275:VAL:HG12	2.03	0.40
2:B:229:GLU:HA	2:B:249:GLY:HA2	2.03	0.40
2:E:1076:ARG:HB3	2:E:1191:VAL:HG23	2.03	0.40
2:E:229:GLU:HA	2:E:249:GLY:HA2	2.03	0.40
2:E:261:ARG:HB3	2:E:283:ARG:HB3	2.02	0.40
2:E:4996:ILE:HD12	4:E:5102:CFF:H123	2.03	0.40
2:G:683:ARG:HG2	2:G:717:ASP:HB3	2.04	0.40
2:I:3658:LYS:HA	2:I:3661:TRP:CE2	2.56	0.40
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.86	0.40
2:B:4996:ILE:HD12	4:B:5102:CFF:H123	2.03	0.40
2:E:113:HIS:O	2:E:399:GLN:NE2	2.55	0.40
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.54	0.40
2:G:261:ARG:HB3	2:G:283:ARG:HB3	2.02	0.40
2:B:4156:HIS:CE1	2:B:5036:LEU:HD11	2.56	0.40
2:E:2144:ILE:HG13	2:E:2144:ILE:H	1.80	0.40
2:E:661:LYS:HB3	2:E:808:TYR:CD1	2.57	0.40
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	2.03	0.40
2:G:4957:LYS:HG2	2:G:4964:GLY:HA2	2.03	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%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2916 (90%)	311 (10%)	8 (0%)	52	86
2	E	3235/4416 (73%)	2915 (90%)	312 (10%)	8 (0%)	52	86
2	G	3235/4416 (73%)	2915 (90%)	312 (10%)	8 (0%)	52	86
2	I	3235/4416 (73%)	2915 (90%)	312 (10%)	8 (0%)	52	86
All	All	13360/18096 (74%)	12037 (90%)	1291 (10%)	32 (0%)	56	86

All (32) 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	B	2291	GLN
2	E	1840	PRO
2	E	2291	GLN
2	I	1840	PRO

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Mol	Chain	Res	Type
2	I	2291	GLN
2	G	1840	PRO
2	G	2291	GLN
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
2	B	4667	PRO
2	E	4667	PRO
2	I	4667	PRO
2	G	4667	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%)	2476 (99%)	17 (1%)	88	94
2	E	2493/3022 (82%)	2476 (99%)	17 (1%)	88	94
2	G	2493/3022 (82%)	2476 (99%)	17 (1%)	88	94
2	I	2493/3022 (82%)	2476 (99%)	17 (1%)	88	94
All	All	10324/12444 (83%)	10256 (99%)	68 (1%)	89	94

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

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG
2	B	553	ARG
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	3787	LYS
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4944	ARG
2	B	4983	HIS
2	B	4995	LEU
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	3787	LYS
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4944	ARG
2	E	4983	HIS
2	E	4995	LEU
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	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	4944	ARG
2	I	4983	HIS
2	I	4995	LEU
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	3787	LYS
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4944	ARG
2	G	4983	HIS
2	G	4995	LEU
2	G	5027	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (119) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS
1	A	87	HIS
1	H	87	HIS
1	J	87	HIS
2	B	57	ASN
2	B	113	HIS
2	B	224	HIS
2	B	379	HIS
2	B	395	GLN
2	B	413	GLN
2	B	479	GLN
2	B	582	HIS
2	B	1206	GLN

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Mol	Chain	Res	Type
2	B	1598	GLN
2	B	1688	HIS
2	B	1693	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	2005	GLN
2	B	2858	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
2	B	3976	ASN
2	B	4034	ASN
2	B	4120	ASN
2	B	4130	ASN
2	B	4983	HIS
2	E	57	ASN
2	E	113	HIS
2	E	224	HIS
2	E	379	HIS
2	E	395	GLN
2	E	413	GLN
2	E	479	GLN
2	E	582	HIS
2	E	765	GLN
2	E	1206	GLN
2	E	1598	GLN
2	E	1688	HIS
2	E	1693	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	2005	GLN
2	E	2858	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

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Mol	Chain	Res	Type
2	E	3960	GLN
2	E	3976	ASN
2	E	4034	ASN
2	E	4120	ASN
2	E	4130	ASN
2	E	4806	ASN
2	E	4983	HIS
2	I	57	ASN
2	I	113	HIS
2	I	224	HIS
2	I	379	HIS
2	I	395	GLN
2	I	413	GLN
2	I	479	GLN
2	I	582	HIS
2	I	765	GLN
2	I	1206	GLN
2	I	1598	GLN
2	I	1688	HIS
2	I	1693	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	2005	GLN
2	I	2858	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	3976	ASN
2	I	4034	ASN
2	I	4120	ASN
2	I	4130	ASN
2	I	4983	HIS
2	G	57	ASN
2	G	113	HIS
2	G	224	HIS
2	G	379	HIS
2	G	395	GLN
2	G	413	GLN

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Mol	Chain	Res	Type
2	G	479	GLN
2	G	582	HIS
2	G	1206	GLN
2	G	1598	GLN
2	G	1688	HIS
2	G	1693	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	2005	GLN
2	G	2858	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	3976	ASN
2	G	4034	ASN
2	G	4120	ASN
2	G	4130	ASN
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	0.92	1 (3%)	26,52,52	1.75	1 (3%)
4	CFF	B	5102	-	8,15,15	2.40	3 (37%)	8,23,23	1.18	1 (12%)
3	ATP	E	5101	-	26,33,33	0.92	1 (3%)	26,52,52	1.77	1 (3%)
4	CFF	E	5102	-	8,15,15	2.40	3 (37%)	8,23,23	1.18	1 (12%)
3	ATP	G	5101	-	26,33,33	0.92	1 (3%)	26,52,52	1.75	1 (3%)
4	CFF	G	5102	-	8,15,15	2.40	3 (37%)	8,23,23	1.18	1 (12%)
3	ATP	I	5101	-	26,33,33	0.91	1 (3%)	26,52,52	1.75	1 (3%)
4	CFF	I	5102	-	8,15,15	2.40	3 (37%)	8,23,23	1.18	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	G	5102	CFF	C4-N3	-4.53	1.33	1.39
4	I	5102	CFF	C4-N3	-4.53	1.33	1.39
4	B	5102	CFF	C4-N3	-4.53	1.33	1.39
4	E	5102	CFF	C4-N3	-4.51	1.33	1.39
4	I	5102	CFF	C6-N1	-4.00	1.32	1.38
4	E	5102	CFF	C6-N1	-3.98	1.32	1.38
4	G	5102	CFF	C6-N1	-3.97	1.32	1.38
4	B	5102	CFF	C6-N1	-3.97	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	5102	CFF	O13-C6	-2.31	1.18	1.24
4	I	5102	CFF	O13-C6	-2.31	1.18	1.24
4	B	5102	CFF	O13-C6	-2.31	1.18	1.24
4	E	5102	CFF	O13-C6	-2.30	1.18	1.24
3	E	5101	ATP	C5-C4	2.95	1.47	1.40
3	B	5101	ATP	C5-C4	2.96	1.47	1.40
3	I	5101	ATP	C5-C4	2.96	1.47	1.40
3	G	5101	ATP	C5-C4	2.96	1.47	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	5101	ATP	N3-C2-N1	-7.26	123.17	128.87
3	I	5101	ATP	N3-C2-N1	-7.20	123.22	128.87
3	B	5101	ATP	N3-C2-N1	-7.19	123.22	128.87
3	G	5101	ATP	N3-C2-N1	-7.19	123.22	128.87
4	G	5102	CFF	C14-N7-C8	-2.55	112.02	125.31
4	E	5102	CFF	C14-N7-C8	-2.54	112.03	125.31
4	B	5102	CFF	C14-N7-C8	-2.54	112.05	125.31
4	I	5102	CFF	C14-N7-C8	-2.53	112.08	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
4	B	5102	CFF	1	0
4	E	5102	CFF	1	0
4	G	5102	CFF	1	0
4	I	5102	CFF	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	72.89
1	E	4345:UNK	C	4540:PHE	N	72.89
1	I	4345:UNK	C	4540:PHE	N	72.89
1	G	4345:UNK	C	4540:PHE	N	72.89
1	B	3613:UNK	C	3639:THR	N	44.63
1	E	3613:UNK	C	3639:THR	N	44.63
1	I	3613:UNK	C	3639:THR	N	44.63
1	G	3613:UNK	C	3639:THR	N	44.63
1	B	4253:GLU	C	4320:UNK	N	25.42
1	E	4253:GLU	C	4320:UNK	N	25.42
1	I	4253:GLU	C	4320:UNK	N	25.42
1	G	4253:GLU	C	4320:UNK	N	25.42
1	B	3163:UNK	C	3170:UNK	N	15.89
1	E	3163:UNK	C	3170:UNK	N	15.89
1	I	3163:UNK	C	3170:UNK	N	15.89
1	G	3163:UNK	C	3170:UNK	N	15.89
1	B	3063:UNK	C	3134:UNK	N	15.28
1	E	3063:UNK	C	3134:UNK	N	15.28
1	I	3063:UNK	C	3134:UNK	N	15.28
1	G	3063:UNK	C	3134:UNK	N	15.28
1	B	3468:UNK	C	3511:UNK	N	14.58
1	E	3468:UNK	C	3511:UNK	N	14.58
1	I	3468:UNK	C	3511:UNK	N	14.58
1	G	3468:UNK	C	3511:UNK	N	14.58
1	I	2703:UNK	C	2734:ASN	N	13.79
1	B	2703:UNK	C	2734:ASN	N	13.78
1	E	2703:UNK	C	2734:ASN	N	13.78
1	G	2703:UNK	C	2734:ASN	N	13.78
1	B	3236:UNK	C	3241:UNK	N	13.29
1	E	3236:UNK	C	3241:UNK	N	13.29
1	I	3236:UNK	C	3241:UNK	N	13.29
1	G	3236:UNK	C	3241:UNK	N	13.29
1	B	2976:UNK	C	2995:UNK	N	12.55
1	E	2976:UNK	C	2995:UNK	N	12.55
1	I	2976:UNK	C	2995:UNK	N	12.55
1	G	2976:UNK	C	2995:UNK	N	12.55

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1564:UNK	C	1573:MET	N	12.52
1	E	1564:UNK	C	1573:MET	N	12.52
1	I	1564:UNK	C	1573:MET	N	12.52
1	G	1564:UNK	C	1573:MET	N	12.52
1	B	3254:UNK	C	3261:UNK	N	8.35
1	E	3254:UNK	C	3261:UNK	N	8.35
1	I	3254:UNK	C	3261:UNK	N	8.35
1	G	3254:UNK	C	3261:UNK	N	8.35
1	B	1297:UNK	C	1430:UNK	N	6.00
1	E	1297:UNK	C	1430:UNK	N	6.00
1	I	1297:UNK	C	1430:UNK	N	6.00
1	G	1297:UNK	C	1430:UNK	N	6.00
1	B	2939:ARG	C	2942:UNK	N	3.26
1	E	2939:ARG	C	2942:UNK	N	3.26
1	I	2939:ARG	C	2942:UNK	N	3.26
1	G	2939:ARG	C	2942:UNK	N	3.26
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