wwPDB EM Map/Model Validation Report (i)

Oct 17, 2016 – 03:39 PM EDT

PDB ID	:	5T15
EMDB ID:	:	EMD-8342
Title	:	Structural basis for gating and activation of RyR1 (30 uM Ca2+ dataset, all particles)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-08-17
Resolution	:	3.60 Å(reported)

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

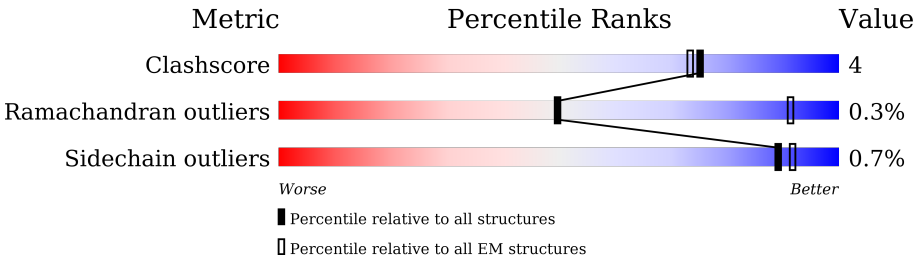
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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	87% 12% •
1	F	108	89% 10% •
1	H	108	88% 11% •
1	J	108	89% 10% •
2	B	4676	80% 8% 11%
2	E	4676	81% 8% 11%
2	G	4676	80% 8% 11%
2	I	4676	80% 8% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 120796 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,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4170	Total	C	N	O	S	0	0
			29379	18614	5204	5404	157		
2	E	4170	Total	C	N	O	S	0	0
			29379	18614	5204	5404	157		
2	I	4170	Total	C	N	O	S	0	0
			29379	18614	5204	5404	157		
2	G	4170	Total	C	N	O	S	0	0
			29379	18614	5204	5404	157		

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

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

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

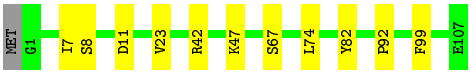
Mol	Chain	Residues	Atoms	AltConf
4	G	1	Total Ca 1 1	0
4	B	1	Total Ca 1 1	0
4	I	1	Total Ca 1 1	0
4	E	1	Total Ca 1 1	0

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

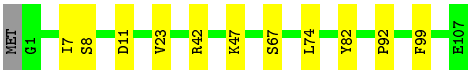
Chain A:

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

Chain H:

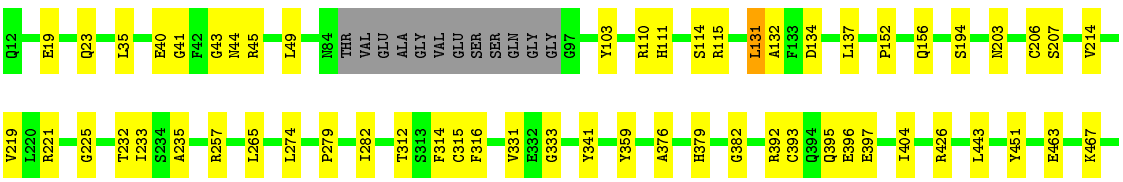
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

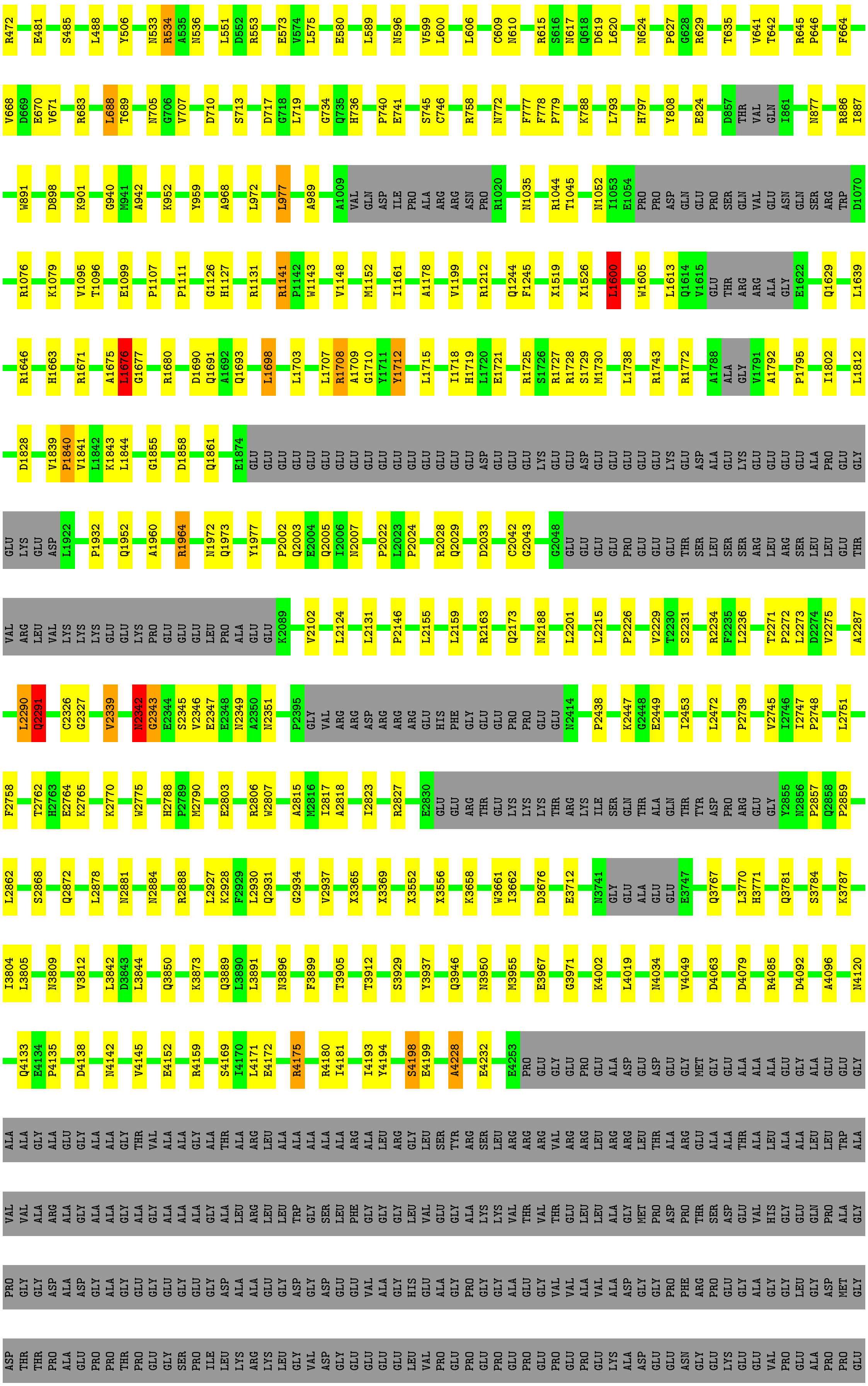
Chain J:

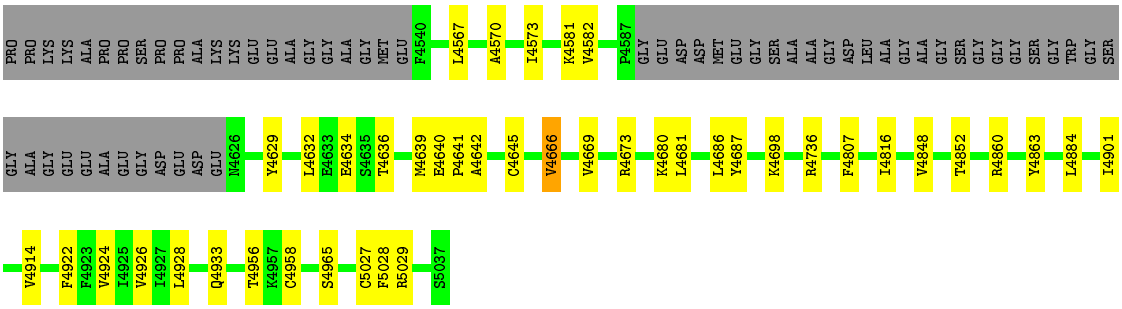


- Molecule 2: Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1

Chain B:

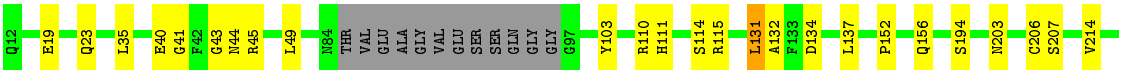


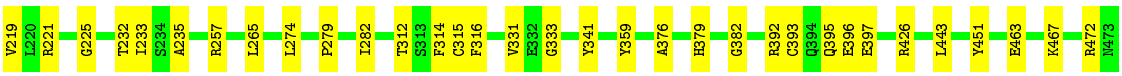

R472 E481 S485 L488 Y506 N533 R534 A535 N536 L551 D552 R553 E573 V574 L575 E580 L589 N596 V599 L600 L606 C609 N610 R615 S616 N617 Q618 D619 L620 N624 P627 G628 R629 T635 V641 T642 R645 P646 F664
V668 D669 E670 V671 R683 L688 T689 N705 G706 V707 D710 S713 D717 G718 L719 G734 Q735 H736 P740 E741 S745 C746 R758 N772 F777 F778 P779 K788 L793 H797 Y808 E824 D857 THR VAL GLN I861 N877 R886 I887
W891 D898 K901 G940 M941 A942 K952 Y959 A968 L972 L977 A989 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 N1035 R1044 T1045 N1052 I1053 E1054 PRO PRO ASP GLN GLN PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070
R1076 K1079 V1095 T1096 E1099 P1107 P1111 G1126 H1127 R1131 R1141 P1142 W1143 V1148 M1152 I1161 A1178 V1199 R1212 Q1244 F1245 X1519 X1526 L1600 W1605 L1613 Q1614 V1615 GLU THR ARG ARG ALA GLY E1622 Q1629 L1639
R1646 H1663 R1671 A1675 L1676 G1677 R1680 D1690 Q1691 A1692 Q1693 L1698 L1703 L1707 R1708 A1709 G1710 Y1711 Y1712 L1715 I1718 H1719 L1720 E1721 R1725 S1726 R1727 R1728 S1729 M1730 L1738 R1743 R1772 A1788 ALA GLY V1791 A1792 P1795 I1802 L1812
D1828 V1839 P1840 V1841 L1842 K1843 L1844 G1855 D1858 Q1861 E1874 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 P1932 Q1952 A1960 R1964 N1972 Q1973 Y1977 P2002 Q2003 E2004 Q2005 I2006 N2007 P2022 L2023 P2024 R2028 Q2029 D2033 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 V2102 L2124 L2131 P2146 L2155 L2159 R2163 Q2173 N2188 L2201 L2215 P2226 V2229 T2230 S2231 R2234 F2235 L2236 T2271 P2272 L2273 D2274 V2275 A2287
L2290 Q2291 C2326 G2327 V2339 N2342 G2343 E2344 S2345 V2346 E2347 E2348 N2349 A2350 N2351 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 P2438 K2447 G2448 E2449 I2453 L2472 P2739 V2745 I2746 I2747 P2748 L2751
F2758 T2762 H2763 E2764 K2765 K2770 W2775 H2788 P2789 M2790 E2803 R2806 W2807 A2815 M2816 I2817 A2818 I2823 R2827 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 N2856 P2857 Q2858 P2859
L2862 S2868 Q2872 L2878 N2881 N2884 R2888 L2927 K2928 F2929 L2930 Q2931 G2934 V2937 X3365 X3369 X3552 X3556 K3658 W3661 I3662 D3676 E3712 N3741 GLY GLU ALA GLU GLU E3747 Q3767 L3770 H3771 Q3781 S3784 K3787
I3804 L3805 N3809 V3812 L3842 D3843 L3844 Q3850 K3873 Q3889 L3890 L3891 N3896 F3899 T3905 T3912 S3929 Y3937 Q3946 N3950 M3955 E3967 G3971 K4002 L4019 N4034 V4049 D4063 D4079 R4085 D4092 A4096 N4120
Q4133 E4134 P4135 D4138 N4142 V4145 E4152 R4159 S4169 I4170 L4171 E4172 R4175 R4180 I4181 I4193 Y4194 S4198 E4199 A4228 E4232 E4253 PRO GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA GLU GLY ALA GLU GLY
ALA ALA GLY ALA GLU GLY ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG LEU ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA ALA LEU LEU TRP ALA
VAL VAL ALA ARG ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU GLU VAL HIS GLY GLU GLN PRO ALA GLY
PRO GLY GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY ASP ALA ALA GLU GLY ASP GLY ASP GLU GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL ALA VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY ALA GLY LEU GLY ASP MET GLY
ASP THR THR PRO ALA GLU PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU LEU VAL PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU LYS ALA ASP GLU GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO GLU

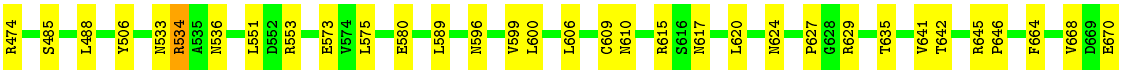


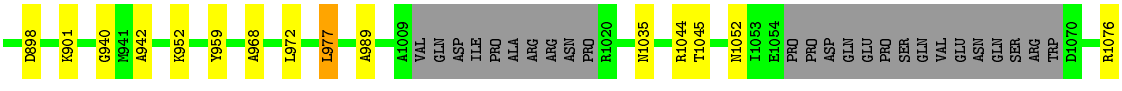
• Molecule 2: Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1

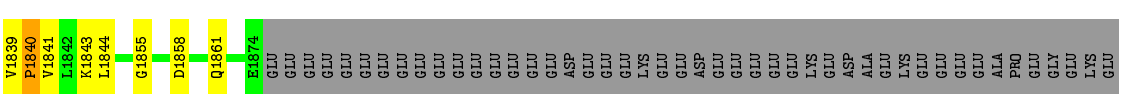
Chain E:

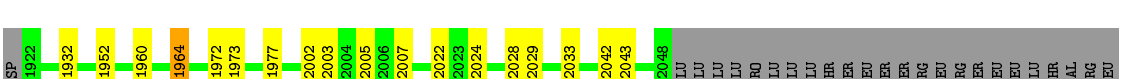


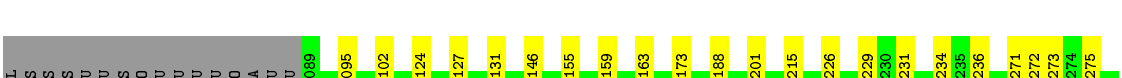


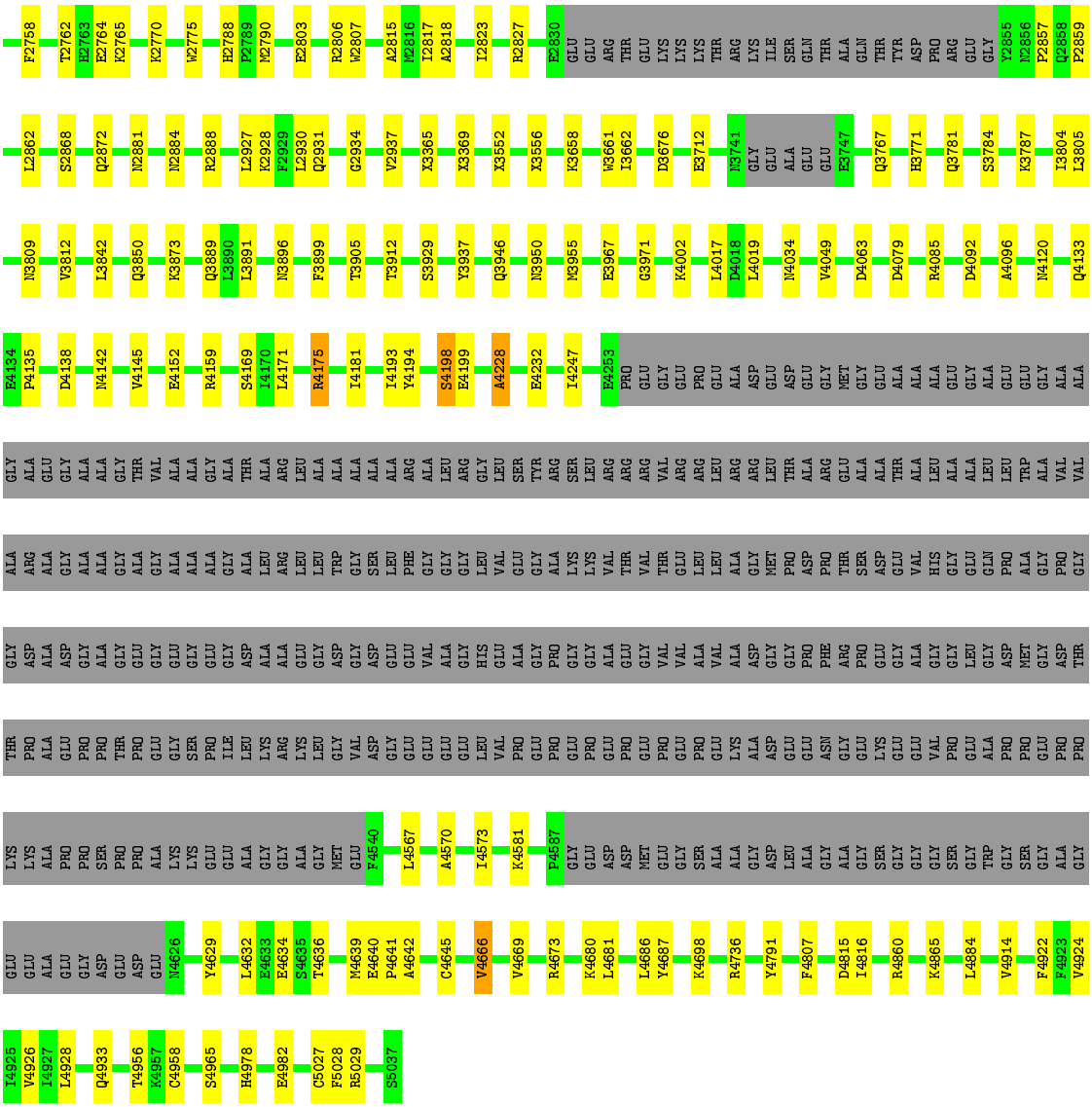






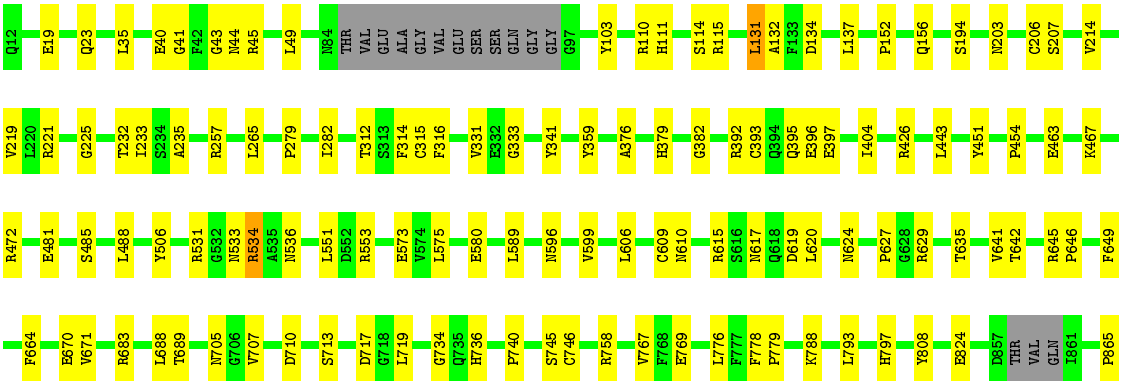


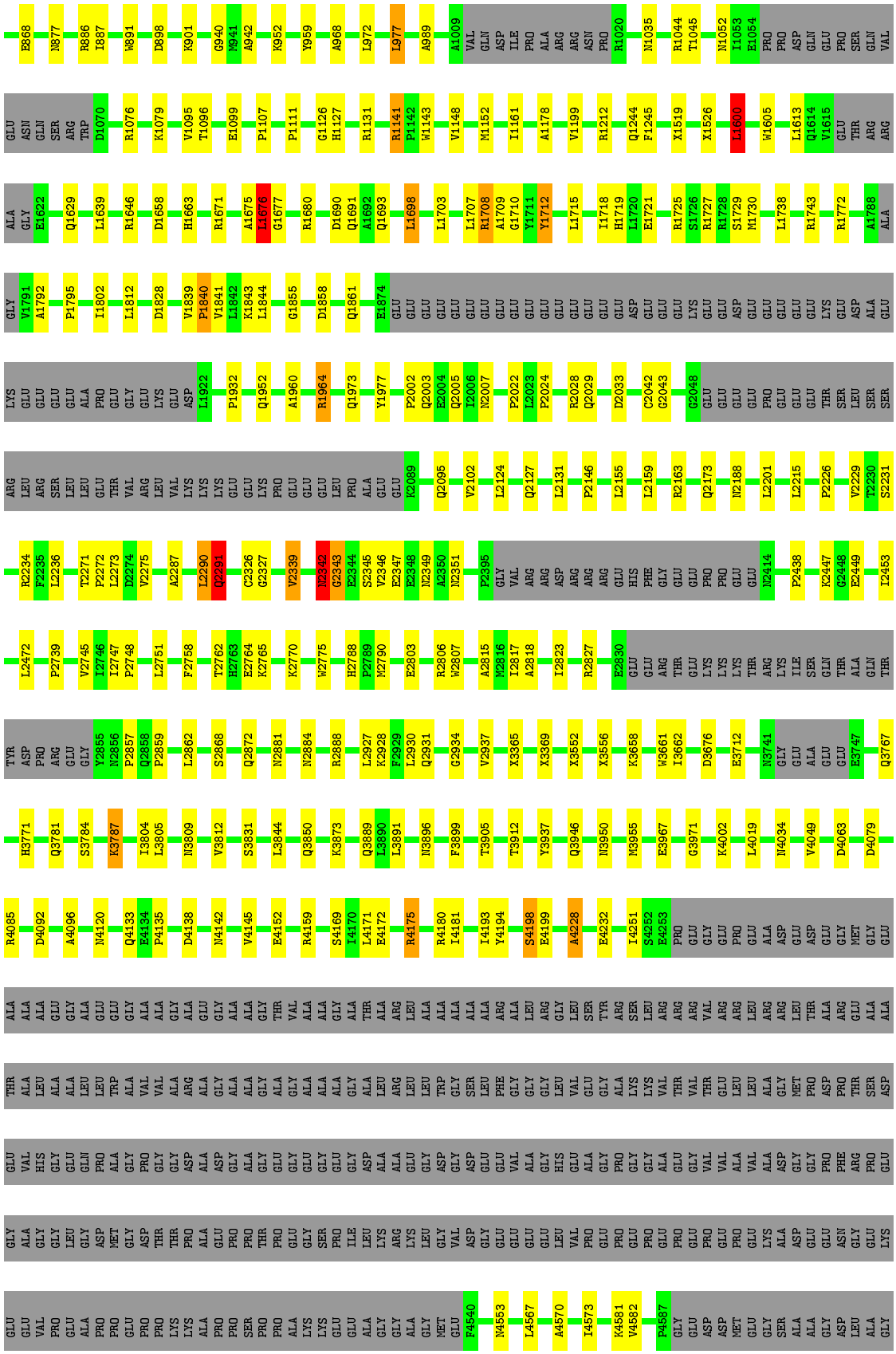




• Molecule 2: Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1

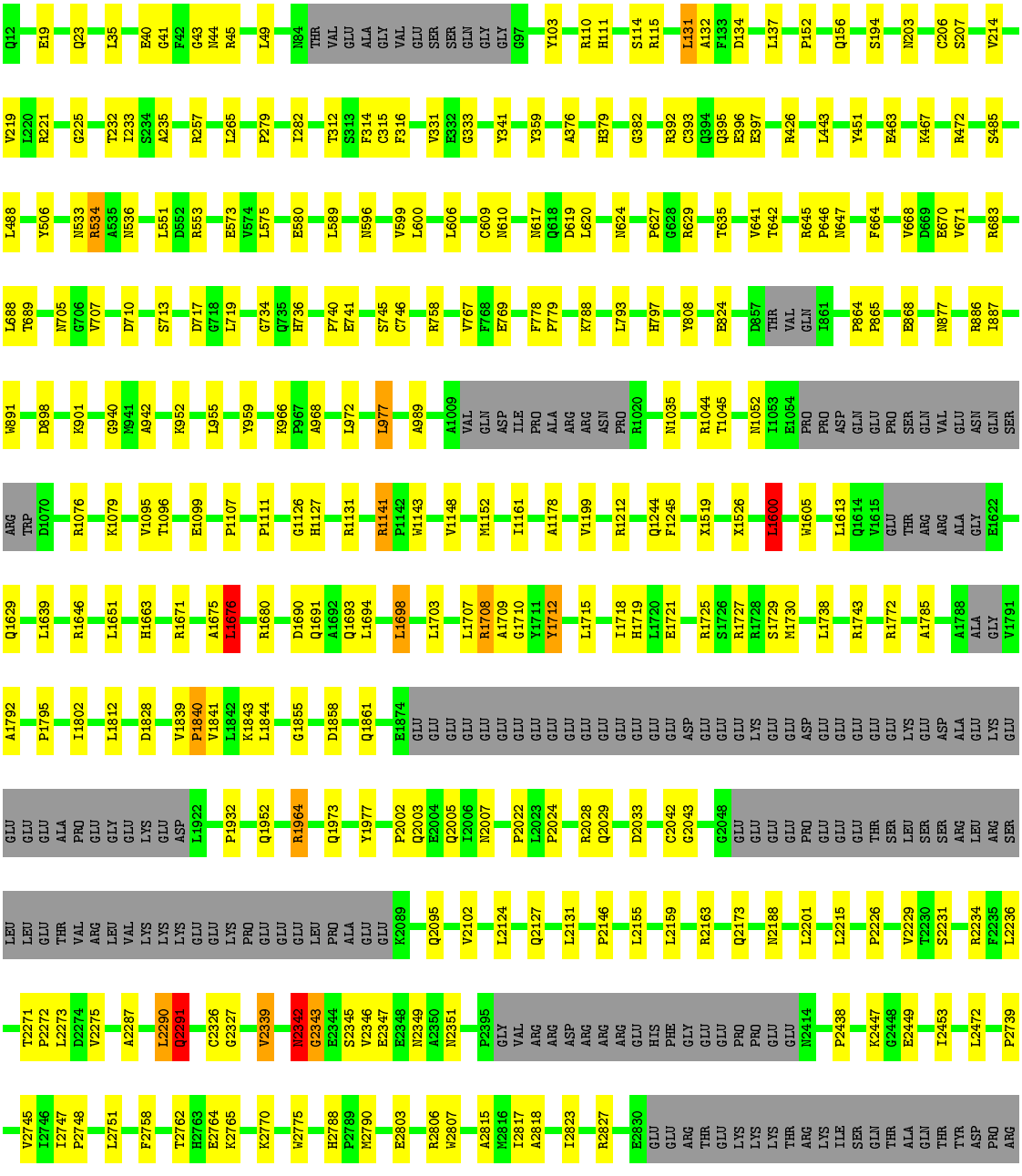
Chain I:

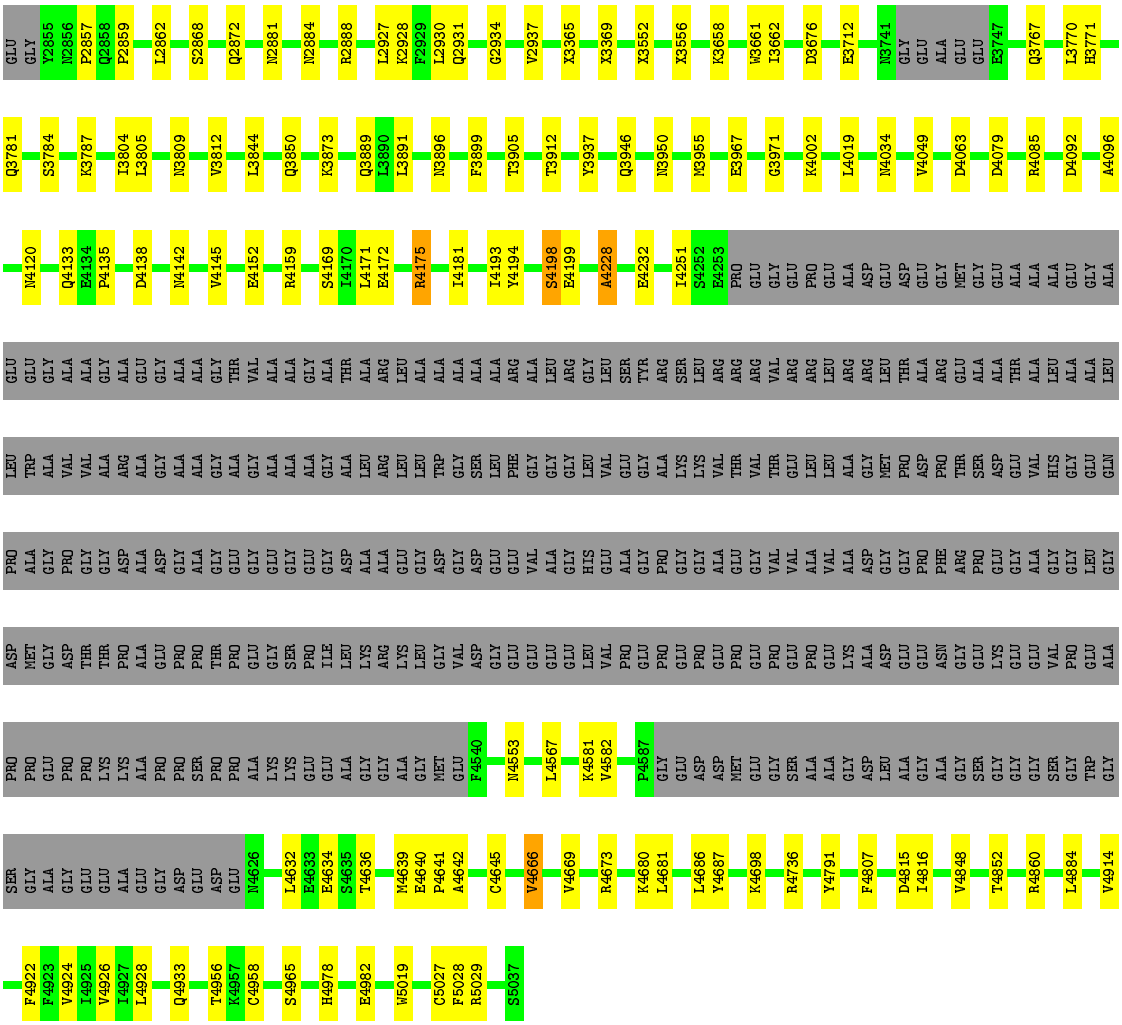




• Molecule 2: Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1

Chain G:




GLU GLY Y2855 N2856 P2857 Q2858 P2859 L2862 S2868 Q2872 N2881 N2884 R2888 L2927 K2928 F2929 L2930 Q2931 G2934 V2937 X3365 X3369 X3552 X3556 K3658 W3661 I3662 D3676 E3712 N3741 GLY GLU ALA GLU GLU E3747 Q3767 L3770 H3771
Q3781 S3784 K3787 I3804 L3805 N3809 V3812 L3844 Q3850 K3873 Q3889 L3890 L3891 N3896 F3899 T3905 T3912 Y3937 Q3946 N3950 M3955 E3967 G3971 K4002 L4019 N4034 V4049 D4063 D4079 R4085 D4092 A4096
N4120 Q4133 E4134 P4135 D4138 N4142 V4145 E4152 R4159 S4169 I4170 L4171 E4172 R4175 I4181 I4193 Y4194 S4198 E4199 A4228 E4232 I4251 S4252 E4253 PRO GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA GLU GLY
GLU GLU GLY ALA ALA GLY ALA GLU GLY ALA ALA ALA GLY THR VAL ALA ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ARG LEU ALA ALA LEU ARG ARG VAL ARG ARG LEU ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA LEU
LEU TRP ALA VAL VAL ALA ARG ALA GLY ALA ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA LEU ARG LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY LYS LYS VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN
PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLU GLY GLU GLY ASP GLY GLU GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL ALA VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY ALA GLY GLY GLY GLU
ASP MET GLY ASP THR THR PRO ALA GLU PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU LEU LEU VAL PRO GLU PRO PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA
PRO PRO GLU PRO PRO LYS LYS ALA PRO PRO SER PRO PRO ALA ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET GLU F4540 N4653 L4567 K4581 V4582 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY 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 L4632 E4633 E4634 S4635 T4636 M4639 E4640 P4641 A4642 C4645 V4666 V4669 R4673 K4680 L4681 L4686 Y4687 K4698 R4736 Y4791 F4807 D4815 I4816 V4848 T4852 R4860 L4884 V4914
F4922 F4923 V4924 I4925 V4926 I4927 L4928 Q4933 T4956 K4957 C4958 S4965 H4978 E4982 W5019 C5027 F5028 R5029 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: ZN, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.37	0/834	0.55	0/1123
1	F	0.37	0/834	0.55	0/1123
1	H	0.37	0/834	0.55	0/1123
1	J	0.37	0/834	0.55	0/1123
2	B	0.40	0/25438	0.60	11/34548 (0.0%)
2	E	0.40	0/25438	0.60	11/34548 (0.0%)
2	G	0.40	0/25438	0.60	11/34548 (0.0%)
2	I	0.40	0/25438	0.60	11/34548 (0.0%)
All	All	0.40	0/105088	0.59	44/142684 (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	3
1	F	0	3
1	H	0	3
1	J	0	3
2	B	0	22
2	E	0	22
2	G	0	22
2	I	0	22
All	All	0	100

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	131	LEU	CA-CB-CG	7.90	133.47	115.30
2	I	131	LEU	CA-CB-CG	7.90	133.47	115.30
2	E	131	LEU	CA-CB-CG	7.89	133.46	115.30
2	G	131	LEU	CA-CB-CG	7.89	133.44	115.30
2	B	2290	LEU	CA-CB-CG	7.21	131.87	115.30
2	E	2290	LEU	CA-CB-CG	7.19	131.84	115.30
2	G	2290	LEU	CA-CB-CG	7.19	131.83	115.30
2	I	2290	LEU	CA-CB-CG	7.18	131.82	115.30
2	I	1600	LEU	CA-CB-CG	7.10	131.63	115.30
2	B	1600	LEU	CA-CB-CG	7.10	131.63	115.30
2	G	1600	LEU	CA-CB-CG	7.10	131.62	115.30
2	E	1600	LEU	CA-CB-CG	7.09	131.61	115.30
2	I	1676	LEU	CA-CB-CG	6.48	130.20	115.30
2	G	1676	LEU	CA-CB-CG	6.47	130.18	115.30
2	B	1676	LEU	CA-CB-CG	6.47	130.18	115.30
2	E	1676	LEU	CA-CB-CG	6.47	130.17	115.30
2	E	4639	MET	C-N-CA	6.20	137.21	121.70
2	B	4639	MET	C-N-CA	6.20	137.20	121.70
2	G	4639	MET	C-N-CA	6.19	137.18	121.70
2	I	4639	MET	C-N-CA	6.18	137.15	121.70
2	I	688	LEU	CA-CB-CG	6.08	129.28	115.30
2	E	688	LEU	CA-CB-CG	6.05	129.22	115.30
2	B	688	LEU	CA-CB-CG	6.05	129.22	115.30
2	G	688	LEU	CA-CB-CG	6.05	129.22	115.30
2	G	1712	TYR	CA-CB-CG	-5.99	102.02	113.40
2	I	1712	TYR	CA-CB-CG	-5.98	102.03	113.40
2	B	1712	TYR	CA-CB-CG	-5.97	102.06	113.40
2	E	1712	TYR	CA-CB-CG	-5.96	102.07	113.40
2	B	977	LEU	CA-CB-CG	5.81	128.66	115.30
2	G	977	LEU	CA-CB-CG	5.81	128.66	115.30
2	E	977	LEU	CA-CB-CG	5.81	128.66	115.30
2	I	977	LEU	CA-CB-CG	5.80	128.63	115.30
2	E	1698	LEU	CA-CB-CG	5.42	127.77	115.30
2	G	1698	LEU	CA-CB-CG	5.42	127.77	115.30
2	B	1698	LEU	CA-CB-CG	5.42	127.76	115.30
2	I	1698	LEU	CA-CB-CG	5.42	127.76	115.30
2	I	2291	GLN	C-N-CA	5.22	134.76	121.70
2	B	2291	GLN	C-N-CA	5.20	134.71	121.70
2	E	2291	GLN	C-N-CA	5.20	134.70	121.70
2	G	2291	GLN	C-N-CA	5.20	134.69	121.70
2	E	4133	GLN	C-N-CA	5.08	134.39	121.70
2	B	4133	GLN	C-N-CA	5.06	134.35	121.70
2	I	4133	GLN	C-N-CA	5.04	134.31	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	4133	GLN	C-N-CA	5.04	134.31	121.70

There are no chirality outliers.

All (100) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	7	ILE	Peptide
1	A	8	SER	Peptide
1	A	82	TYR	Peptide
2	B	137	LEU	Peptide
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	2342	ASN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	312	THR	Peptide
2	B	3771	HIS	Peptide
2	B	3971	GLY	Peptide
2	B	4096	ALA	Peptide
2	B	4175	ARG	Peptide
2	B	4198	SER	Peptide
2	B	4228	ALA	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	4958	CYS	Peptide
2	B	624	ASN	Peptide
2	B	808	TYR	Peptide
2	B	977	LEU	Peptide
2	E	137	LEU	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	2342	ASN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	312	THR	Peptide
2	E	3771	HIS	Peptide

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Mol	Chain	Res	Type	Group
2	E	3971	GLY	Peptide
2	E	4096	ALA	Peptide
2	E	4175	ARG	Peptide
2	E	4198	SER	Peptide
2	E	4228	ALA	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	4958	CYS	Peptide
2	E	624	ASN	Peptide
2	E	808	TYR	Peptide
2	E	977	LEU	Peptide
1	F	7	ILE	Peptide
1	F	8	SER	Peptide
1	F	82	TYR	Peptide
2	G	137	LEU	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	2342	ASN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	312	THR	Peptide
2	G	3771	HIS	Peptide
2	G	3971	GLY	Peptide
2	G	4096	ALA	Peptide
2	G	4175	ARG	Peptide
2	G	4198	SER	Peptide
2	G	4228	ALA	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	4958	CYS	Peptide
2	G	624	ASN	Peptide
2	G	808	TYR	Peptide
2	G	977	LEU	Peptide
1	H	7	ILE	Peptide
1	H	8	SER	Peptide
1	H	82	TYR	Peptide
2	I	137	LEU	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	2342	ASN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	312	THR	Peptide
2	I	3771	HIS	Peptide
2	I	3971	GLY	Peptide
2	I	4096	ALA	Peptide
2	I	4175	ARG	Peptide
2	I	4198	SER	Peptide
2	I	4228	ALA	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	4958	CYS	Peptide
2	I	624	ASN	Peptide
2	I	808	TYR	Peptide
2	I	977	LEU	Peptide
1	J	7	ILE	Peptide
1	J	8	SER	Peptide
1	J	82	TYR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	6	0
1	F	818	0	824	5	0
1	H	818	0	824	6	0
1	J	818	0	824	5	0
2	B	29379	0	24730	221	0
2	E	29379	0	24729	219	0
2	G	29379	0	24730	223	0
2	I	29379	0	24729	221	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	120796	0	102214	875	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 (875) 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:379:HIS:HD2	2:G:382:GLY:H	1.40	0.70
2:I:379:HIS:HD2	2:I:382:GLY:H	1.40	0.70
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	1.75	0.69
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	1.75	0.69
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.74	0.69
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.74	0.69
2:B:379:HIS:HD2	2:B:382:GLY:H	1.40	0.67
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	1.75	0.67
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.74	0.67
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	1.75	0.67
2:E:379:HIS:HD2	2:E:382:GLY:H	1.40	0.67
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.74	0.67
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.77	0.67
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.78	0.66
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.77	0.66
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.78	0.66
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.78	0.66
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.77	0.66
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.78	0.65
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.77	0.65
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.71	0.64
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.71	0.64
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.79	0.64
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.79	0.64
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.71	0.64
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.71	0.64
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.81	0.63
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:670:GLU:HG3	2:I:788:LYS:H	1.64	0.63
2:G:670:GLU:HG3	2:G:788:LYS:H	1.64	0.63
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.81	0.63
2:B:670:GLU:HG3	2:B:788:LYS:H	1.64	0.63
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.79	0.62
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.81	0.62
2:E:670:GLU:HG3	2:E:788:LYS:H	1.64	0.62
2:B:3767:GLN:OE1	2:B:3809:ASN:ND2	2.33	0.62
2:E:3767:GLN:OE1	2:E:3809:ASN:ND2	2.33	0.62
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.81	0.62
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.81	0.62
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.33	0.61
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.34	0.61
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.33	0.61
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.34	0.61
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.34	0.61
2:G:3767:GLN:OE1	2:G:3809:ASN:ND2	2.33	0.61
2:I:4567:LEU:HA	2:I:4816:ILE:HD12	1.83	0.61
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.33	0.60
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.33	0.60
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.34	0.60
2:E:4567:LEU:HA	2:E:4816:ILE:HD12	1.83	0.60
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.66	0.60
2:I:645:ARG:HH11	2:I:778:PHE:HE1	1.49	0.60
2:G:4567:LEU:HA	2:G:4816:ILE:HD12	1.83	0.60
2:B:41:GLY:O	2:B:45:ARG:NH1	2.35	0.60
2:B:1148:VAL:HG21	2:B:1212:ARG:HG2	1.84	0.59
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.66	0.59
2:I:3767:GLN:OE1	2:I:3809:ASN:ND2	2.33	0.59
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.85	0.59
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.66	0.59
2:B:4567:LEU:HA	2:B:4816:ILE:HD12	1.83	0.59
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.85	0.59
2:B:645:ARG:HH11	2:B:778:PHE:HE1	1.49	0.59
2:G:1148:VAL:HG21	2:G:1212:ARG:HG2	1.84	0.59
2:I:41:GLY:O	2:I:45:ARG:NH1	2.35	0.59
2:B:2764:GLU:HG3	2:B:2857:PRO:HB2	1.84	0.59
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.85	0.59
2:I:2764:GLU:HG3	2:I:2857:PRO:HB2	1.84	0.59
2:E:41:GLY:O	2:E:45:ARG:NH1	2.35	0.59
2:E:2764:GLU:HG3	2:E:2857:PRO:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.85	0.59
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.67	0.59
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.66	0.59
2:E:1148:VAL:HG21	2:E:1212:ARG:HG2	1.84	0.58
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.67	0.58
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.85	0.58
2:E:645:ARG:HH11	2:E:778:PHE:HE1	1.49	0.58
2:G:41:GLY:O	2:G:45:ARG:NH1	2.35	0.58
2:I:1148:VAL:HG21	2:I:1212:ARG:HG2	1.84	0.58
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.35	0.58
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.36	0.58
2:G:2764:GLU:HG3	2:G:2857:PRO:HB2	1.84	0.58
2:G:645:ARG:HH11	2:G:778:PHE:HE1	1.49	0.58
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.85	0.58
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.67	0.58
2:B:2758:PHE:O	2:B:2762:THR:N	2.36	0.58
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.86	0.58
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.85	0.58
2:E:359:TYR:HA	2:E:376:ALA:HA	1.85	0.58
2:I:359:TYR:HA	2:I:376:ALA:HA	1.85	0.58
2:B:359:TYR:HA	2:B:376:ALA:HA	1.85	0.58
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.67	0.58
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.85	0.58
2:G:359:TYR:HA	2:G:376:ALA:HA	1.85	0.57
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.85	0.57
2:I:2758:PHE:O	2:I:2762:THR:N	2.36	0.57
2:B:3809:ASN:HB3	2:B:3812:VAL:HG22	1.86	0.57
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.37	0.57
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.86	0.57
2:B:1703:LEU:HD12	2:B:1708:ARG:HB2	1.87	0.57
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.37	0.57
2:G:1244:GLN:OE1	2:G:1646:ARG:NH1	2.38	0.57
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.85	0.57
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.86	0.57
2:E:1244:GLN:OE1	2:E:1646:ARG:NH1	2.38	0.57
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.85	0.57
2:G:1703:LEU:HD12	2:G:1708:ARG:HB2	1.87	0.57
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.35	0.57
2:B:4933:GLN:OE1	2:E:4933:GLN:NE2	2.37	0.57
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.85	0.57
2:I:4933:GLN:NE2	2:G:4933:GLN:OE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.38	0.57
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.78	0.57
2:B:4914:VAL:HG21	2:E:4884:LEU:HD11	1.87	0.57
2:I:1244:GLN:OE1	2:I:1646:ARG:NH1	2.38	0.57
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.78	0.57
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.86	0.57
2:I:1703:LEU:HD12	2:I:1708:ARG:HB2	1.87	0.57
2:I:627:PRO:O	2:I:629:ARG:NH1	2.38	0.57
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.37	0.56
2:G:2758:PHE:O	2:G:2762:THR:N	2.36	0.56
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.38	0.56
2:G:627:PRO:O	2:G:629:ARG:NH1	2.38	0.56
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.38	0.56
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.85	0.56
2:E:627:PRO:O	2:E:629:ARG:NH1	2.38	0.56
2:G:3809:ASN:HB3	2:G:3812:VAL:HG22	1.86	0.56
2:I:3809:ASN:HB3	2:I:3812:VAL:HG22	1.86	0.56
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.87	0.56
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.38	0.56
2:E:23:GLN:OE1	2:E:203:ASN:ND2	2.38	0.56
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.38	0.56
2:G:23:GLN:OE1	2:G:203:ASN:ND2	2.38	0.56
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.86	0.56
2:B:132:ALA:HA	2:B:194:SER:HB2	1.87	0.56
2:B:4933:GLN:NE2	2:I:4933:GLN:OE1	2.38	0.56
2:E:1703:LEU:HD12	2:E:1708:ARG:HB2	1.87	0.56
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.37	0.56
2:E:132:ALA:HA	2:E:194:SER:HB2	1.88	0.56
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.86	0.56
2:E:3809:ASN:HB3	2:E:3812:VAL:HG22	1.86	0.56
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.88	0.56
2:E:4933:GLN:OE1	2:G:4933:GLN:NE2	2.37	0.56
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.86	0.56
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.88	0.56
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.86	0.56
2:B:1244:GLN:OE1	2:B:1646:ARG:NH1	2.38	0.56
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.87	0.56
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.38	0.56
2:I:793:LEU:HD12	2:I:797:HIS:H	1.71	0.56
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.38	0.56
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.38	0.56
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.88	0.56
2:B:627:PRO:O	2:B:629:ARG:NH1	2.38	0.56
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.88	0.56
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.35	0.55
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.88	0.55
2:I:609:CYS:SG	2:I:610:ASN:N	2.80	0.55
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.78	0.55
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.38	0.55
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.88	0.55
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.80	0.55
2:E:331:VAL:HG12	2:E:333:GLY:H	1.72	0.55
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.87	0.55
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.88	0.55
2:I:23:GLN:OE1	2:I:203:ASN:ND2	2.38	0.55
2:B:4581:LYS:HD2	2:B:4632:LEU:HD22	1.89	0.55
2:G:609:CYS:SG	2:G:610:ASN:N	2.79	0.55
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.38	0.55
2:B:609:CYS:SG	2:B:610:ASN:N	2.79	0.55
2:E:2758:PHE:O	2:E:2762:THR:N	2.36	0.55
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.80	0.55
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.80	0.55
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.87	0.55
2:E:4914:VAL:HG21	2:G:4884:LEU:HD11	1.89	0.55
2:G:793:LEU:HD12	2:G:797:HIS:H	1.71	0.55
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.80	0.55
2:G:331:VAL:HG12	2:G:333:GLY:H	1.72	0.55
2:I:132:ALA:HA	2:I:194:SER:HB2	1.88	0.55
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.88	0.55
2:B:4079:ASP:OD2	2:I:4736:ARG:NH1	2.40	0.55
2:I:4171:LEU:O	2:I:4175:ARG:NH2	2.41	0.54
2:E:609:CYS:SG	2:E:610:ASN:N	2.79	0.54
2:G:132:ALA:HA	2:G:194:SER:HB2	1.88	0.54
2:G:4171:LEU:O	2:G:4175:ARG:NH2	2.41	0.54
2:I:4884:LEU:HD11	2:G:4914:VAL:HG21	1.88	0.54
2:I:4581:LYS:HD2	2:I:4632:LEU:HD22	1.89	0.54
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	1.90	0.54
2:B:793:LEU:HD12	2:B:797:HIS:H	1.71	0.54
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.78	0.54
2:B:331:VAL:HG12	2:B:333:GLY:H	1.72	0.54
2:I:331:VAL:HG12	2:I:333:GLY:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.38	0.54
2:B:4171:LEU:O	2:B:4175:ARG:NH2	2.41	0.54
2:E:793:LEU:HD12	2:E:797:HIS:H	1.71	0.54
2:I:4198:SER:OG	2:I:4199:GLU:N	2.41	0.54
2:B:2347:GLU:O	2:B:2351:ASN:N	2.41	0.54
2:B:4198:SER:OG	2:B:4199:GLU:N	2.41	0.53
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	1.90	0.53
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	1.90	0.53
2:G:2347:GLU:O	2:G:2351:ASN:N	2.41	0.53
2:I:2347:GLU:O	2:I:2351:ASN:N	2.41	0.53
2:B:4884:LEU:HD11	2:I:4914:VAL:HG21	1.90	0.53
2:G:4581:LYS:HD2	2:G:4632:LEU:HD22	1.89	0.53
2:B:4736:ARG:NH1	2:E:4079:ASP:OD2	2.41	0.53
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.90	0.53
2:I:1663:HIS:HD2	2:I:1707:LEU:HD11	1.73	0.53
2:E:4171:LEU:O	2:E:4175:ARG:NH2	2.41	0.53
2:E:4581:LYS:HD2	2:E:4632:LEU:HD22	1.89	0.53
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.91	0.53
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	1.90	0.53
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.90	0.53
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.42	0.53
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.34	0.53
2:E:2347:GLU:O	2:E:2351:ASN:N	2.41	0.53
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.38	0.53
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.42	0.53
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.42	0.53
2:I:606:LEU:O	2:I:617:ASN:ND2	2.42	0.53
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.90	0.52
2:B:1663:HIS:HD2	2:B:1707:LEU:HD11	1.74	0.52
2:E:606:LEU:O	2:E:617:ASN:ND2	2.42	0.52
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.42	0.52
2:I:4956:THR:O	2:I:4965:SER:N	2.43	0.52
2:B:156:GLN:HE22	2:E:225:GLY:HA2	1.75	0.52
2:E:4198:SER:OG	2:E:4199:GLU:N	2.41	0.52
2:G:4198:SER:OG	2:G:4199:GLU:N	2.41	0.52
2:I:1973:GLN:O	2:I:1977:TYR:N	2.43	0.52
2:G:606:LEU:O	2:G:617:ASN:ND2	2.42	0.52
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.43	0.52
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.90	0.52
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.91	0.52
2:G:1663:HIS:HD2	2:G:1707:LEU:HD11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1131:ARG:HH12	2:G:1178:ALA:HB3	1.75	0.52
2:B:4956:THR:O	2:B:4965:SER:N	2.43	0.52
2:E:1131:ARG:HH12	2:E:1178:ALA:HB3	1.75	0.52
2:B:606:LEU:O	2:B:617:ASN:ND2	2.42	0.52
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.43	0.52
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.92	0.52
2:I:225:GLY:HA2	2:G:156:GLN:HE22	1.74	0.52
2:G:1973:GLN:O	2:G:1977:TYR:N	2.43	0.52
2:G:4956:THR:O	2:G:4965:SER:N	2.43	0.52
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.91	0.51
2:G:2815:ALA:HB3	2:G:2881:ASN:HD21	1.75	0.51
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.91	0.51
2:B:1131:ARG:HH12	2:B:1178:ALA:HB3	1.75	0.51
2:I:1738:LEU:HB3	2:I:2146:PRO:HD3	1.93	0.51
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.34	0.51
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.91	0.51
2:E:1663:HIS:HD2	2:E:1707:LEU:HD11	1.74	0.51
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.43	0.51
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.91	0.51
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.93	0.51
2:B:225:GLY:HA2	2:I:156:GLN:HE22	1.74	0.51
2:E:1738:LEU:HB3	2:E:2146:PRO:HD3	1.93	0.51
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.92	0.51
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.91	0.51
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.91	0.51
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.92	0.51
2:B:1973:GLN:O	2:B:1977:TYR:N	2.43	0.51
2:B:2290:LEU:HG	2:B:2291:GLN:H	1.76	0.51
2:B:2131:LEU:HB3	2:B:3662:ILE:HD13	1.93	0.51
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.93	0.51
2:E:1973:GLN:O	2:E:1977:TYR:N	2.43	0.51
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.92	0.51
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.91	0.51
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.93	0.51
2:G:1738:LEU:HB3	2:G:2146:PRO:HD3	1.92	0.51
2:E:156:GLN:HE22	2:G:225:GLY:HA2	1.76	0.51
2:I:2131:LEU:HB3	2:I:3662:ILE:HD13	1.93	0.51
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.46	0.51
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.43	0.51
2:E:2290:LEU:HG	2:E:2291:GLN:H	1.76	0.51
2:G:1729:SER:HB3	2:G:2163:ARG:HH11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.91	0.50
2:E:4956:THR:O	2:E:4965:SER:N	2.43	0.50
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.93	0.50
2:B:1738:LEU:HB3	2:B:2146:PRO:HD3	1.92	0.50
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.91	0.50
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.44	0.50
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.45	0.50
2:B:2815:ALA:HB3	2:B:2881:ASN:HD21	1.75	0.50
2:G:1245:PHE:HD1	2:G:1600:LEU:HB3	1.76	0.50
2:I:1729:SER:HB3	2:I:2163:ARG:HH11	1.76	0.50
2:I:4079:ASP:OD2	2:G:4736:ARG:NH1	2.41	0.50
2:E:235:ALA:HA	2:E:257:ARG:HD3	1.93	0.50
2:I:1131:ARG:HH12	2:I:1178:ALA:HB3	1.75	0.50
2:I:2236:LEU:HD23	2:I:2275:VAL:HG21	1.94	0.50
2:I:2290:LEU:HG	2:I:2291:GLN:H	1.76	0.50
2:B:4848:VAL:O	2:B:4852:THR:OG1	2.28	0.50
2:E:2236:LEU:HD23	2:E:2275:VAL:HG21	1.94	0.50
2:E:2815:ALA:HB3	2:E:2881:ASN:HD21	1.76	0.50
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.94	0.50
2:G:2131:LEU:HB3	2:G:3662:ILE:HD13	1.93	0.50
2:G:2236:LEU:HD23	2:G:2275:VAL:HG21	1.94	0.50
2:B:2236:LEU:HD23	2:B:2275:VAL:HG21	1.94	0.50
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.93	0.50
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.94	0.50
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.92	0.50
2:B:1729:SER:HB3	2:B:2163:ARG:HH11	1.76	0.50
2:B:235:ALA:HA	2:B:257:ARG:HD3	1.93	0.50
2:I:1245:PHE:HD1	2:I:1600:LEU:HB3	1.76	0.50
2:I:235:ALA:HA	2:I:257:ARG:HD3	1.93	0.50
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.46	0.50
2:B:1245:PHE:HD1	2:B:1600:LEU:HB3	1.76	0.50
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.46	0.50
2:E:2131:LEU:HB3	2:E:3662:ILE:HD13	1.93	0.50
2:G:1675:ALA:HB1	2:G:1676:LEU:HD13	1.94	0.50
2:I:1730:MET:O	2:I:1772:ARG:NH1	2.45	0.50
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.94	0.49
2:E:1675:ALA:HB1	2:E:1676:LEU:HD13	1.94	0.49
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.45	0.49
2:G:4092:ASP:OD1	2:G:4092:ASP:N	2.45	0.49
2:I:1840:PRO:O	2:I:1844:LEU:N	2.45	0.49
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1840:PRO:O	2:G:1844:LEU:N	2.45	0.49
2:G:2290:LEU:HG	2:G:2291:GLN:H	1.76	0.49
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.45	0.49
2:B:1840:PRO:O	2:B:1844:LEU:N	2.45	0.49
2:E:1245:PHE:HD1	2:E:1600:LEU:HB3	1.76	0.49
2:E:1729:SER:HB3	2:E:2163:ARG:HH11	1.76	0.49
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.46	0.49
2:I:2815:ALA:HB3	2:I:2881:ASN:HD21	1.75	0.49
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.31	0.49
2:I:3889:GLN:HG3	2:I:3967:GLU:HG3	1.95	0.49
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.45	0.49
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.45	0.49
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.31	0.49
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.95	0.49
2:B:4092:ASP:OD1	2:B:4092:ASP:N	2.45	0.49
2:E:1730:MET:O	2:E:1772:ARG:NH1	2.45	0.49
2:I:2868:SER:O	2:I:2872:GLN:N	2.46	0.49
2:E:580:GLU:HG3	2:E:620:LEU:HD22	1.94	0.49
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.95	0.49
2:G:1730:MET:O	2:G:1772:ARG:NH1	2.45	0.49
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.45	0.49
2:I:1096:THR:HG23	2:I:1199:VAL:HG22	1.95	0.49
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.95	0.49
2:B:1096:THR:HG23	2:B:1199:VAL:HG22	1.95	0.49
2:B:1730:MET:O	2:B:1772:ARG:NH1	2.45	0.49
2:E:2159:LEU:HD22	2:E:2201:LEU:HD23	1.94	0.49
2:G:221:ARG:NH2	2:G:397:GLU:OE2	2.45	0.49
2:G:580:GLU:HG3	2:G:620:LEU:HD22	1.94	0.49
2:I:580:GLU:HG3	2:I:620:LEU:HD22	1.94	0.49
2:E:2823:ILE:HG12	2:E:2937:VAL:HG22	1.95	0.49
2:G:3889:GLN:HG3	2:G:3967:GLU:HG3	1.95	0.49
2:I:1675:ALA:HB1	2:I:1676:LEU:HD13	1.94	0.49
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.45	0.49
2:I:2823:ILE:HG12	2:I:2937:VAL:HG22	1.95	0.49
2:I:4634:GLU:HG3	2:I:4636:THR:H	1.77	0.49
2:B:1675:ALA:HB1	2:B:1676:LEU:HD13	1.94	0.48
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.95	0.48
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.95	0.48
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.95	0.48
2:E:3889:GLN:HG3	2:E:3967:GLU:HG3	1.95	0.48
2:G:1096:THR:HG23	2:G:1199:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:11:ASP:OD1	1:H:67:SER:OG	2.31	0.48
2:B:4634:GLU:HG3	2:B:4636:THR:H	1.77	0.48
2:G:235:ALA:HA	2:G:257:ARG:HD3	1.93	0.48
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.31	0.48
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.95	0.48
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.78	0.48
2:E:1096:THR:HG23	2:E:1199:VAL:HG22	1.95	0.48
2:E:1840:PRO:O	2:E:1844:LEU:N	2.45	0.48
2:G:4634:GLU:HG3	2:G:4636:THR:H	1.77	0.48
2:B:2823:ILE:HG12	2:B:2937:VAL:HG22	1.95	0.48
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.31	0.48
2:E:4634:GLU:HG3	2:E:4636:THR:H	1.77	0.48
2:G:2823:ILE:HG12	2:G:2937:VAL:HG22	1.95	0.48
2:I:2159:LEU:HD22	2:I:2201:LEU:HD23	1.94	0.48
2:E:940:GLY:O	2:E:1052:ASN:N	2.47	0.48
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	1.96	0.48
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	1.96	0.48
2:B:2159:LEU:HD22	2:B:2201:LEU:HD23	1.94	0.48
2:B:3889:GLN:HG3	2:B:3967:GLU:HG3	1.95	0.48
2:B:2342:ASN:N	2:B:2342:ASN:OD1	2.34	0.48
2:E:645:ARG:O	2:E:824:GLU:N	2.47	0.48
2:I:940:GLY:O	2:I:1052:ASN:N	2.47	0.48
2:B:940:GLY:O	2:B:1052:ASN:N	2.47	0.48
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	1.96	0.48
2:G:2159:LEU:HD22	2:G:2201:LEU:HD23	1.94	0.48
2:E:2868:SER:O	2:E:2872:GLN:N	2.46	0.48
2:G:2868:SER:O	2:G:2872:GLN:N	2.46	0.48
2:G:3552:UNK:O	2:G:3556:UNK:N	2.47	0.48
2:G:689:THR:H	2:G:778:PHE:HE2	1.62	0.48
2:B:645:ARG:O	2:B:824:GLU:N	2.47	0.47
2:B:734:GLY:O	2:B:736:HIS:ND1	2.47	0.47
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.96	0.47
2:I:4092:ASP:OD1	2:I:4092:ASP:N	2.45	0.47
2:I:4629:TYR:OH	2:G:4860:ARG:NH2	2.42	0.47
2:E:4092:ASP:N	2:E:4092:ASP:OD1	2.45	0.47
2:I:3552:UNK:O	2:I:3556:UNK:N	2.47	0.47
2:B:221:ARG:NH2	2:B:397:GLU:OE2	2.45	0.47
2:B:689:THR:H	2:B:778:PHE:HE2	1.61	0.47
2:G:940:GLY:O	2:G:1052:ASN:N	2.47	0.47
2:G:265:LEU:HD12	2:G:279:PRO:HB2	1.97	0.47
2:B:2022:PRO:HB2	2:B:2024:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	1.96	0.47
2:E:4736:ARG:NH1	2:G:4079:ASP:OD2	2.42	0.47
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.78	0.47
2:B:219:VAL:O	2:B:392:ARG:NH1	2.48	0.47
2:E:265:LEU:HD12	2:E:279:PRO:HB2	1.96	0.47
2:I:219:VAL:O	2:I:392:ARG:NH1	2.48	0.47
2:I:534:ARG:NH2	2:I:573:GLU:OE2	2.42	0.47
2:B:580:GLU:HG3	2:B:620:LEU:HD22	1.94	0.47
2:E:1839:VAL:O	2:E:1841:VAL:N	2.48	0.47
2:I:4228:ALA:O	2:I:4232:GLU:N	2.48	0.47
2:B:2868:SER:O	2:B:2872:GLN:N	2.46	0.47
2:G:219:VAL:O	2:G:392:ARG:NH1	2.48	0.47
2:G:645:ARG:O	2:G:824:GLU:N	2.47	0.47
2:I:734:GLY:O	2:I:736:HIS:ND1	2.47	0.47
2:E:3552:UNK:O	2:E:3556:UNK:N	2.47	0.47
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.95	0.47
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.78	0.47
2:G:4978:HIS:ND1	2:G:4982:GLU:OE1	2.32	0.47
2:E:4978:HIS:ND1	2:E:4982:GLU:OE1	2.32	0.47
2:G:3770:LEU:HD12	2:G:3770:LEU:HA	1.74	0.47
2:G:4228:ALA:O	2:G:4232:GLU:N	2.48	0.47
2:I:1839:VAL:O	2:I:1841:VAL:N	2.48	0.47
2:B:111:HIS:CD2	2:B:114:SER:H	2.33	0.47
2:B:615:ARG:NH1	2:B:1677:GLY:O	2.39	0.47
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.97	0.47
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.80	0.47
2:E:2022:PRO:HB2	2:E:2024:PRO:HD2	1.96	0.47
2:E:4181:ILE:HG22	2:E:4193:ILE:HB	1.97	0.47
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.95	0.47
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.80	0.47
2:I:1792:ALA:HB2	2:I:2173:GLN:HG3	1.97	0.47
2:I:265:LEU:HD12	2:I:279:PRO:HB2	1.97	0.47
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.80	0.47
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.96	0.47
2:E:111:HIS:CD2	2:E:114:SER:H	2.33	0.47
2:G:111:HIS:CD2	2:G:114:SER:H	2.33	0.47
2:I:111:HIS:CD2	2:I:114:SER:H	2.33	0.47
2:I:2022:PRO:HB2	2:I:2024:PRO:HD2	1.96	0.47
2:I:221:ARG:NH2	2:I:397:GLU:OE2	2.45	0.47
2:I:689:THR:H	2:I:778:PHE:HE2	1.62	0.47
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1839:VAL:O	2:B:1841:VAL:N	2.48	0.46
2:E:1715:LEU:HD12	2:E:1719:HIS:HD2	1.80	0.46
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.78	0.46
2:G:1792:ALA:HB2	2:G:2173:GLN:HG3	1.97	0.46
2:B:3552:UNK:O	2:B:3556:UNK:N	2.48	0.46
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.80	0.46
2:G:1715:LEU:HD12	2:G:1719:HIS:HD2	1.80	0.46
2:G:734:GLY:O	2:G:736:HIS:ND1	2.47	0.46
2:B:265:LEU:HD12	2:B:279:PRO:HB2	1.96	0.46
2:B:4228:ALA:O	2:B:4232:GLU:N	2.48	0.46
2:E:689:THR:H	2:E:778:PHE:HE2	1.62	0.46
2:E:898:ASP:HB3	2:E:901:LYS:HB2	1.98	0.46
2:G:1839:VAL:O	2:G:1841:VAL:N	2.48	0.46
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	1.96	0.46
2:G:4181:ILE:HG22	2:G:4193:ILE:HB	1.97	0.46
2:G:898:ASP:HB3	2:G:901:LYS:HB2	1.98	0.46
2:I:645:ARG:O	2:I:824:GLU:N	2.47	0.46
2:B:396:GLU:OE2	2:B:451:TYR:OH	2.34	0.46
2:G:4848:VAL:O	2:G:4852:THR:OG1	2.28	0.46
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.97	0.46
2:B:1715:LEU:HD12	2:B:1719:HIS:HD2	1.80	0.46
2:G:534:ARG:NH2	2:G:573:GLU:OE2	2.42	0.46
2:G:617:ASN:OD1	2:G:617:ASN:N	2.49	0.46
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.40	0.46
2:I:2827:ARG:HH21	2:I:2931:GLN:HG3	1.81	0.46
2:G:2827:ARG:HH21	2:G:2931:GLN:HG3	1.81	0.46
2:I:898:ASP:HB3	2:I:901:LYS:HB2	1.98	0.46
2:B:2827:ARG:HH21	2:B:2931:GLN:HG3	1.81	0.46
2:B:898:ASP:HB3	2:B:901:LYS:HB2	1.98	0.46
2:E:219:VAL:O	2:E:392:ARG:NH1	2.48	0.46
2:G:2745:VAL:HG21	2:G:2818:ALA:HB2	1.98	0.46
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.96	0.46
2:I:1772:ARG:HH21	2:I:1952:GLN:NE2	2.14	0.46
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.97	0.46
2:I:396:GLU:OE2	2:I:451:TYR:OH	2.34	0.46
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.98	0.46
2:B:1772:ARG:HH21	2:B:1952:GLN:NE2	2.14	0.46
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.98	0.46
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.98	0.46
2:E:111:HIS:HD2	2:E:114:SER:H	1.64	0.46
2:E:2745:VAL:HG21	2:E:2818:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.98	0.46
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.97	0.46
2:I:1715:LEU:HD12	2:I:1719:HIS:HD2	1.80	0.46
2:I:4181:ILE:HG22	2:I:4193:ILE:HB	1.97	0.46
2:I:485:SER:HA	2:I:488:LEU:HB2	1.98	0.46
2:B:1792:ALA:HB2	2:B:2173:GLN:HG3	1.97	0.45
2:E:1772:ARG:HH21	2:E:1952:GLN:NE2	2.14	0.45
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.81	0.45
1:J:11:ASP:OD1	1:J:67:SER:OG	2.31	0.45
2:B:4181:ILE:HG22	2:B:4193:ILE:HB	1.97	0.45
2:B:4629:TYR:OH	2:I:4860:ARG:NH2	2.41	0.45
2:B:4860:ARG:NH2	2:E:4629:TYR:OH	2.40	0.45
2:E:4791:TYR:OH	2:E:4815:ASP:O	2.33	0.45
2:G:485:SER:HA	2:G:488:LEU:HB2	1.98	0.45
2:I:2029:GLN:O	2:I:2033:ASP:N	2.49	0.45
2:E:1099:GLU:OE2	2:E:1127:HIS:ND1	2.38	0.45
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.98	0.45
2:E:2827:ARG:HH21	2:E:2931:GLN:HG3	1.81	0.45
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.97	0.45
2:E:5027:CYS:O	2:E:5029:ARG:N	2.48	0.45
2:B:668:VAL:O	2:B:741:GLU:N	2.47	0.45
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.82	0.45
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.50	0.45
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.82	0.45
2:I:2024:PRO:O	2:I:2028:ARG:NE	2.40	0.45
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.40	0.45
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.81	0.45
2:E:1792:ALA:HB2	2:E:2173:GLN:HG3	1.97	0.45
2:E:485:SER:HA	2:E:488:LEU:HB2	1.98	0.45
2:G:596:ASN:HB3	2:G:599:VAL:HG22	1.99	0.45
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.82	0.45
2:I:596:ASN:HB3	2:I:599:VAL:HG22	1.99	0.45
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.50	0.45
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.98	0.45
2:E:221:ARG:NH2	2:E:397:GLU:OE2	2.45	0.45
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.98	0.45
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.82	0.45
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.98	0.45
2:B:596:ASN:HB3	2:B:599:VAL:HG22	1.99	0.45
2:E:4228:ALA:O	2:E:4232:GLU:N	2.48	0.45
2:E:396:GLU:OE2	2:E:451:TYR:OH	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:596:ASN:HB3	2:E:599:VAL:HG22	1.99	0.45
2:E:668:VAL:O	2:E:741:GLU:N	2.47	0.45
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.98	0.45
2:B:617:ASN:N	2:B:617:ASN:OD1	2.49	0.45
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	1.98	0.45
2:E:2747:ILE:HG12	2:E:2817:ILE:HD12	1.99	0.45
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.50	0.45
2:I:111:HIS:HD2	2:I:114:SER:H	1.64	0.45
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	1.98	0.45
2:B:485:SER:HA	2:B:488:LEU:HB2	1.98	0.45
2:B:534:ARG:NH2	2:B:573:GLU:OE2	2.42	0.45
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.81	0.45
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.25	0.45
1:A:11:ASP:OD1	1:A:67:SER:OG	2.31	0.44
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.50	0.44
2:B:2765:LYS:HA	2:B:2859:PRO:HG3	1.99	0.44
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.99	0.44
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.99	0.44
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.98	0.44
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.98	0.44
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.50	0.44
2:I:232:THR:OG1	2:I:233:ILE:N	2.50	0.44
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.98	0.44
2:B:1855:GLY:H	2:B:1858:ASP:HB2	1.83	0.44
2:E:615:ARG:NH1	2:E:1677:GLY:O	2.39	0.44
2:E:788:LYS:HG2	2:E:1629:GLN:HA	1.99	0.44
2:G:1855:GLY:H	2:G:1858:ASP:HB2	1.82	0.44
2:G:396:GLU:OE2	2:G:451:TYR:OH	2.34	0.44
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.99	0.44
2:G:788:LYS:HG2	2:G:1629:GLN:HA	1.99	0.44
2:I:1099:GLU:OE2	2:I:1127:HIS:ND1	2.38	0.44
2:B:2231:SER:HA	2:B:2234:ARG:HG2	2.00	0.44
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.99	0.44
2:G:2024:PRO:O	2:G:2028:ARG:NE	2.40	0.44
2:I:1855:GLY:H	2:I:1858:ASP:HB2	1.82	0.44
2:I:2231:SER:HA	2:I:2234:ARG:HG2	2.00	0.44
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	1.98	0.44
2:B:111:HIS:HD2	2:B:114:SER:H	1.64	0.44
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.99	0.44
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.81	0.44
2:B:2029:GLN:O	2:B:2033:ASP:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2745:VAL:HG21	2:B:2818:ALA:HB2	1.98	0.44
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.99	0.44
2:G:2342:ASN:N	2:G:2342:ASN:OD1	2.34	0.44
2:I:2188:ASN:OD1	2:I:2188:ASN:N	2.49	0.44
2:I:2745:VAL:HG21	2:I:2818:ALA:HB2	1.98	0.44
2:I:2747:ILE:HG12	2:I:2817:ILE:HD12	1.99	0.44
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.99	0.44
2:B:788:LYS:HG2	2:B:1629:GLN:HA	1.99	0.44
2:E:1855:GLY:H	2:E:1858:ASP:HB2	1.82	0.44
2:G:111:HIS:HD2	2:G:114:SER:H	1.64	0.44
2:G:4138:ASP:N	2:G:4138:ASP:OD1	2.51	0.44
2:I:4642:ALA:HA	2:I:4645:CYS:HB2	2.00	0.44
2:B:5027:CYS:O	2:B:5029:ARG:N	2.48	0.44
2:E:4642:ALA:HA	2:E:4645:CYS:HB2	2.00	0.44
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.50	0.44
2:G:2029:GLN:O	2:G:2033:ASP:N	2.49	0.44
2:G:43:GLY:HA2	2:G:443:LEU:HG	2.00	0.44
2:B:3770:LEU:HD12	2:B:3770:LEU:HA	1.74	0.44
2:E:2231:SER:HA	2:E:2234:ARG:HG2	2.00	0.44
2:E:617:ASN:N	2:E:617:ASN:OD1	2.49	0.44
2:G:2102:VAL:HB	2:G:2124:LEU:HD12	1.99	0.44
2:I:2765:LYS:HA	2:I:2859:PRO:HG3	1.99	0.44
2:E:2102:VAL:HB	2:E:2124:LEU:HD12	1.99	0.44
2:E:2765:LYS:HA	2:E:2859:PRO:HG3	1.98	0.44
2:G:1772:ARG:HH21	2:G:1952:GLN:NE2	2.14	0.44
2:G:2747:ILE:HG12	2:G:2817:ILE:HD12	1.99	0.44
2:G:4642:ALA:HA	2:G:4645:CYS:HB2	2.00	0.44
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	2.00	0.44
2:B:134:ASP:OD1	2:B:134:ASP:N	2.51	0.44
2:B:2747:ILE:HG12	2:B:2817:ILE:HD12	1.99	0.44
2:B:3365:UNK:O	2:B:3369:UNK:N	2.51	0.44
2:E:134:ASP:N	2:E:134:ASP:OD1	2.51	0.44
2:E:4138:ASP:N	2:E:4138:ASP:OD1	2.51	0.44
1:F:11:ASP:OD1	1:F:67:SER:OG	2.31	0.44
2:G:232:THR:OG1	2:G:233:ILE:N	2.50	0.44
2:G:4815:ASP:N	2:G:4815:ASP:OD1	2.50	0.44
2:I:615:ARG:NH1	2:I:1677:GLY:O	2.39	0.44
2:I:2739:PRO:HD2	2:I:2888:ARG:HH21	1.83	0.44
2:I:788:LYS:HG2	2:I:1629:GLN:HA	1.99	0.44
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.50	0.44
2:B:4642:ALA:HA	2:B:4645:CYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	2.00	0.43
2:E:43:GLY:HA2	2:E:443:LEU:HG	2.00	0.43
2:G:2231:SER:HA	2:G:2234:ARG:HG2	2.00	0.43
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.98	0.43
2:B:2447:LYS:HG3	2:B:2449:GLU:H	1.83	0.43
2:B:2739:PRO:HD2	2:B:2888:ARG:HH21	1.83	0.43
2:E:2447:LYS:HG3	2:E:2449:GLU:H	1.83	0.43
2:E:4063:ASP:OD1	2:E:4169:SER:OG	2.28	0.43
2:G:206:CYS:SG	2:G:207:SER:N	2.92	0.43
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	1.98	0.43
2:G:668:VAL:O	2:G:741:GLU:N	2.47	0.43
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	2.00	0.43
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	2.00	0.43
2:G:1707:LEU:O	2:G:1709:ALA:N	2.51	0.43
2:I:4138:ASP:N	2:I:4138:ASP:OD1	2.51	0.43
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	2.00	0.43
2:E:4681:LEU:HD21	2:E:4687:TYR:HD2	1.84	0.43
2:E:734:GLY:O	2:E:736:HIS:ND1	2.47	0.43
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.99	0.43
2:I:206:CYS:SG	2:I:207:SER:N	2.92	0.43
2:B:1707:LEU:O	2:B:1709:ALA:N	2.51	0.43
2:E:206:CYS:SG	2:E:207:SER:N	2.92	0.43
2:G:2188:ASN:OD1	2:G:2188:ASN:N	2.49	0.43
2:G:2765:LYS:HA	2:G:2859:PRO:HG3	1.98	0.43
2:B:206:CYS:SG	2:B:207:SER:N	2.92	0.43
2:B:2102:VAL:HB	2:B:2124:LEU:HD12	1.99	0.43
1:A:92:PRO:HD3	2:B:627:PRO:HB2	2.00	0.43
2:E:1707:LEU:O	2:E:1709:ALA:N	2.51	0.43
2:E:2739:PRO:HD2	2:E:2888:ARG:HH21	1.83	0.43
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.52	0.43
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	2.00	0.43
2:I:2447:LYS:HG3	2:I:2449:GLU:H	1.83	0.43
2:I:43:GLY:HA2	2:I:443:LEU:HG	2.00	0.43
2:B:43:GLY:HA2	2:B:443:LEU:HG	2.00	0.43
2:E:635:THR:HG23	2:E:1693:GLN:HE22	1.84	0.43
2:E:2188:ASN:OD1	2:E:2188:ASN:N	2.49	0.43
2:E:232:THR:OG1	2:E:233:ILE:N	2.51	0.43
2:G:5027:CYS:O	2:G:5029:ARG:N	2.48	0.43
2:G:635:THR:HG23	2:G:1693:GLN:HE22	1.84	0.43
2:I:4681:LEU:HD21	2:I:4687:TYR:HD2	1.84	0.43
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4142:ASN:HA	2:E:4145:VAL:HG12	2.01	0.43
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	2.00	0.43
2:G:134:ASP:OD1	2:G:134:ASP:N	2.51	0.43
2:G:3905:THR:HA	2:G:3912:THR:HG23	2.01	0.43
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.84	0.43
2:I:2102:VAL:HB	2:I:2124:LEU:HD12	1.99	0.43
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.54	0.43
2:B:232:THR:OG1	2:B:233:ILE:N	2.50	0.43
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	2.00	0.43
2:G:2447:LYS:HG3	2:G:2449:GLU:H	1.83	0.43
2:I:710:ASP:OD1	2:I:710:ASP:N	2.52	0.43
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.25	0.43
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.84	0.43
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.50	0.43
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	2.00	0.43
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.54	0.43
2:G:4791:TYR:OH	2:G:4815:ASP:O	2.33	0.43
2:I:4063:ASP:OD1	2:I:4169:SER:OG	2.28	0.43
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.54	0.42
2:B:710:ASP:N	2:B:710:ASP:OD1	2.52	0.42
2:G:2739:PRO:HD2	2:G:2888:ARG:HH21	1.83	0.42
2:G:4063:ASP:OD1	2:G:4169:SER:OG	2.28	0.42
2:I:3804:ILE:HG22	2:I:3812:VAL:HG21	2.01	0.42
2:B:2188:ASN:N	2:B:2188:ASN:OD1	2.49	0.42
2:B:4063:ASP:OD1	2:B:4169:SER:OG	2.28	0.42
2:G:315:CYS:SG	2:G:316:PHE:N	2.92	0.42
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	2.01	0.42
2:E:2788:HIS:HE1	2:E:2790:MET:HB2	1.84	0.42
2:E:534:ARG:NH2	2:E:573:GLU:OE2	2.43	0.42
2:G:2827:ARG:H	2:G:2934:GLY:HA3	1.85	0.42
2:G:3365:UNK:O	2:G:3369:UNK:N	2.52	0.42
2:I:1707:LEU:O	2:I:1709:ALA:N	2.51	0.42
2:I:2788:HIS:HE1	2:I:2790:MET:HB2	1.84	0.42
2:I:2827:ARG:H	2:I:2934:GLY:HA3	1.85	0.42
2:I:315:CYS:SG	2:I:316:PHE:N	2.92	0.42
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.40	0.42
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.52	0.42
2:E:2029:GLN:O	2:E:2033:ASP:N	2.49	0.42
2:E:2339:VAL:HG12	2:E:2345:SER:H	1.85	0.42
2:E:3365:UNK:O	2:E:3369:UNK:N	2.52	0.42
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1840:PRO:HB3	2:I:1843:LYS:HB3	2.02	0.42
2:I:3365:UNK:O	2:I:3369:UNK:N	2.52	0.42
2:I:3905:THR:HA	2:I:3912:THR:HG23	2.01	0.42
2:I:4142:ASN:HA	2:I:4145:VAL:HG12	2.01	0.42
2:I:4815:ASP:N	2:I:4815:ASP:OD1	2.50	0.42
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	2.00	0.42
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.94	0.42
2:B:1840:PRO:HB3	2:B:1843:LYS:HB3	2.02	0.42
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.49	0.42
2:B:2788:HIS:HE1	2:B:2790:MET:HB2	1.84	0.42
2:B:2827:ARG:H	2:B:2934:GLY:HA3	1.85	0.42
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.49	0.42
2:G:3804:ILE:HG22	2:G:3812:VAL:HG21	2.01	0.42
2:G:4922:PHE:HA	2:G:4926:VAL:HG12	2.01	0.42
2:I:2215:LEU:HD21	2:I:2272:PRO:HG3	2.02	0.42
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	2.01	0.42
2:B:4142:ASN:HA	2:B:4145:VAL:HG12	2.01	0.42
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.52	0.42
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.52	0.42
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.52	0.42
2:G:4142:ASN:HA	2:G:4145:VAL:HG12	2.01	0.42
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	2.01	0.42
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.52	0.42
2:I:4922:PHE:HA	2:I:4926:VAL:HG12	2.01	0.42
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	2.00	0.42
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	2.01	0.42
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	2.00	0.42
2:B:635:THR:HG23	2:B:1693:GLN:HE22	1.84	0.42
2:E:2827:ARG:H	2:E:2934:GLY:HA3	1.85	0.42
2:E:315:CYS:SG	2:E:316:PHE:N	2.92	0.42
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	2.01	0.42
2:E:710:ASP:N	2:E:710:ASP:OD1	2.52	0.42
2:G:1099:GLU:OE2	2:G:1127:HIS:ND1	2.38	0.42
2:G:2788:HIS:CE1	2:G:2790:MET:HB2	2.55	0.42
2:G:2788:HIS:HE1	2:G:2790:MET:HB2	1.85	0.42
2:G:282:ILE:HD12	2:G:314:PHE:HD2	1.85	0.42
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	2.01	0.42
2:B:3905:THR:HA	2:B:3912:THR:HG23	2.01	0.42
2:B:4922:PHE:HA	2:B:4926:VAL:HG12	2.01	0.42
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	2.01	0.42
2:E:2788:HIS:CE1	2:E:2790:MET:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	2.00	0.42
2:I:635:THR:HG23	2:I:1693:GLN:HE22	1.84	0.42
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.54	0.42
2:I:2788:HIS:CE1	2:I:2790:MET:HB2	2.55	0.42
2:I:886:ARG:HB3	2:I:891:TRP:HB2	2.02	0.42
2:B:2215:LEU:HD21	2:B:2272:PRO:HG3	2.02	0.42
2:B:282:ILE:HD12	2:B:314:PHE:HD2	1.85	0.42
2:B:3891:LEU:HB3	2:B:3899:PHE:CE2	2.55	0.42
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.54	0.42
2:G:3891:LEU:HB3	2:G:3899:PHE:CE2	2.55	0.42
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.54	0.42
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.52	0.42
2:I:5027:CYS:O	2:I:5029:ARG:N	2.48	0.42
2:B:642:THR:HG23	2:B:1613:LEU:HD12	2.02	0.42
2:B:2339:VAL:HG12	2:B:2345:SER:H	1.85	0.42
2:B:599:VAL:HG23	2:B:600:LEU:HD12	2.02	0.42
2:E:2290:LEU:HD21	2:E:2349:ASN:HA	2.01	0.42
2:E:3891:LEU:HB3	2:E:3899:PHE:CE2	2.55	0.42
1:H:54:GLU:O	2:G:1785:ALA:N	2.53	0.42
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	2.01	0.42
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.52	0.42
2:G:886:ARG:HB3	2:G:891:TRP:HB2	2.02	0.42
2:B:1727:ARG:HH12	2:B:1772:ARG:HB3	1.85	0.41
2:B:2290:LEU:HD21	2:B:2349:ASN:HA	2.01	0.41
2:B:2346:VAL:O	2:B:2349:ASN:ND2	2.53	0.41
2:E:282:ILE:HD12	2:E:314:PHE:HD2	1.85	0.41
2:E:864:PRO:HA	2:E:865:PRO:HD3	1.89	0.41
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.54	0.41
2:G:2215:LEU:HD21	2:G:2272:PRO:HG3	2.02	0.41
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.49	0.41
2:I:2290:LEU:HD21	2:I:2349:ASN:HA	2.01	0.41
2:B:1099:GLU:OE2	2:B:1127:HIS:ND1	2.38	0.41
2:E:1245:PHE:CD1	2:E:1600:LEU:HB3	2.54	0.41
2:E:395:GLN:HG3	2:E:397:GLU:H	1.85	0.41
2:E:474:ARG:HD2	2:E:474:ARG:HH11	1.75	0.41
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	2.02	0.41
2:I:282:ILE:HD12	2:I:314:PHE:HD2	1.85	0.41
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.85	0.41
2:B:2788:HIS:CE1	2:B:2790:MET:HB2	2.54	0.41
2:E:2215:LEU:HD21	2:E:2272:PRO:HG3	2.02	0.41
2:E:2346:VAL:O	2:E:2349:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1141:ARG:HD2	2:G:1141:ARG:H	1.86	0.41
2:G:3844:LEU:HD23	2:G:3844:LEU:HA	1.88	0.41
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	2.02	0.41
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.86	0.41
2:I:1245:PHE:CD1	2:I:1600:LEU:HB3	2.54	0.41
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.25	0.41
2:I:3844:LEU:HA	2:I:3844:LEU:HD23	1.88	0.41
2:B:3804:ILE:HG22	2:B:3812:VAL:HG21	2.01	0.41
2:B:4152:GLU:OE2	2:B:4180:ARG:NH1	2.50	0.41
2:G:1840:PRO:HB3	2:G:1843:LYS:HB3	2.02	0.41
2:G:2290:LEU:HD21	2:G:2349:ASN:HA	2.01	0.41
2:G:426:ARG:HB2	2:G:506:TYR:HA	2.03	0.41
2:G:599:VAL:HG23	2:G:600:LEU:HD12	2.02	0.41
2:I:1727:ARG:HH12	2:I:1772:ARG:HB3	1.85	0.41
2:I:2339:VAL:HG12	2:I:2345:SER:H	1.85	0.41
2:B:315:CYS:SG	2:B:316:PHE:N	2.92	0.41
2:B:3842:LEU:O	2:B:3929:SER:OG	2.39	0.41
2:E:1727:ARG:HH12	2:E:1772:ARG:HB3	1.85	0.41
2:I:642:THR:HG23	2:I:1613:LEU:HD12	2.02	0.41
2:I:426:ARG:HB2	2:I:506:TYR:HA	2.03	0.41
2:B:3844:LEU:HA	2:B:3844:LEU:HD23	1.88	0.41
2:E:3804:ILE:HG22	2:E:3812:VAL:HG21	2.01	0.41
2:E:3905:THR:HA	2:E:3912:THR:HG23	2.01	0.41
2:E:4922:PHE:HA	2:E:4926:VAL:HG12	2.01	0.41
2:G:395:GLN:HG3	2:G:397:GLU:H	1.85	0.41
2:G:4232:GLU:OE1	2:G:5019:TRP:NE1	2.53	0.41
2:I:3891:LEU:HB3	2:I:3899:PHE:CE2	2.55	0.41
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	2.01	0.41
2:E:3658:LYS:HA	2:E:3661:TRP:CE2	2.56	0.41
2:E:3842:LEU:O	2:E:3929:SER:OG	2.39	0.41
2:G:1727:ARG:HH12	2:G:1772:ARG:HB3	1.85	0.41
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.85	0.41
2:G:2346:VAL:O	2:G:2349:ASN:ND2	2.53	0.41
2:G:642:THR:HG23	2:G:1613:LEU:HD12	2.02	0.41
2:G:647:ASN:N	2:G:647:ASN:OD1	2.53	0.41
2:I:2346:VAL:O	2:I:2349:ASN:ND2	2.53	0.41
2:I:3658:LYS:HA	2:I:3661:TRP:CE2	2.56	0.41
2:B:214:VAL:HG12	2:B:274:LEU:HD12	2.03	0.41
2:B:772:ASN:OD1	2:B:772:ASN:N	2.54	0.41
2:E:214:VAL:HG22	2:E:341:TYR:CE1	2.56	0.41
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:214:VAL:HG12	2:E:274:LEU:HD12	2.03	0.41
2:E:4570:ALA:HA	2:E:4573:ILE:HG22	2.03	0.41
2:G:1245:PHE:CD1	2:G:1600:LEU:HB3	2.54	0.41
2:G:955:LEU:O	2:G:966:LYS:NZ	2.43	0.41
2:I:404:ILE:HG21	2:I:481:GLU:HG3	2.03	0.41
2:B:1245:PHE:CD1	2:B:1600:LEU:HB3	2.54	0.41
2:B:214:VAL:HG22	2:B:341:TYR:CE1	2.56	0.41
2:B:404:ILE:HG21	2:B:481:GLU:HG3	2.03	0.41
2:B:886:ARG:HB3	2:B:891:TRP:HB2	2.02	0.41
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.25	0.41
2:E:4247:ILE:HA	2:E:4247:ILE:HD12	1.98	0.41
2:I:134:ASP:OD1	2:I:134:ASP:N	2.51	0.41
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.86	0.41
2:I:865:PRO:HA	2:I:868:GLU:HB2	2.03	0.41
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.86	0.41
2:B:1725:ARG:HD2	2:B:1725:ARG:HH21	1.72	0.41
2:B:4138:ASP:OD1	2:B:4138:ASP:N	2.51	0.41
2:E:1141:ARG:HD2	2:E:1141:ARG:H	1.86	0.41
2:G:2339:VAL:HG12	2:G:2345:SER:H	1.85	0.41
2:G:710:ASP:OD1	2:G:710:ASP:N	2.52	0.41
2:G:865:PRO:HA	2:G:868:GLU:HB2	2.03	0.41
2:I:214:VAL:HG22	2:I:341:TYR:CE1	2.56	0.41
2:B:426:ARG:HB2	2:B:506:TYR:HA	2.03	0.41
2:B:4570:ALA:HA	2:B:4573:ILE:HG22	2.03	0.41
2:E:1840:PRO:HB3	2:E:1843:LYS:HB3	2.02	0.41
2:E:1972:ASN:HD21	2:E:2024:PRO:HB3	1.86	0.41
2:E:4865:LYS:HD2	2:E:4865:LYS:HA	1.90	0.41
2:E:599:VAL:HG23	2:E:600:LEU:HD12	2.02	0.41
2:I:2095:GLN:NE2	2:I:2127:GLN:O	2.54	0.41
2:I:395:GLN:HG3	2:I:397:GLU:H	1.85	0.41
2:I:767:VAL:HG12	2:I:769:GLU:HG3	2.03	0.41
2:B:395:GLN:HG3	2:B:397:GLU:H	1.85	0.40
2:E:1725:ARG:HD2	2:E:1725:ARG:HH21	1.71	0.40
2:E:2095:GLN:NE2	2:E:2127:GLN:O	2.54	0.40
2:E:426:ARG:HB2	2:E:506:TYR:HA	2.03	0.40
2:G:767:VAL:HG12	2:G:769:GLU:HG3	2.03	0.40
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	2.02	0.40
2:I:4172:GLU:OE1	2:I:4175:ARG:NH1	2.55	0.40
2:I:4570:ALA:HA	2:I:4573:ILE:HG22	2.03	0.40
2:E:1671:ARG:NH2	2:E:1713:ASP:HB3	2.36	0.40
2:E:688:LEU:HB3	2:E:777:PHE:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1694:LEU:O	2:G:1712:TYR:OH	2.23	0.40
2:G:214:VAL:HG22	2:G:341:TYR:CE1	2.56	0.40
2:G:3658:LYS:HA	2:G:3661:TRP:CE2	2.56	0.40
2:B:4863:TYR:HA	2:B:4901:ILE:HG23	2.04	0.40
2:B:688:LEU:HB3	2:B:777:PHE:CE1	2.57	0.40
2:E:642:THR:HG23	2:E:1613:LEU:HD12	2.03	0.40
2:G:4251:ILE:HG22	2:G:4553:ASN:HD22	1.87	0.40
2:I:4152:GLU:OE2	2:I:4180:ARG:NH1	2.50	0.40
2:I:4251:ILE:HG22	2:I:4553:ASN:HD22	1.87	0.40
2:I:5036:LEU:HD12	2:I:5036:LEU:HA	1.91	0.40
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.03	0.40
2:B:1972:ASN:HD21	2:B:2024:PRO:HB3	1.86	0.40
2:B:2878:LEU:HD23	2:B:2878:LEU:HA	1.94	0.40
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	2.02	0.40
2:G:2095:GLN:NE2	2:G:2127:GLN:O	2.54	0.40
2:G:4172:GLU:OE1	2:G:4175:ARG:NH1	2.55	0.40
2:G:864:PRO:HA	2:G:865:PRO:HD3	1.89	0.40
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.87	0.40
2:I:649:PHE:HB3	2:I:776:LEU:HB3	2.04	0.40
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	2.02	0.40
2:B:4172:GLU:OE1	2:B:4175:ARG:NH1	2.55	0.40
2:E:4017:LEU:HA	2:E:4017:LEU:HD23	1.87	0.40
2:E:886:ARG:HB3	2:E:891:TRP:HB2	2.02	0.40
2:G:1651:LEU:HD23	2:G:1651:LEU:HA	1.86	0.40
2:I:1658:ASP:N	2:I:1658:ASP:OD1	2.55	0.40
2:I:3787:LYS:HB2	2:I:3831:SER:HA	2.04	0.40
2:I:4863:TYR:HA	2:I:4901:ILE:HG23	2.04	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%)	91 (87%)	14 (13%)	0	100	100
1	F	105/108 (97%)	91 (87%)	14 (13%)	0	100	100
1	H	105/108 (97%)	91 (87%)	14 (13%)	0	100	100
1	J	105/108 (97%)	91 (87%)	14 (13%)	0	100	100
2	B	3237/4676 (69%)	2857 (88%)	371 (12%)	9 (0%)	46	83
2	E	3237/4676 (69%)	2859 (88%)	369 (11%)	9 (0%)	46	83
2	G	3237/4676 (69%)	2858 (88%)	370 (11%)	9 (0%)	46	83
2	I	3237/4676 (69%)	2859 (88%)	369 (11%)	9 (0%)	46	83
All	All	13368/19136 (70%)	11797 (88%)	1535 (12%)	36 (0%)	50	83

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	B	1932	PRO
2	E	1708	ARG
2	E	1932	PRO
2	I	1708	ARG
2	I	1932	PRO
2	G	1708	ARG
2	G	1932	PRO
2	B	1840	PRO
2	B	4641	PRO
2	B	5028	PHE
2	E	1840	PRO
2	E	4641	PRO
2	E	5028	PHE
2	I	1840	PRO
2	I	4641	PRO
2	I	5028	PHE
2	G	1840	PRO
2	G	4641	PRO
2	G	5028	PHE
2	B	2291	GLN
2	E	2291	GLN
2	I	2291	GLN
2	G	2291	GLN
2	B	4640	GLU
2	E	4135	PRO
2	E	4640	GLU

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Mol	Chain	Res	Type
2	I	4135	PRO
2	I	4640	GLU
2	G	4640	GLU
2	B	4135	PRO
2	G	4135	PRO
2	B	2343	GLY
2	E	2343	GLY
2	I	2343	GLY
2	G	2343	GLY

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	2493/3202 (78%)	2476 (99%)	17 (1%)	88	96
2	E	2493/3202 (78%)	2476 (99%)	17 (1%)	88	96
2	G	2493/3202 (78%)	2476 (99%)	17 (1%)	88	96
2	I	2493/3202 (78%)	2476 (99%)	17 (1%)	88	96
All	All	10324/13164 (78%)	10256 (99%)	68 (1%)	89	96

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

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG
2	B	553	ARG
2	B	719	LEU
2	B	1076	ARG
2	B	1141	ARG

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Mol	Chain	Res	Type
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	2339	VAL
2	B	2342	ASN
2	B	3787	LYS
2	B	3805	LEU
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	719	LEU
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	2339	VAL
2	E	2342	ASN
2	E	3787	LYS
2	E	3805	LEU
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	719	LEU
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	2339	VAL
2	I	2342	ASN
2	I	3787	LYS
2	I	3805	LEU
2	I	3896	ASN

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Mol	Chain	Res	Type
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	719	LEU
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
2	G	2339	VAL
2	G	2342	ASN
2	G	3787	LYS
2	G	3805	LEU
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) 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	105	HIS
2	B	111	HIS
2	B	113	HIS
2	B	156	GLN
2	B	203	ASN
2	B	224	HIS
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	479	GLN
2	B	520	ASN
2	B	949	ASN
2	B	1158	ASN

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Mol	Chain	Res	Type
2	B	1598	GLN
2	B	1663	HIS
2	B	1688	HIS
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	1952	GLN
2	B	1972	ASN
2	B	2005	GLN
2	B	2881	ASN
2	B	3781	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	4034	ASN
2	B	4120	ASN
2	B	4553	ASN
2	B	4728	HIS
2	E	57	ASN
2	E	105	HIS
2	E	111	HIS
2	E	113	HIS
2	E	156	GLN
2	E	203	ASN
2	E	224	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	479	GLN
2	E	520	ASN
2	E	1158	ASN
2	E	1598	GLN
2	E	1663	HIS
2	E	1688	HIS
2	E	1691	GLN
2	E	1693	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	1952	GLN
2	E	1972	ASN
2	E	2005	GLN

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Mol	Chain	Res	Type
2	E	2127	GLN
2	E	2881	ASN
2	E	3781	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	4034	ASN
2	E	4120	ASN
2	E	4142	ASN
2	E	4553	ASN
2	E	4728	HIS
2	I	57	ASN
2	I	105	HIS
2	I	111	HIS
2	I	113	HIS
2	I	156	GLN
2	I	203	ASN
2	I	224	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	479	GLN
2	I	520	ASN
2	I	949	ASN
2	I	1158	ASN
2	I	1598	GLN
2	I	1663	HIS
2	I	1688	HIS
2	I	1691	GLN
2	I	1693	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	1952	GLN
2	I	2005	GLN
2	I	2881	ASN
2	I	3781	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	4034	ASN
2	I	4120	ASN
2	I	4553	ASN

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Mol	Chain	Res	Type
2	I	4728	HIS
2	G	57	ASN
2	G	105	HIS
2	G	111	HIS
2	G	113	HIS
2	G	156	GLN
2	G	203	ASN
2	G	224	HIS
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	479	GLN
2	G	520	ASN
2	G	949	ASN
2	G	1158	ASN
2	G	1598	GLN
2	G	1663	HIS
2	G	1691	GLN
2	G	1693	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	1952	GLN
2	G	1972	ASN
2	G	2005	GLN
2	G	2127	GLN
2	G	2881	ASN
2	G	3781	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	4034	ASN
2	G	4120	ASN
2	G	4553	ASN
2	G	4728	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3613:UNK	C	3639:THR	N	42.64
1	G	3613:UNK	C	3639:THR	N	42.57
1	I	3613:UNK	C	3639:THR	N	42.56
1	E	3613:UNK	C	3639:THR	N	42.54
1	E	3163:UNK	C	3170:UNK	N	16.55
1	I	3163:UNK	C	3170:UNK	N	16.55
1	G	3163:UNK	C	3170:UNK	N	16.55
1	B	3163:UNK	C	3170:UNK	N	16.52
1	E	3468:UNK	C	3511:UNK	N	15.29

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	3468:UNK	C	3511:UNK	N	15.29
1	G	3468:UNK	C	3511:UNK	N	15.29
1	B	3468:UNK	C	3511:UNK	N	15.27
1	E	3063:UNK	C	3134:UNK	N	14.87
1	G	3063:UNK	C	3134:UNK	N	14.87
1	I	3063:UNK	C	3134:UNK	N	14.86
1	B	3063:UNK	C	3134:UNK	N	14.83
1	E	2703:UNK	C	2734:ASN	N	14.48
1	I	2703:UNK	C	2734:ASN	N	14.47
1	G	2703:UNK	C	2734:ASN	N	14.44
1	B	2703:UNK	C	2734:ASN	N	14.41
1	B	3236:UNK	C	3241:UNK	N	13.70
1	G	3236:UNK	C	3241:UNK	N	13.62
1	I	3236:UNK	C	3241:UNK	N	13.61
1	E	3236:UNK	C	3241:UNK	N	13.60
1	E	1564:UNK	C	1573:MET	N	12.83
1	I	1564:UNK	C	1573:MET	N	12.83
1	G	1564:UNK	C	1573:MET	N	12.81
1	B	1564:UNK	C	1573:MET	N	12.75
1	E	2976:UNK	C	2995:UNK	N	12.39
1	I	2976:UNK	C	2995:UNK	N	12.39
1	G	2976:UNK	C	2995:UNK	N	12.39
1	B	2976:UNK	C	2995:UNK	N	12.36
1	E	3254:UNK	C	3261:UNK	N	8.63
1	I	3254:UNK	C	3261:UNK	N	8.62
1	G	3254:UNK	C	3261:UNK	N	8.62
1	B	3254:UNK	C	3261:UNK	N	8.56
1	B	1297:UNK	C	1430:UNK	N	5.72
1	E	1297:UNK	C	1430:UNK	N	5.72
1	I	1297:UNK	C	1430:UNK	N	5.72
1	G	1297:UNK	C	1430:UNK	N	5.72
1	B	2479:LEU	C	2487:UNK	N	3.59
1	G	2479:LEU	C	2487:UNK	N	3.53
1	I	2479:LEU	C	2487:UNK	N	3.52
1	E	2479:LEU	C	2487:UNK	N	3.51
1	E	2939:ARG	C	2942:UNK	N	3.37
1	I	2939:ARG	C	2942:UNK	N	3.34
1	G	2939:ARG	C	2942:UNK	N	3.33
1	B	2939:ARG	C	2942:UNK	N	3.26