Full wwPDB EM Validation Report ⓘ

Nov 2, 2022 – 02:34 AM EDT

PDB ID	:	5T9S
EMDB ID	:	EMD-8375
Title	:	Structure of rabbit RyR1 (Ca2+-only dataset, class 4)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-09
Resolution	:	4.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

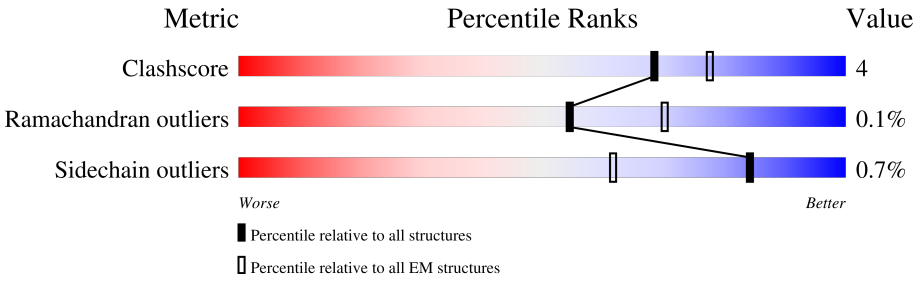
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	84% 15% .
1	F	108	83% 16% .
1	H	108	84% 15% .
1	J	108	84% 15% .
2	B	4676	80% 8% 11%
2	E	4676	80% 8% 11%
2	G	4676	81% 8% 11%
2	I	4676	81% 8% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 120756 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

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

- Molecule 2 is a protein called Ryanodine receptor 1.

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

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

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

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

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

3 Residue-property plots (i)

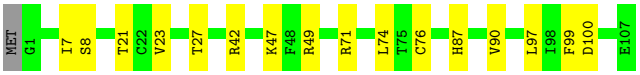
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

Chain F:

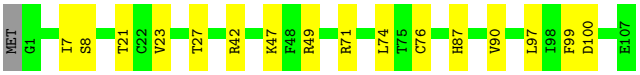
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



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

Chain H:

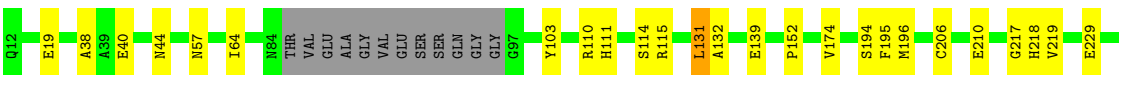


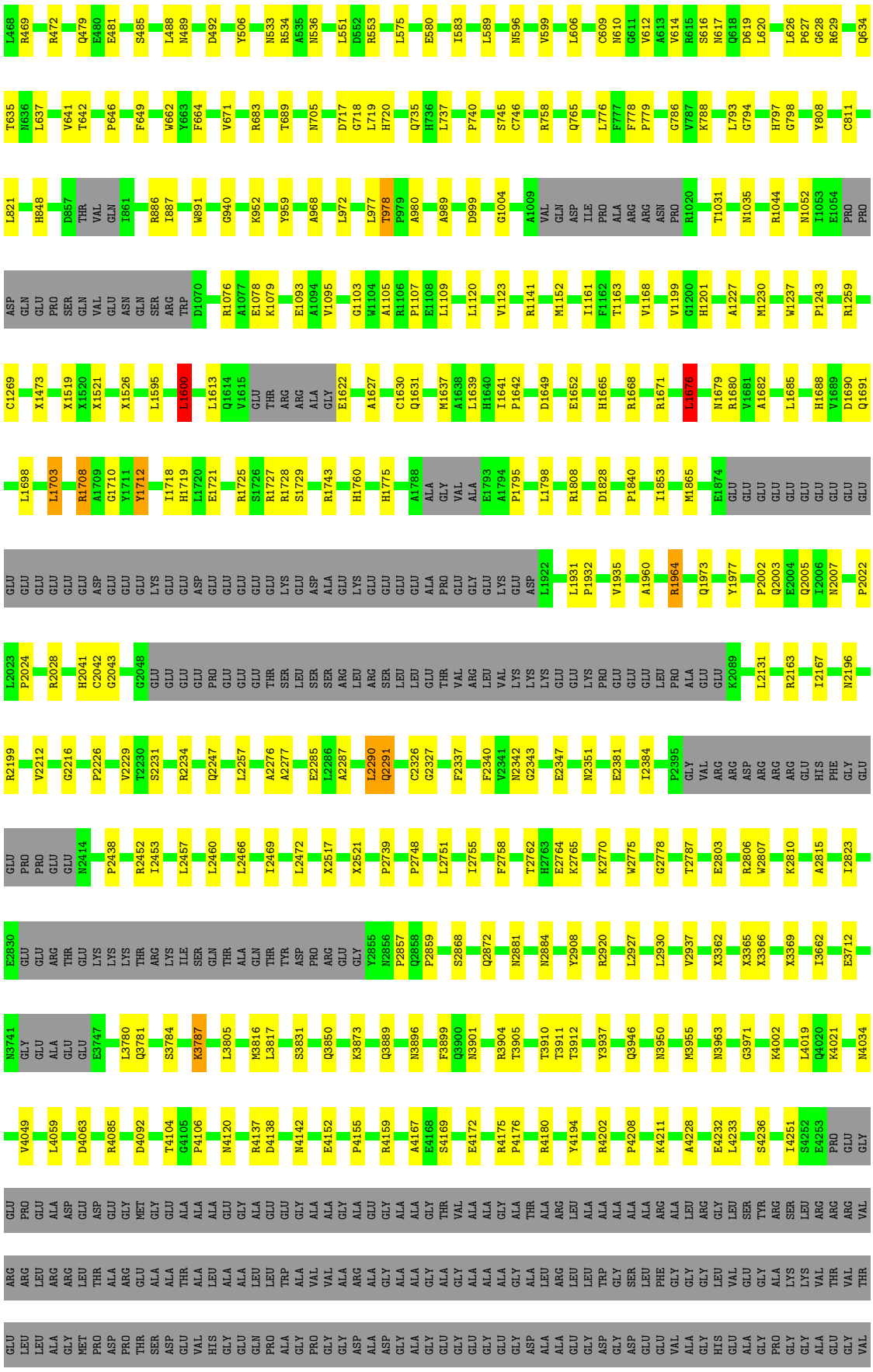
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

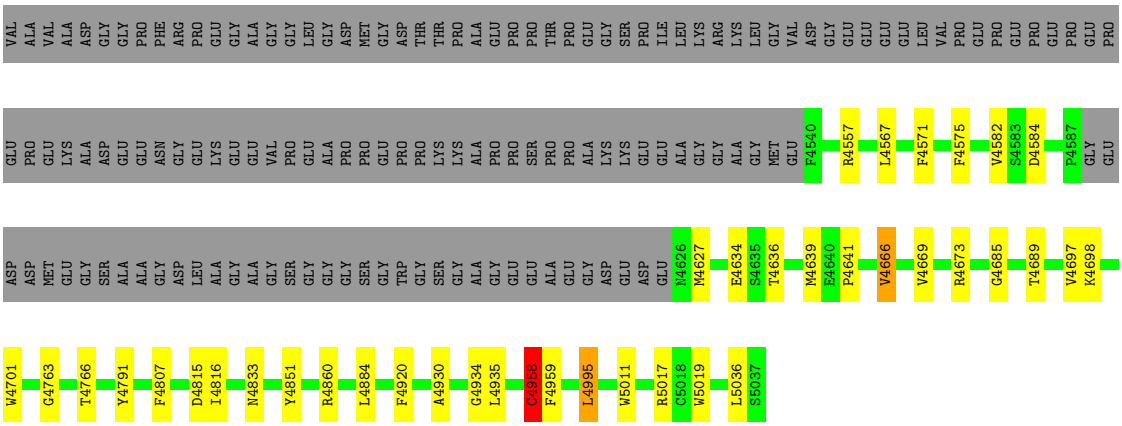
Chain J:

• Molecule 2: Ryanodine receptor 1

Chain B:

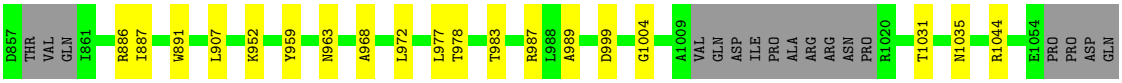


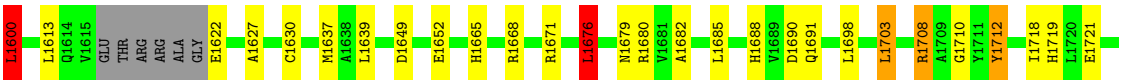


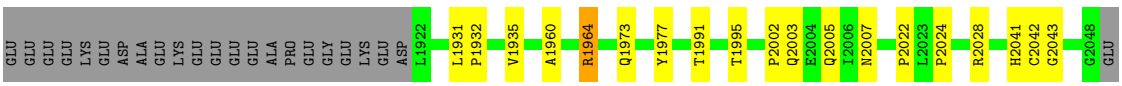


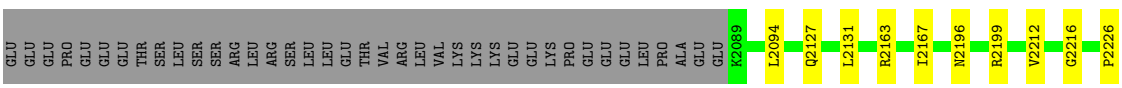
• Molecule 2: Ryanodine receptor 1

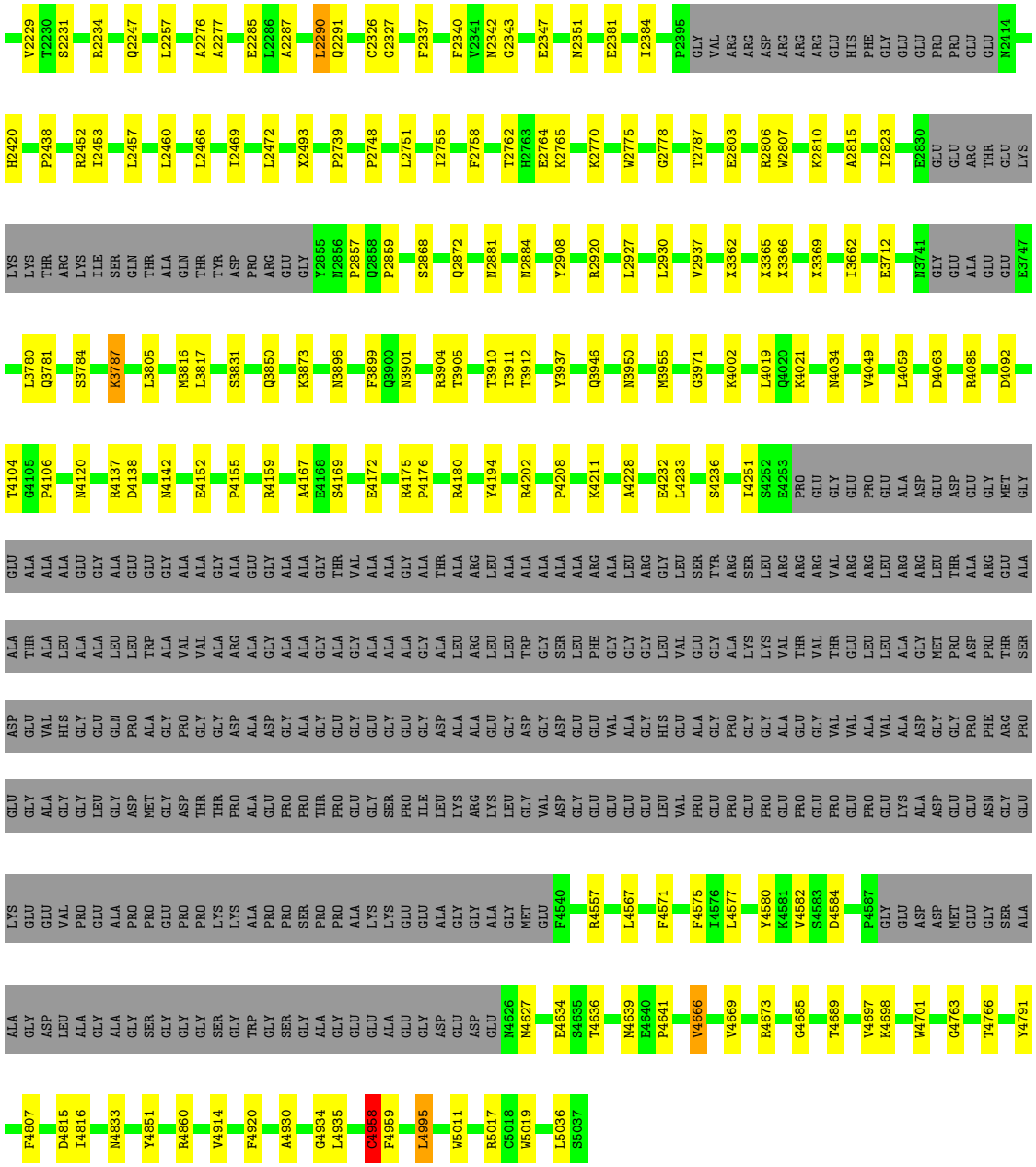
Chain E:





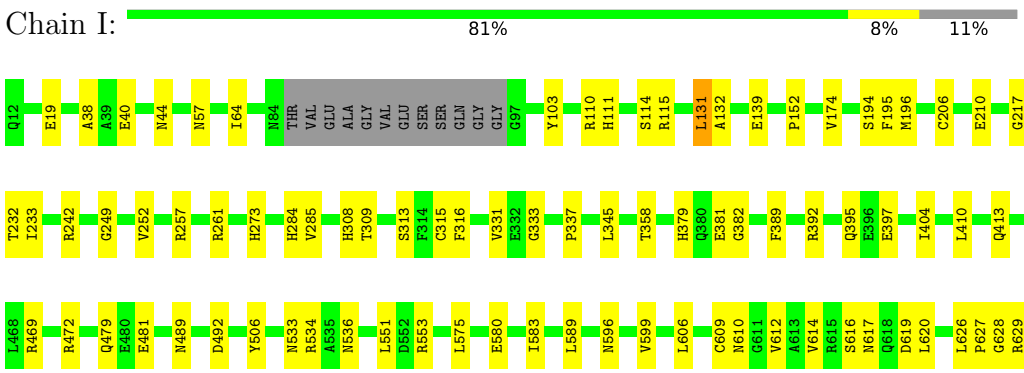


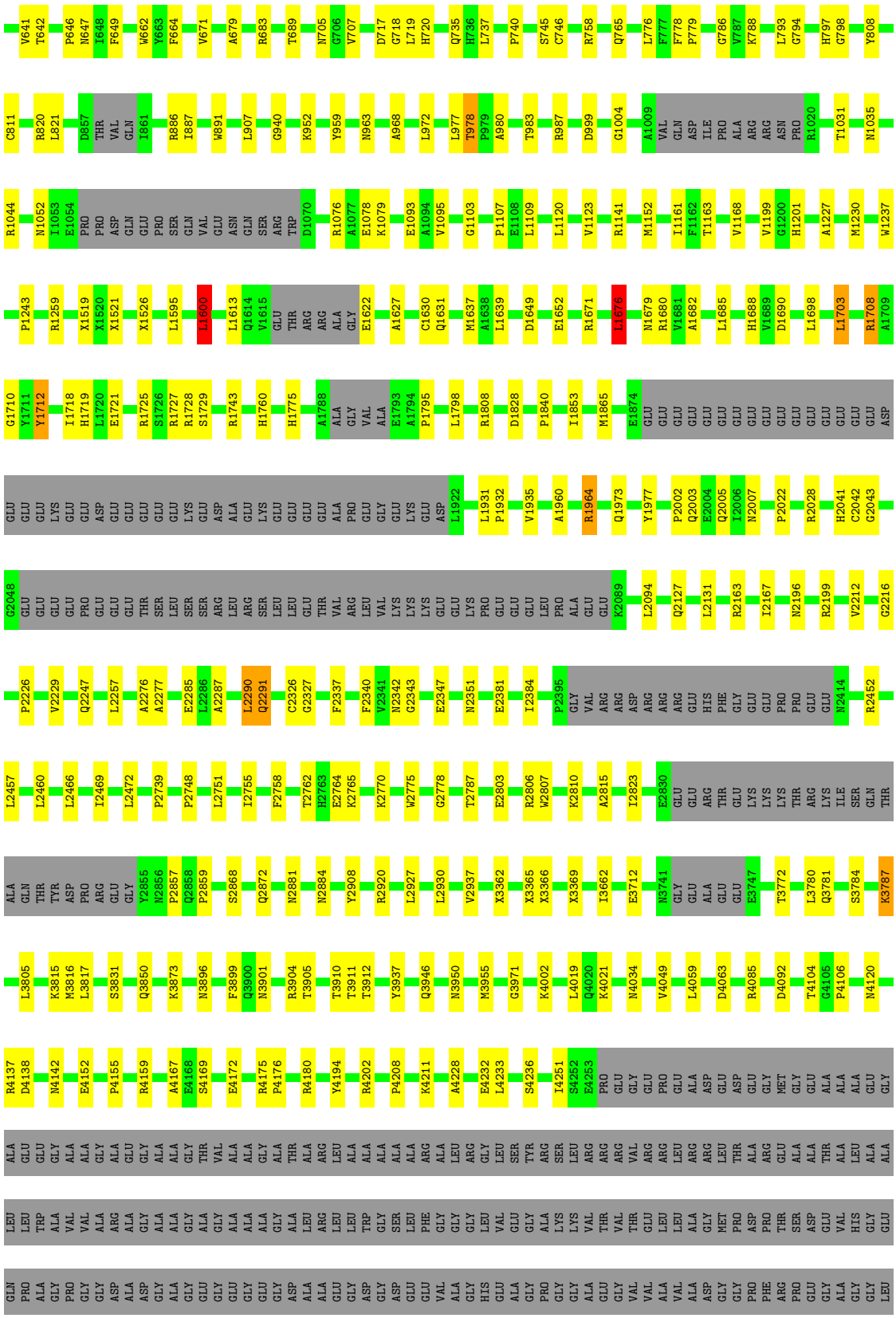


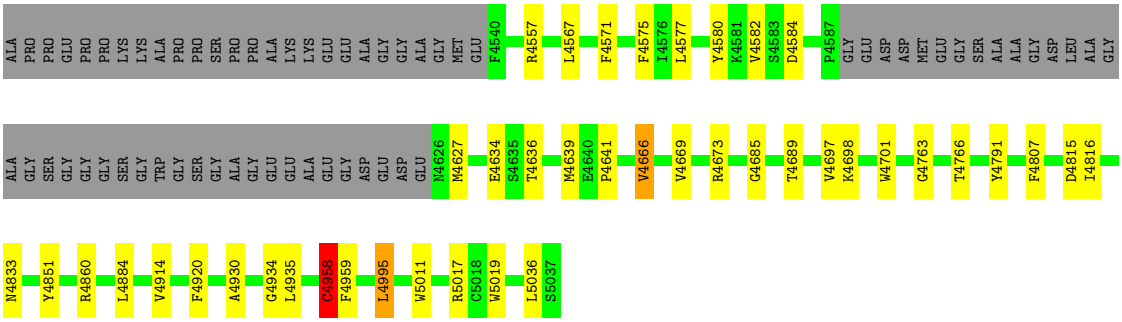


• Molecule 2: Ryanodine receptor 1

Chain I:

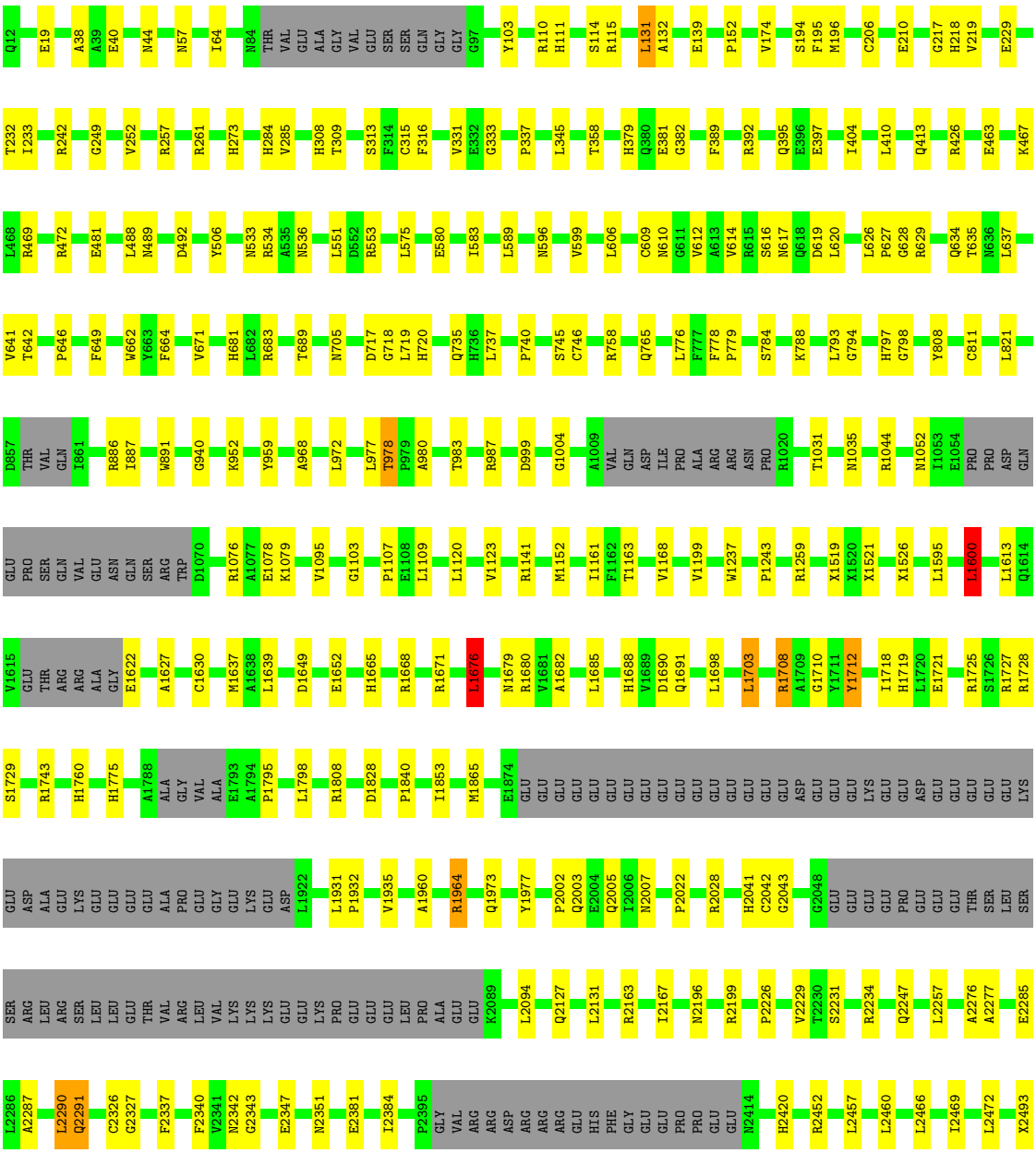


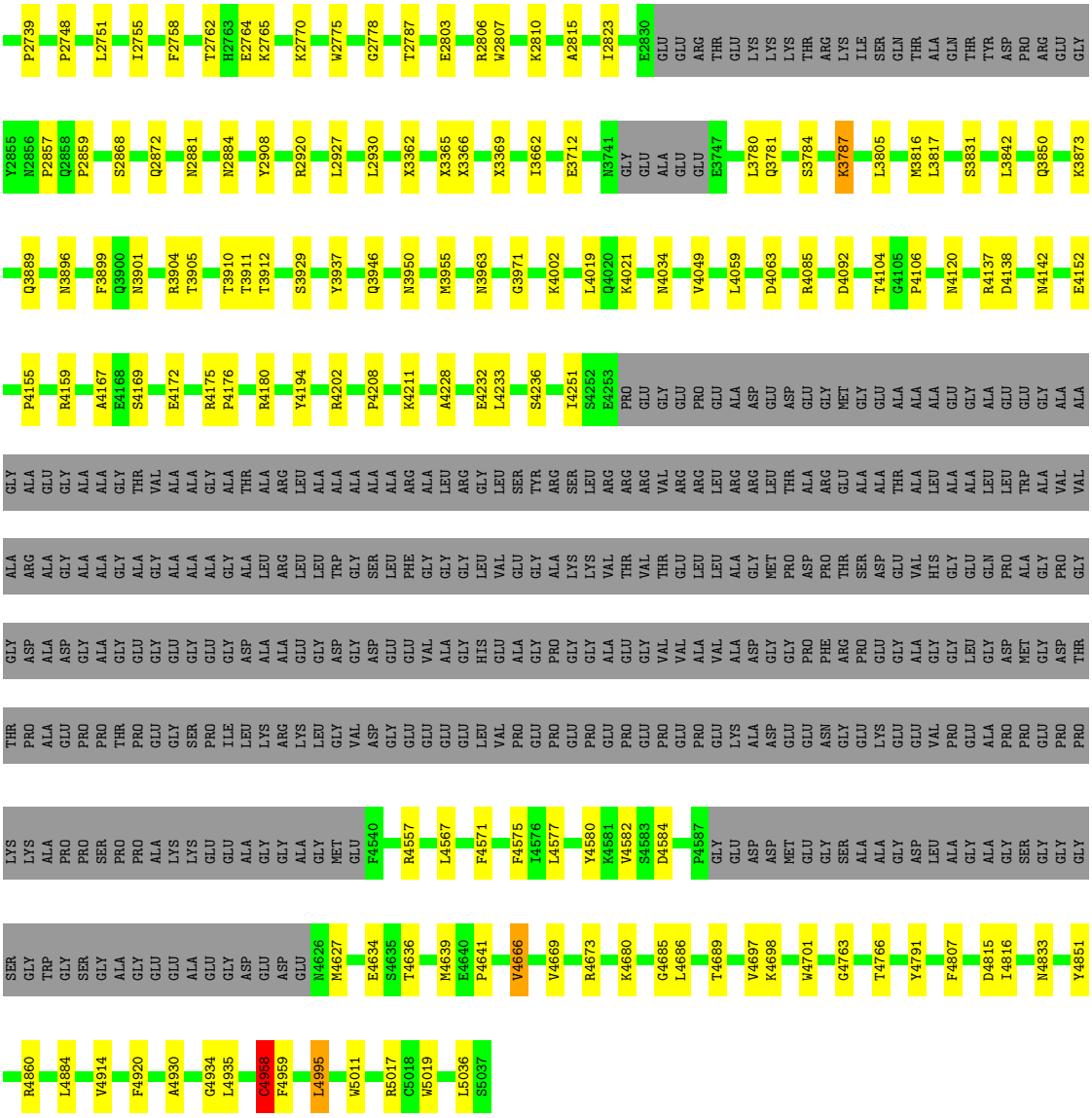




• Molecule 2: Ryanodine receptor 1

Chain G:




P2739 P2748 L2751 I2755 F2758 T2762 H2763 E2764 K2765 K2770 W2775 G2778 T2787 E2803 R2806 W2807 K2810 A2815 I2823 E2830
Y2855 N2856 P2857 Q2858 P2859 S2868 Q2872 N2881 N2884 Y2908 R2920 L2927 L2930 X3362 X3365 X3366 X3369 I3662 E3712 N3741 E3747 L3780 Q3781 S3784 K3787 L3805 M3816 L3817 S3831 L3842 Q3850 K3873
Q3889 N3896 F3899 Q3900 N3901 R3904 T3905 T3910 T3911 T3912 S3929 Y3937 Q3946 N3950 M3955 N3963 G3971 K4002 L4019 Q4020 K4021 N4034 V4049 L4059 D4063 R4085 D4092 T4104 G4105 P4106 N4120 R4137 D4138 N4142 E4152
P4155 R4159 A4167 E4168 S4169 E4172 R4175 P4176 R4180 Y4194 R4202 P4208 K4211 A4228 E4232 L4233 S4236 I4251 S4252 E4253
GLY ALA GLU GLY ALA ALA GLY THR VAL ALA ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ALA ALA ALA LEU ALA ARG GLY SER ARG ARG VAL ARG ARG LEU ARG ARG ARG LEU ARG ARG ARG LEU THR ALA ARG GLU ALA ALA ALA LEU ALA GLU GLY ALA ALA ALA
ALA ARG ALA GLY ALA ALA GLY ALA ALA ALA GLY ALA LEU LEU VAL GLU GLY ALA 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 ASP GLY
GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLU ALA GLY PRO GLY GLY ALA ALA GLU GLY 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 PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU VAL ALA GLU GLU VAL PRO GLU PRO GLU GLU GLY GLU GLU PRO GLU PRO GLU LYS ALA ASP GLU GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO PRO
LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA LYS GLY MET GLU F4540 R4557 L4567 F4571 F4575 I4576 L4577 Y4580 K4581 V4582 S4583 D4584 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY SER GLY GLY GLY
SER GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU ASP N4626 M4627 E4634 S4635 T4636 M4639 E4640 P4641 V4666 V4669 R4673 K4680 G4685 L4686 T4689 V4697 K4698 W4701 G4763 T4766 Y4791 F4807 D4815 I4816 N4833 Y4851
R4860 L4884 V4914 F4920 A4930 G4934 L4935 C4958 F4959 L4995 W5011 R5017 C5018 W5019 L5036 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.31	0/834	0.51	0/1123
1	F	0.31	0/834	0.51	0/1123
1	H	0.30	0/834	0.51	0/1123
1	J	0.31	0/834	0.51	0/1123
2	B	0.30	0/25428	0.54	6/34534 (0.0%)
2	E	0.30	0/25428	0.54	6/34534 (0.0%)
2	G	0.30	0/25428	0.54	6/34534 (0.0%)
2	I	0.30	0/25428	0.54	6/34534 (0.0%)
All	All	0.30	0/105048	0.54	24/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	16
2	E	0	16
2	G	0	16
2	I	0	16
All	All	0	68

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	131	LEU	CA-CB-CG	8.13	134.00	115.30
2	E	131	LEU	CA-CB-CG	8.11	133.96	115.30
2	I	131	LEU	CA-CB-CG	8.11	133.96	115.30
2	B	131	LEU	CA-CB-CG	8.10	133.94	115.30
2	E	1600	LEU	CA-CB-CG	7.05	131.51	115.30
2	B	1600	LEU	CA-CB-CG	7.03	131.48	115.30
2	G	1600	LEU	CA-CB-CG	7.03	131.47	115.30
2	I	1600	LEU	CA-CB-CG	7.01	131.43	115.30
2	E	1676	LEU	CA-CB-CG	6.33	129.86	115.30
2	I	1676	LEU	CA-CB-CG	6.33	129.85	115.30
2	B	1676	LEU	CA-CB-CG	6.32	129.84	115.30
2	G	1676	LEU	CA-CB-CG	6.32	129.84	115.30
2	B	2290	LEU	CA-CB-CG	6.11	129.35	115.30
2	I	2290	LEU	CA-CB-CG	6.10	129.34	115.30
2	E	2290	LEU	CA-CB-CG	6.10	129.33	115.30
2	G	2290	LEU	CA-CB-CG	6.09	129.31	115.30
2	G	977	LEU	CA-CB-CG	5.68	128.38	115.30
2	I	977	LEU	CA-CB-CG	5.68	128.36	115.30
2	E	977	LEU	CA-CB-CG	5.67	128.35	115.30
2	B	977	LEU	CA-CB-CG	5.66	128.32	115.30
2	E	4639	MET	C-N-CA	5.07	134.38	121.70
2	G	4639	MET	C-N-CA	5.07	134.37	121.70
2	I	4639	MET	C-N-CA	5.06	134.36	121.70
2	B	4639	MET	C-N-CA	5.04	134.31	121.70

There are no chirality outliers.

All (68) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1712	TYR	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	2291	GLN	Peptide
2	B	2342	ASN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	B	4807	PHE	Peptide
2	B	4958	CYS	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide
2	E	1712	TYR	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	2291	GLN	Peptide
2	E	2342	ASN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	4958	CYS	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	Peptide
2	G	1712	TYR	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	2291	GLN	Peptide
2	G	2342	ASN	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	4958	CYS	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	Peptide
2	I	1712	TYR	Peptide
2	I	1795	PRO	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	I	1828	ASP	Peptide
2	I	2291	GLN	Peptide
2	I	2342	ASN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	4958	CYS	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	8	0
1	F	818	0	824	9	0
1	H	818	0	824	8	0
1	J	818	0	824	9	0
2	B	29369	0	24721	212	0
2	E	29369	0	24721	206	0
2	G	29369	0	24719	205	0
2	I	29369	0	24721	208	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	120756	0	102178	849	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 (849) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.78	0.66
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.78	0.66
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.78	0.66
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.78	0.65
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.77	0.64
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.80	0.64
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.80	0.63
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.80	0.63
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.31	0.63
2:B:2452:ARG:NH1	2:I:174:VAL:O	2.31	0.63
2:E:627:PRO:O	2:E:629:ARG:NH1	2.32	0.63
2:I:627:PRO:O	2:I:629:ARG:NH1	2.32	0.63
2:B:627:PRO:O	2:B:629:ARG:NH1	2.32	0.62
2:G:627:PRO:O	2:G:629:ARG:NH1	2.32	0.62
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.80	0.62
2:B:2764:GLU:HG3	2:B:2857:PRO:HB2	1.82	0.62
2:E:2764:GLU:HG3	2:E:2857:PRO:HB2	1.82	0.62
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.33	0.62
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.30	0.61
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.33	0.61
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.33	0.61
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.82	0.61
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.82	0.61
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.83	0.61
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.83	0.61
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.83	0.61
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.83	0.61
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.83	0.61
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.33	0.61
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.83	0.61
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.83	0.60
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.30	0.60
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.83	0.60
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.82	0.60
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.82	0.60
2:G:1703:LEU:HB3	2:G:1708:ARG:HH21	1.67	0.60
2:E:379:HIS:HD2	2:E:382:GLY:H	1.49	0.60
2:I:2764:GLU:HG3	2:I:2857:PRO:HB2	1.82	0.60
2:E:4251:ILE:O	2:E:4557:ARG:NH1	2.35	0.60
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.84	0.60
2:G:4251:ILE:O	2:G:4557:ARG:NH1	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.83	0.60
2:B:1703:LEU:HB3	2:B:1708:ARG:HH21	1.67	0.59
2:E:111:HIS:HD2	2:E:114:SER:H	1.48	0.59
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.66	0.59
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.83	0.59
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.30	0.59
2:G:2764:GLU:HG3	2:G:2857:PRO:HB2	1.82	0.59
2:B:111:HIS:HD2	2:B:114:SER:H	1.48	0.59
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.84	0.59
2:E:1703:LEU:HB3	2:E:1708:ARG:HH21	1.67	0.59
2:B:379:HIS:HD2	2:B:382:GLY:H	1.49	0.59
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.36	0.59
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.66	0.59
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.83	0.59
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.85	0.59
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.83	0.59
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.83	0.59
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.84	0.59
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.66	0.59
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.36	0.59
2:B:4251:ILE:O	2:B:4557:ARG:NH1	2.35	0.59
2:E:609:CYS:SG	2:E:610:ASN:N	2.76	0.59
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.36	0.59
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.84	0.59
2:B:614:VAL:HG22	2:B:616:SER:H	1.68	0.59
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.85	0.59
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.85	0.59
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.66	0.59
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.36	0.59
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.85	0.59
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.85	0.58
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.36	0.58
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.85	0.58
2:I:4251:ILE:O	2:I:4557:ARG:NH1	2.35	0.58
2:E:4791:TYR:OH	2:E:4815:ASP:O	2.22	0.58
2:G:379:HIS:HD2	2:G:382:GLY:H	1.49	0.58
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.85	0.58
2:I:1703:LEU:HB3	2:I:1708:ARG:HH21	1.67	0.58
2:G:4791:TYR:OH	2:G:4815:ASP:O	2.22	0.58
2:E:614:VAL:HG22	2:E:616:SER:H	1.68	0.58
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4233:LEU:HA	2:I:4236:SER:HB3	1.86	0.58
2:G:111:HIS:HD2	2:G:114:SER:H	1.49	0.58
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.86	0.58
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.86	0.58
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.37	0.58
2:G:609:CYS:SG	2:G:610:ASN:N	2.76	0.58
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.86	0.58
2:B:609:CYS:SG	2:B:610:ASN:N	2.76	0.58
2:B:4791:TYR:OH	2:B:4815:ASP:O	2.22	0.58
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.86	0.58
2:I:614:VAL:HG22	2:I:616:SER:H	1.68	0.58
2:I:4791:TYR:OH	2:I:4815:ASP:O	2.22	0.58
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.37	0.58
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.36	0.58
2:I:111:HIS:HD2	2:I:114:SER:H	1.48	0.58
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.85	0.58
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.85	0.58
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.85	0.58
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.37	0.58
2:I:379:HIS:HD2	2:I:382:GLY:H	1.49	0.58
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.86	0.57
2:G:4233:LEU:HA	2:G:4236:SER:HB3	1.86	0.57
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.35	0.57
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.37	0.57
2:I:609:CYS:SG	2:I:610:ASN:N	2.76	0.57
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.35	0.57
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.70	0.57
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.87	0.57
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.86	0.57
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.36	0.57
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.38	0.57
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.36	0.57
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.38	0.57
2:I:2452:ARG:NH1	2:G:174:VAL:O	2.38	0.57
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.70	0.57
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.70	0.57
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.38	0.57
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.30	0.57
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.38	0.57
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.87	0.57
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.38	0.57
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.87	0.57
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.70	0.56
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.38	0.56
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.87	0.56
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.85	0.56
2:E:4233:LEU:HA	2:E:4236:SER:HB3	1.86	0.56
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.87	0.56
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.38	0.56
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.38	0.56
2:B:4233:LEU:HA	2:B:4236:SER:HB3	1.86	0.56
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.86	0.56
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.38	0.56
2:G:614:VAL:HG22	2:G:616:SER:H	1.68	0.56
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.87	0.56
2:E:174:VAL:O	2:G:2452:ARG:NH1	2.39	0.56
2:E:626:LEU:HG	2:E:628:GLY:H	1.70	0.56
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.88	0.56
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.38	0.56
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.38	0.56
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.35	0.56
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.88	0.56
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.88	0.56
2:E:217:GLY:O	2:E:261:ARG:NH1	2.39	0.56
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.88	0.56
2:I:4176:PRO:O	2:I:4202:ARG:NH1	2.39	0.56
2:G:626:LEU:HG	2:G:628:GLY:H	1.70	0.56
2:B:217:GLY:O	2:B:261:ARG:NH1	2.39	0.56
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.39	0.56
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.38	0.56
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.89	0.55
2:G:4176:PRO:O	2:G:4202:ARG:NH1	2.39	0.55
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.78	0.55
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.40	0.55
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.87	0.55
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.87	0.55
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.39	0.55
2:B:309:THR:O	2:B:313:SER:OG	2.24	0.55
2:E:4176:PRO:O	2:E:4202:ARG:NH1	2.39	0.55
2:I:626:LEU:HG	2:I:628:GLY:H	1.70	0.55
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:345:LEU:HD23	2:E:389:PHE:HB3	1.89	0.55
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.78	0.55
2:G:217:GLY:O	2:G:261:ARG:NH1	2.39	0.55
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.35	0.55
2:B:626:LEU:HG	2:B:628:GLY:H	1.70	0.55
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.87	0.55
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.87	0.55
2:I:217:GLY:O	2:I:261:ARG:NH1	2.39	0.55
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.40	0.55
2:G:132:ALA:HA	2:G:194:SER:HB2	1.88	0.55
2:G:345:LEU:HD23	2:G:389:PHE:HB3	1.89	0.55
2:B:4152:GLU:OE2	2:B:4180:ARG:NH1	2.40	0.55
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.39	0.55
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.72	0.55
2:I:309:THR:O	2:I:313:SER:OG	2.24	0.55
2:G:309:THR:O	2:G:313:SER:OG	2.24	0.55
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.40	0.55
2:G:4152:GLU:OE2	2:G:4180:ARG:NH1	2.40	0.55
2:B:4176:PRO:O	2:B:4202:ARG:NH1	2.39	0.54
2:E:132:ALA:HA	2:E:194:SER:HB2	1.88	0.54
2:I:345:LEU:HD23	2:I:389:PHE:HB3	1.89	0.54
2:I:132:ALA:HA	2:I:194:SER:HB2	1.88	0.54
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.40	0.54
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.73	0.54
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.78	0.54
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.89	0.54
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.72	0.54
2:B:345:LEU:HD23	2:B:389:PHE:HB3	1.89	0.54
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.90	0.54
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.72	0.54
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.72	0.54
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.41	0.54
2:B:132:ALA:HA	2:B:194:SER:HB2	1.88	0.54
2:E:309:THR:O	2:E:313:SER:OG	2.24	0.54
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.90	0.54
2:E:4152:GLU:OE2	2:E:4180:ARG:NH1	2.40	0.54
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.91	0.53
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.40	0.53
2:I:4152:GLU:OE2	2:I:4180:ARG:NH1	2.40	0.53
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.73	0.53
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.41	0.53
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.82	0.53
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.41	0.53
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.91	0.53
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.91	0.53
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.82	0.53
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.41	0.53
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.91	0.53
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.91	0.53
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.90	0.53
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.42	0.53
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.82	0.53
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.90	0.53
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.82	0.53
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.42	0.53
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.91	0.52
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.42	0.52
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	1.92	0.52
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.91	0.52
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.91	0.52
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	1.92	0.52
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.91	0.52
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	1.92	0.52
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.78	0.52
2:G:4958:CYS:SG	2:G:4959:PHE:N	2.82	0.52
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.92	0.52
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.34	0.52
2:I:1973:GLN:O	2:I:1977:TYR:N	2.43	0.52
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.92	0.52
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.42	0.52
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.91	0.52
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.92	0.52
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	1.91	0.52
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.92	0.52
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.91	0.52
2:B:4567:LEU:HD12	2:B:4816:ILE:HD12	1.92	0.52
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.91	0.52
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.91	0.52
2:B:1973:GLN:O	2:B:1977:TYR:N	2.43	0.52
2:B:4958:CYS:SG	2:B:4959:PHE:N	2.82	0.52
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.73	0.52
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.92	0.52
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.91	0.52
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.91	0.52
2:E:395:GLN:HG3	2:E:397:GLU:H	1.75	0.52
2:B:1729:SER:HB3	2:B:2163:ARG:HH11	1.75	0.52
2:B:4884:LEU:HD11	2:I:4914:VAL:HG21	1.92	0.52
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.91	0.52
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.92	0.52
2:I:1729:SER:HB3	2:I:2163:ARG:HH11	1.75	0.52
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.91	0.52
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.75	0.52
2:E:315:CYS:SG	2:E:316:PHE:N	2.83	0.52
2:E:4958:CYS:SG	2:E:4959:PHE:N	2.82	0.52
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.92	0.51
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.92	0.51
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.91	0.51
2:I:395:GLN:HG3	2:I:397:GLU:H	1.75	0.51
2:G:315:CYS:SG	2:G:316:PHE:N	2.83	0.51
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.93	0.51
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.75	0.51
2:B:315:CYS:SG	2:B:316:PHE:N	2.83	0.51
2:B:395:GLN:HG3	2:B:397:GLU:H	1.75	0.51
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.91	0.51
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.75	0.51
2:I:315:CYS:SG	2:I:316:PHE:N	2.83	0.51
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.92	0.51
2:E:765:GLN:NE2	2:E:1521:UNK:O	2.43	0.51
2:I:4567:LEU:HD12	2:I:4816:ILE:HD12	1.92	0.51
2:G:1973:GLN:O	2:G:1977:TYR:N	2.43	0.51
2:G:395:GLN:HG3	2:G:397:GLU:H	1.75	0.51
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.92	0.51
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.91	0.51
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.92	0.51
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.92	0.51
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.75	0.51
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.43	0.51
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.92	0.51
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.44	0.51
2:E:4172:GLU:HA	2:E:4175:ARG:HE	1.76	0.51
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.92	0.51
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.44	0.51
2:E:4567:LEU:HD12	2:E:4816:ILE:HD12	1.92	0.51
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.44	0.51
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.44	0.51
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.93	0.51
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.44	0.50
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.92	0.50
2:E:2908:TYR:OH	2:E:2920:ARG:NE	2.44	0.50
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.93	0.50
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.44	0.50
2:G:4567:LEU:HD12	2:G:4816:ILE:HD12	1.92	0.50
2:E:1973:GLN:O	2:E:1977:TYR:N	2.43	0.50
2:I:4958:CYS:SG	2:I:4959:PHE:N	2.82	0.50
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.43	0.50
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.44	0.50
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	1.94	0.50
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.40	0.50
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	1.94	0.50
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.94	0.50
2:G:4172:GLU:HA	2:G:4175:ARG:HE	1.76	0.50
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.40	0.50
2:B:1622:GLU:N	2:B:1627:ALA:O	2.45	0.50
2:B:4172:GLU:HA	2:B:4175:ARG:HE	1.76	0.50
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.76	0.50
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.76	0.50
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.94	0.50
2:E:1729:SER:HB3	2:E:2163:ARG:HH11	1.75	0.50
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.43	0.50
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	1.94	0.50
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.93	0.50
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.94	0.50
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.76	0.50
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	1.94	0.50
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.77	0.50
2:G:1729:SER:HB3	2:G:2163:ARG:HH11	1.75	0.50
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	1.94	0.50
2:B:689:THR:H	2:B:778:PHE:HE2	1.60	0.50
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.77	0.50
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.94	0.50
2:E:689:THR:H	2:E:778:PHE:HE2	1.60	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:689:THR:H	2:I:778:PHE:HE2	1.60	0.49
2:G:4584:ASP:HA	2:G:4627:MET:HA	1.94	0.49
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.77	0.49
2:E:38:ALA:HB1	2:E:64:ILE:HG13	1.94	0.49
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.93	0.49
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.77	0.49
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.92	0.49
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.94	0.49
2:G:689:THR:H	2:G:778:PHE:HE2	1.60	0.49
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	1.94	0.49
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.95	0.49
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.93	0.49
2:E:1259:ARG:NH2	2:E:1595:LEU:O	2.46	0.49
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.76	0.49
2:G:606:LEU:O	2:G:617:ASN:ND2	2.45	0.49
2:G:2347:GLU:O	2:G:2351:ASN:N	2.45	0.49
2:B:2347:GLU:O	2:B:2351:ASN:N	2.45	0.49
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.94	0.49
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	1.94	0.49
2:I:2347:GLU:O	2:I:2351:ASN:N	2.45	0.49
2:G:38:ALA:HB1	2:G:64:ILE:HG13	1.95	0.49
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.94	0.49
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.94	0.49
2:G:4251:ILE:HD12	2:G:4557:ARG:HA	1.94	0.49
2:B:331:VAL:HG12	2:B:333:GLY:H	1.77	0.49
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.95	0.49
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	1.94	0.49
2:B:4251:ILE:HD12	2:B:4557:ARG:HA	1.94	0.49
2:B:4584:ASP:HA	2:B:4627:MET:HA	1.94	0.49
2:E:2347:GLU:O	2:E:2351:ASN:N	2.45	0.49
2:E:4138:ASP:OD1	2:E:4138:ASP:N	2.46	0.49
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.93	0.49
2:I:1622:GLU:N	2:I:1627:ALA:O	2.45	0.49
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.77	0.49
2:G:4138:ASP:OD1	2:G:4138:ASP:N	2.46	0.49
2:B:38:ALA:HB1	2:B:64:ILE:HG13	1.95	0.49
2:B:195:PHE:HB3	2:B:196:MET:HG2	1.95	0.49
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.94	0.49
2:B:233:ILE:HD11	2:B:242:ARG:HH21	1.77	0.49
2:B:1259:ARG:NH2	2:B:1595:LEU:O	2.46	0.49
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.95	0.49
2:I:4138:ASP:OD1	2:I:4138:ASP:N	2.46	0.49
2:G:765:GLN:NE2	2:G:1521:UNK:O	2.46	0.49
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	1.94	0.49
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	1.94	0.49
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.95	0.49
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.95	0.49
2:I:606:LEU:O	2:I:617:ASN:ND2	2.46	0.49
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.95	0.49
2:G:1622:GLU:N	2:G:1627:ALA:O	2.45	0.49
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.77	0.49
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.95	0.48
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.77	0.48
2:E:606:LEU:O	2:E:617:ASN:ND2	2.45	0.48
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	1.94	0.48
2:E:4251:ILE:HD12	2:E:4557:ARG:HA	1.94	0.48
2:I:765:GLN:NE2	2:I:1521:UNK:O	2.46	0.48
2:I:4172:GLU:HA	2:I:4175:ARG:HE	1.76	0.48
2:G:111:HIS:CD2	2:G:114:SER:H	2.29	0.48
2:G:1259:ARG:NH2	2:G:1595:LEU:O	2.46	0.48
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.95	0.48
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.95	0.48
2:B:111:HIS:CD2	2:B:114:SER:H	2.29	0.48
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.94	0.48
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.95	0.48
2:I:233:ILE:HD11	2:I:242:ARG:HH21	1.77	0.48
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.95	0.48
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.95	0.48
2:B:606:LEU:O	2:B:617:ASN:ND2	2.45	0.48
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.96	0.48
2:E:233:ILE:HD11	2:E:242:ARG:HH21	1.77	0.48
2:I:38:ALA:HB1	2:I:64:ILE:HG13	1.94	0.48
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.95	0.48
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	1.94	0.48
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.43	0.48
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.94	0.48
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.95	0.48
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.95	0.48
2:E:195:PHE:HB3	2:E:196:MET:HG2	1.95	0.48
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.95	0.48
2:I:111:HIS:CD2	2:I:114:SER:H	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:257:ARG:O	2:I:284:HIS:NE2	2.36	0.48
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.77	0.48
2:G:331:VAL:HG12	2:G:333:GLY:H	1.77	0.48
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.95	0.48
2:E:331:VAL:HG12	2:E:333:GLY:H	1.77	0.48
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.96	0.48
2:E:1622:GLU:N	2:E:1627:ALA:O	2.45	0.48
2:E:4584:ASP:HA	2:E:4627:MET:HA	1.94	0.48
2:I:4584:ASP:HA	2:I:4627:MET:HA	1.94	0.48
2:G:2908:TYR:OH	2:G:2920:ARG:NE	2.44	0.48
2:B:580:GLU:HG3	2:B:620:LEU:HD22	1.96	0.48
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.94	0.48
2:E:580:GLU:HG3	2:E:620:LEU:HD22	1.96	0.48
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.95	0.48
2:I:1259:ARG:NH2	2:I:1595:LEU:O	2.46	0.48
2:I:4228:ALA:O	2:I:4232:GLU:N	2.46	0.48
2:E:793:LEU:HD12	2:E:797:HIS:HB2	1.96	0.48
2:I:331:VAL:HG12	2:I:333:GLY:H	1.77	0.48
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.49	0.48
2:I:4251:ILE:HD12	2:I:4557:ARG:HA	1.94	0.48
2:G:195:PHE:HB3	2:G:196:MET:HG2	1.95	0.48
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.95	0.48
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.96	0.48
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.95	0.48
2:G:233:ILE:HD11	2:G:242:ARG:HH21	1.77	0.48
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.95	0.48
2:E:111:HIS:CD2	2:E:114:SER:H	2.29	0.48
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.49	0.48
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.95	0.48
2:B:257:ARG:O	2:B:284:HIS:NE2	2.36	0.47
2:I:642:THR:HG23	2:I:1613:LEU:HD12	1.96	0.47
2:B:642:THR:HG23	2:B:1613:LEU:HD12	1.96	0.47
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.95	0.47
2:I:793:LEU:HD12	2:I:797:HIS:HB2	1.96	0.47
2:G:4063:ASP:OD1	2:G:4169:SER:OG	2.30	0.47
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.49	0.47
2:I:195:PHE:HB3	2:I:196:MET:HG2	1.95	0.47
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.94	0.47
2:G:649:PHE:HB3	2:G:776:LEU:HD13	1.97	0.47
2:B:649:PHE:HB3	2:B:776:LEU:HD13	1.97	0.47
2:B:3901:ASN:OD1	2:B:3904:ARG:NH1	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:649:PHE:HB3	2:E:776:LEU:HD13	1.97	0.47
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.96	0.47
2:I:1679:ASN:HA	2:I:1682:ALA:HB3	1.97	0.47
2:I:2196:ASN:OD1	2:I:2199:ARG:NH1	2.34	0.47
2:E:3901:ASN:OD1	2:E:3904:ARG:NH1	2.46	0.47
2:G:1679:ASN:HA	2:G:1682:ALA:HB3	1.97	0.47
2:B:793:LEU:HD12	2:B:797:HIS:HB2	1.96	0.47
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.95	0.47
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.96	0.47
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	1.97	0.47
2:I:580:GLU:HG3	2:I:620:LEU:HD22	1.96	0.47
2:B:1679:ASN:HA	2:B:1682:ALA:HB3	1.97	0.47
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.96	0.47
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.96	0.47
2:I:232:THR:HB	2:I:252:VAL:HG11	1.96	0.47
2:I:649:PHE:HB3	2:I:776:LEU:HD13	1.97	0.47
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.96	0.47
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.96	0.47
2:G:580:GLU:HG3	2:G:620:LEU:HD22	1.96	0.47
2:G:4228:ALA:O	2:G:4232:GLU:N	2.46	0.47
2:E:232:THR:HB	2:E:252:VAL:HG11	1.96	0.47
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.95	0.47
2:G:232:THR:HB	2:G:252:VAL:HG11	1.96	0.47
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.40	0.47
2:G:2758:PHE:O	2:G:2762:THR:N	2.45	0.47
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.96	0.47
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.49	0.47
2:B:4228:ALA:O	2:B:4232:GLU:N	2.46	0.47
2:G:793:LEU:HD12	2:G:797:HIS:HB2	1.96	0.47
2:B:404:ILE:HG21	2:B:481:GLU:HG3	1.97	0.47
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.97	0.47
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.97	0.47
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.96	0.47
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.96	0.47
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.97	0.46
2:B:232:THR:HB	2:B:252:VAL:HG11	1.96	0.46
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.96	0.46
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	1.97	0.46
2:E:2196:ASN:OD1	2:E:2199:ARG:NH1	2.34	0.46
2:E:4571:PHE:O	2:E:4575:PHE:N	2.48	0.46
2:B:4138:ASP:OD1	2:B:4138:ASP:N	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:642:THR:HG23	2:E:1613:LEU:HD12	1.96	0.46
2:I:404:ILE:HG21	2:I:481:GLU:HG3	1.97	0.46
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.97	0.46
2:I:4063:ASP:OD1	2:I:4169:SER:OG	2.29	0.46
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.96	0.46
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.81	0.46
2:I:2908:TYR:OH	2:I:2920:ARG:NE	2.44	0.46
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.97	0.46
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.97	0.46
2:B:2868:SER:O	2:B:2872:GLN:N	2.47	0.46
2:B:4571:PHE:O	2:B:4575:PHE:N	2.48	0.46
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.81	0.46
2:G:3905:THR:HA	2:G:3912:THR:HG23	1.97	0.46
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.97	0.46
2:I:358:THR:HG21	2:I:382:GLY:HA2	1.98	0.46
2:I:3905:THR:HA	2:I:3912:THR:HG23	1.97	0.46
2:E:358:THR:HG21	2:E:382:GLY:HA2	1.98	0.46
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.98	0.46
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.81	0.46
2:B:2908:TYR:OH	2:B:2920:ARG:NE	2.44	0.46
2:E:3905:THR:HA	2:E:3912:THR:HG23	1.97	0.46
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.81	0.46
2:G:4571:PHE:O	2:G:4575:PHE:N	2.48	0.46
2:B:485:SER:O	2:B:489:ASN:N	2.42	0.46
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	1.97	0.46
2:G:642:THR:HG23	2:G:1613:LEU:HD12	1.96	0.46
2:G:662:TRP:HZ3	2:G:811:CYS:HA	1.81	0.46
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.97	0.45
2:E:662:TRP:HZ3	2:E:811:CYS:HA	1.81	0.45
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.34	0.45
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.41	0.45
2:G:358:THR:HG21	2:G:382:GLY:HA2	1.98	0.45
2:G:404:ILE:HG21	2:G:481:GLU:HG3	1.97	0.45
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.81	0.45
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.98	0.45
2:E:4697:VAL:O	2:E:4701:TRP:N	2.49	0.45
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.96	0.45
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.98	0.45
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.34	0.45
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.96	0.45
2:B:358:THR:HG21	2:B:382:GLY:HA2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.97	0.45
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.97	0.45
2:E:4914:VAL:HG21	2:G:4884:LEU:HD11	1.98	0.45
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.98	0.45
2:E:404:ILE:HG21	2:E:481:GLU:HG3	1.97	0.45
2:E:999:ASP:O	2:E:1004:GLY:N	2.50	0.45
2:I:4571:PHE:O	2:I:4575:PHE:N	2.48	0.45
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.97	0.45
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.98	0.45
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.97	0.45
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	1.97	0.45
2:I:2758:PHE:O	2:I:2762:THR:N	2.45	0.45
2:B:2131:LEU:HB3	2:B:3662:ILE:HD13	1.99	0.45
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.81	0.45
2:E:2765:LYS:HA	2:E:2859:PRO:HG3	1.99	0.45
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.81	0.45
2:I:999:ASP:O	2:I:1004:GLY:N	2.50	0.45
2:I:2868:SER:O	2:I:2872:GLN:N	2.47	0.45
2:I:3901:ASN:OD1	2:I:3904:ARG:NH1	2.46	0.45
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.34	0.45
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.97	0.45
2:B:3905:THR:HA	2:B:3912:THR:HG23	1.97	0.45
2:I:2131:LEU:HB3	2:I:3662:ILE:HD13	1.99	0.45
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.99	0.45
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.99	0.45
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.34	0.45
2:E:488:LEU:O	2:E:492:ASP:N	2.45	0.45
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.97	0.45
2:E:1031:THR:O	2:E:1035:ASN:N	2.46	0.45
2:G:999:ASP:O	2:G:1004:GLY:N	2.50	0.45
2:G:2765:LYS:HA	2:G:2859:PRO:HG3	1.99	0.45
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.99	0.45
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.97	0.45
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.81	0.45
2:B:1269:CYS:HA	2:B:1473:UNK:HA	1.99	0.45
2:I:662:TRP:HZ3	2:I:811:CYS:HA	1.81	0.45
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.99	0.45
2:B:999:ASP:O	2:B:1004:GLY:N	2.50	0.45
2:B:1865:MET:SD	2:B:1865:MET:N	2.90	0.45
2:E:4763:GLY:O	2:E:4766:THR:OG1	2.34	0.45
2:G:3901:ASN:OD1	2:G:3904:ARG:NH1	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1031:THR:O	2:B:1035:ASN:N	2.46	0.44
2:E:1865:MET:SD	2:E:1865:MET:N	2.90	0.44
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.98	0.44
2:B:2457:LEU:HD23	2:B:2460:LEU:HD12	1.98	0.44
2:B:2758:PHE:O	2:B:2762:THR:N	2.46	0.44
2:E:4063:ASP:OD1	2:E:4169:SER:OG	2.29	0.44
2:G:683:ARG:HG2	2:G:717:ASP:HB3	2.00	0.44
2:G:2868:SER:O	2:G:2872:GLN:N	2.47	0.44
2:B:683:ARG:HG2	2:B:717:ASP:HB3	2.00	0.44
2:E:257:ARG:O	2:E:284:HIS:NE2	2.36	0.44
2:I:2457:LEU:HD23	2:I:2460:LEU:HD12	1.98	0.44
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	2.00	0.44
2:G:1243:PRO:HB2	2:G:1600:LEU:HD22	1.97	0.44
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.98	0.44
2:B:662:TRP:HZ3	2:B:811:CYS:HA	1.81	0.44
2:B:1163:THR:HA	2:B:1168:VAL:HA	2.00	0.44
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.98	0.44
2:I:2765:LYS:HA	2:I:2859:PRO:HG3	1.99	0.44
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.97	0.44
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.98	0.44
2:E:2457:LEU:HD23	2:E:2460:LEU:HD12	1.98	0.44
2:I:1865:MET:SD	2:I:1865:MET:N	2.90	0.44
1:H:21:THR:HA	1:H:49:ARG:HA	2.00	0.44
2:B:1093:GLU:OE1	2:B:1201:HIS:NE2	2.42	0.44
2:E:629:ARG:HD3	2:E:634:GLN:HG2	2.00	0.44
2:E:1163:THR:HA	2:E:1168:VAL:HA	2.00	0.44
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	2.00	0.44
2:E:4228:ALA:O	2:E:4232:GLU:N	2.46	0.44
2:I:4697:VAL:O	2:I:4701:TRP:N	2.49	0.44
2:G:488:LEU:O	2:G:492:ASP:N	2.45	0.44
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.34	0.44
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	2.00	0.44
2:B:2765:LYS:HA	2:B:2859:PRO:HG3	1.99	0.44
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.41	0.44
2:I:683:ARG:HG2	2:I:717:ASP:HB3	2.00	0.44
2:I:4059:LEU:HD11	2:I:4167:ALA:HB2	2.00	0.44
2:G:629:ARG:HD3	2:G:634:GLN:HG2	2.00	0.44
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.99	0.44
2:G:1163:THR:HA	2:G:1168:VAL:HA	2.00	0.44
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	2.00	0.44
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.34	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:THR:HA	1:F:49:ARG:HA	2.00	0.44
2:E:2131:LEU:HB3	2:E:3662:ILE:HD13	1.99	0.44
2:E:4930:ALA:O	2:E:4934:GLY:N	2.51	0.44
2:G:1865:MET:SD	2:G:1865:MET:N	2.90	0.44
2:G:4208:PRO:HA	2:G:4211:LYS:HB3	2.00	0.44
2:G:4697:VAL:O	2:G:4701:TRP:N	2.49	0.44
1:J:21:THR:HA	1:J:49:ARG:HA	2.00	0.43
2:E:683:ARG:HG2	2:E:717:ASP:HB3	2.00	0.43
2:E:1093:GLU:OE1	2:E:1201:HIS:NE2	2.42	0.43
2:B:488:LEU:O	2:B:492:ASP:N	2.45	0.43
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.50	0.43
2:I:1163:THR:HA	2:I:1168:VAL:HA	2.00	0.43
2:I:4930:ALA:O	2:I:4934:GLY:N	2.51	0.43
2:G:4930:ALA:O	2:G:4934:GLY:N	2.51	0.43
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.99	0.43
2:B:765:GLN:NE2	2:B:1521:UNK:O	2.51	0.43
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.99	0.43
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	2.00	0.43
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	2.00	0.43
2:B:629:ARG:HD3	2:B:634:GLN:HG2	2.00	0.43
2:B:4063:ASP:OD1	2:B:4169:SER:OG	2.29	0.43
2:E:1760:HIS:CE1	2:E:2041:HIS:HA	2.54	0.43
2:G:3787:LYS:HB2	2:G:3831:SER:HA	2.01	0.43
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	2.00	0.43
2:I:1760:HIS:CE1	2:I:2041:HIS:HA	2.54	0.43
2:G:2131:LEU:HB3	2:G:3662:ILE:HD13	1.99	0.43
2:G:2457:LEU:HD23	2:G:2460:LEU:HD12	1.98	0.43
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.99	0.43
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	2.00	0.43
2:I:1093:GLU:OE1	2:I:1201:HIS:NE2	2.42	0.43
2:I:3787:LYS:HB2	2:I:3831:SER:HA	2.01	0.43
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.41	0.43
2:B:1760:HIS:CE1	2:B:2041:HIS:HA	2.54	0.43
2:E:2024:PRO:O	2:E:2028:ARG:NE	2.48	0.43
2:I:4208:PRO:HA	2:I:4211:LYS:HB3	2.00	0.43
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.34	0.43
2:B:4833:ASN:HB3	2:B:4935:LEU:HD23	2.01	0.43
2:I:629:ARG:HD3	2:I:634:GLN:HG2	2.00	0.43
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	2.01	0.43
2:G:4232:GLU:OE1	2:G:5019:TRP:NE1	2.52	0.43
1:A:21:THR:HA	1:A:49:ARG:HA	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4208:PRO:HA	2:B:4211:LYS:HB3	2.00	0.43
2:E:907:LEU:O	2:E:963:ASN:ND2	2.38	0.43
2:E:4833:ASN:HB3	2:E:4935:LEU:HD23	2.01	0.43
2:I:4995:LEU:HD11	2:I:5011:TRP:HB2	2.01	0.43
2:G:983:THR:O	2:G:987:ARG:N	2.51	0.43
2:B:4930:ALA:O	2:B:4934:GLY:N	2.51	0.43
2:E:4232:GLU:OE1	2:E:5019:TRP:NE1	2.52	0.43
2:I:647:ASN:ND2	2:I:820:ARG:O	2.43	0.43
2:G:4833:ASN:HB3	2:G:4935:LEU:HD23	2.01	0.43
2:E:2381:GLU:HA	2:E:2384:ILE:HD12	2.01	0.42
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	2.01	0.42
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.36	0.42
2:G:4059:LEU:HD11	2:G:4167:ALA:HB2	2.00	0.42
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	2.01	0.42
2:B:4995:LEU:HD11	2:B:5011:TRP:HB2	2.01	0.42
2:E:2758:PHE:O	2:E:2762:THR:N	2.45	0.42
2:E:4851:TYR:HD2	2:E:4920:PHE:HD1	1.68	0.42
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	2.01	0.42
2:I:907:LEU:O	2:I:963:ASN:ND2	2.38	0.42
2:I:983:THR:O	2:I:987:ARG:N	2.51	0.42
2:I:2778:GLY:HA3	2:I:2787:THR:HB	2.02	0.42
2:I:4092:ASP:OD1	2:I:4092:ASP:N	2.53	0.42
2:G:1760:HIS:CE1	2:G:2041:HIS:HA	2.54	0.42
2:B:4697:VAL:O	2:B:4701:TRP:N	2.49	0.42
2:E:4059:LEU:HD11	2:E:4167:ALA:HB2	2.00	0.42
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.49	0.42
2:I:4833:ASN:HB3	2:I:4935:LEU:HD23	2.01	0.42
2:G:218:HIS:HB3	2:G:392:ARG:HD3	2.02	0.42
2:G:4851:TYR:HD2	2:G:4920:PHE:HD1	1.67	0.42
2:B:218:HIS:HB3	2:B:392:ARG:HD3	2.02	0.42
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.53	0.42
2:I:379:HIS:CD2	2:I:381:GLU:H	2.38	0.42
2:I:2381:GLU:HA	2:I:2384:ILE:HD12	2.01	0.42
2:G:4092:ASP:N	2:G:4092:ASP:OD1	2.53	0.42
1:J:71:ARG:HH22	2:I:679:ALA:HB2	1.85	0.42
2:E:983:THR:O	2:E:987:ARG:N	2.51	0.42
2:I:683:ARG:NH1	2:I:707:VAL:O	2.45	0.42
2:G:379:HIS:CD2	2:G:381:GLU:H	2.38	0.42
2:G:2815:ALA:HB3	2:G:2881:ASN:HD21	1.85	0.42
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.53	0.42
2:B:2381:GLU:HA	2:B:2384:ILE:HD12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3362:UNK:O	2:B:3366:UNK:N	2.53	0.42
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.53	0.42
2:B:4092:ASP:OD1	2:B:4092:ASP:N	2.53	0.42
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.34	0.42
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.53	0.42
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.53	0.42
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	2.02	0.42
2:B:4059:LEU:HD11	2:B:4167:ALA:HB2	2.00	0.42
2:B:4851:TYR:HD2	2:B:4920:PHE:HD1	1.68	0.42
2:E:3787:LYS:HB2	2:E:3831:SER:HA	2.01	0.42
2:E:4092:ASP:N	2:E:4092:ASP:OD1	2.53	0.42
2:E:4208:PRO:HA	2:E:4211:LYS:HB3	2.00	0.42
2:I:218:HIS:HB3	2:I:392:ARG:HD3	2.02	0.42
2:G:257:ARG:O	2:G:284:HIS:NE2	2.36	0.42
2:G:1031:THR:O	2:G:1035:ASN:N	2.46	0.42
2:B:978:THR:HB	2:B:980:ALA:H	1.85	0.42
2:E:4685:GLY:HA3	2:E:4689:THR:HB	2.02	0.42
2:I:4851:TYR:HD2	2:I:4920:PHE:HD1	1.68	0.42
2:G:2778:GLY:HA3	2:G:2787:THR:HB	2.02	0.42
2:B:4021:LYS:HG3	2:B:4142:ASN:HD22	1.85	0.41
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	2.02	0.41
2:E:1078:GLU:HG3	2:E:1237:TRP:HE1	1.85	0.41
2:E:4021:LYS:HG3	2:E:4142:ASN:HD22	1.85	0.41
2:G:940:GLY:O	2:G:1052:ASN:N	2.53	0.41
2:G:4685:GLY:HA3	2:G:4689:THR:HB	2.02	0.41
2:B:379:HIS:CD2	2:B:381:GLU:H	2.38	0.41
2:B:596:ASN:HB3	2:B:599:VAL:HG22	2.03	0.41
2:B:3787:LYS:HB2	2:B:3831:SER:HA	2.01	0.41
2:E:218:HIS:HB3	2:E:392:ARG:HD3	2.02	0.41
2:E:4995:LEU:HD11	2:E:5011:TRP:HB2	2.01	0.41
2:I:1078:GLU:HG3	2:I:1237:TRP:HE1	1.85	0.41
2:I:4232:GLU:OE1	2:I:5019:TRP:NE1	2.52	0.41
2:G:596:ASN:HB3	2:G:599:VAL:HG22	2.03	0.41
2:G:978:THR:HB	2:G:980:ALA:H	1.85	0.41
2:G:2381:GLU:HA	2:G:2384:ILE:HD12	2.01	0.41
2:G:4634:GLU:HG3	2:G:4636:THR:H	1.86	0.41
2:G:4995:LEU:HD11	2:G:5011:TRP:HB2	2.01	0.41
2:E:2778:GLY:HA3	2:E:2787:THR:HB	2.02	0.41
2:E:2815:ALA:HB3	2:E:2881:ASN:HD21	1.85	0.41
2:E:4634:GLU:HG3	2:E:4636:THR:H	1.85	0.41
2:B:612:VAL:HG12	2:B:2167:ILE:HA	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:379:HIS:CD2	2:E:381:GLU:H	2.38	0.41
2:I:612:VAL:HG12	2:I:2167:ILE:HA	2.03	0.41
2:I:1227:ALA:HB1	2:I:1230:MET:HG3	2.02	0.41
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.53	0.41
2:G:273:HIS:CE1	2:G:337:PRO:HB3	2.56	0.41
2:G:612:VAL:HG12	2:G:2167:ILE:HA	2.02	0.41
1:F:87:HIS:HA	1:F:88:PRO:HD3	1.93	0.41
2:B:273:HIS:CE1	2:B:337:PRO:HB3	2.56	0.41
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.41	0.41
2:B:940:GLY:O	2:B:1052:ASN:N	2.53	0.41
2:B:1078:GLU:HG3	2:B:1237:TRP:HE1	1.85	0.41
2:B:1641:ILE:HA	2:B:1642:PRO:HD3	1.92	0.41
2:B:4232:GLU:OE1	2:B:5019:TRP:NE1	2.52	0.41
2:E:273:HIS:CE1	2:E:337:PRO:HB3	2.56	0.41
2:E:2868:SER:O	2:E:2872:GLN:N	2.47	0.41
2:I:273:HIS:CE1	2:I:337:PRO:HB3	2.56	0.41
2:I:978:THR:HB	2:I:980:ALA:H	1.85	0.41
2:I:1031:THR:O	2:I:1035:ASN:N	2.46	0.41
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	2.03	0.41
2:B:793:LEU:HD22	2:B:821:LEU:HD13	2.03	0.41
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.53	0.41
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.53	0.41
2:B:3365:UNK:O	2:B:3369:UNK:N	2.54	0.41
2:E:596:ASN:HB3	2:E:599:VAL:HG22	2.03	0.41
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.86	0.41
2:I:793:LEU:HD22	2:I:821:LEU:HD13	2.03	0.41
2:I:4685:GLY:HA3	2:I:4689:THR:HB	2.02	0.41
2:G:2094:LEU:HD23	2:G:2127:GLN:HE22	1.86	0.41
2:B:786:GLY:HA2	2:B:1631:GLN:HA	2.03	0.41
2:B:4634:GLU:HG3	2:B:4636:THR:H	1.86	0.41
2:B:4685:GLY:HA3	2:B:4689:THR:HB	2.02	0.41
2:E:489:ASN:HA	2:E:492:ASP:HB2	2.03	0.41
2:E:683:ARG:NH1	2:E:707:VAL:O	2.45	0.41
2:G:793:LEU:HD22	2:G:821:LEU:HD13	2.03	0.41
2:G:3362:UNK:O	2:G:3366:UNK:N	2.54	0.41
2:B:1227:ALA:HB1	2:B:1230:MET:HG3	2.02	0.41
2:E:2212:VAL:O	2:E:2216:GLY:N	2.48	0.41
2:E:3362:UNK:O	2:E:3366:UNK:N	2.54	0.41
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	2.02	0.41
2:I:786:GLY:HA2	2:I:1631:GLN:HA	2.03	0.41
2:I:940:GLY:O	2:I:1052:ASN:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2815:ALA:HB3	2:I:2881:ASN:HD21	1.85	0.41
2:I:3362:UNK:O	2:I:3366:UNK:N	2.54	0.41
2:I:4577:LEU:HG	2:I:4580:TYR:HE2	1.86	0.41
2:I:4634:GLU:HG3	2:I:4636:THR:H	1.85	0.41
2:G:489:ASN:HA	2:G:492:ASP:HB2	2.03	0.41
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	2.03	0.41
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.53	0.41
1:F:27:THR:HB	1:F:100:ASP:HB3	2.03	0.41
2:B:2024:PRO:O	2:B:2028:ARG:NE	2.48	0.41
2:B:2815:ALA:HB3	2:B:2881:ASN:HD21	1.85	0.41
2:E:612:VAL:HG12	2:E:2167:ILE:HA	2.03	0.41
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.53	0.41
2:E:1991:THR:O	2:E:1995:THR:OG1	2.32	0.41
2:I:479:GLN:HE21	2:I:536:ASN:ND2	2.19	0.41
2:I:596:ASN:HB3	2:I:599:VAL:HG22	2.03	0.41
2:I:4884:LEU:HD11	2:G:4914:VAL:HG21	2.03	0.41
2:G:2290:LEU:HG	2:G:2291:GLN:H	1.86	0.41
2:G:2466:LEU:HD23	2:G:2469:ILE:HD12	2.02	0.41
1:J:27:THR:HB	1:J:100:ASP:HB3	2.03	0.41
2:E:776:LEU:HG	2:E:848:HIS:HA	2.03	0.41
2:E:793:LEU:HD22	2:E:821:LEU:HD13	2.03	0.41
2:E:794:GLY:H	2:E:798:GLY:HA3	1.86	0.41
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	2.03	0.41
2:I:2290:LEU:HG	2:I:2291:GLN:H	1.86	0.41
2:I:4021:LYS:HG3	2:I:4142:ASN:HD22	1.86	0.41
1:H:27:THR:HB	1:H:100:ASP:HB3	2.03	0.40
2:B:2231:SER:HA	2:B:2234:ARG:HG2	2.03	0.40
2:B:2778:GLY:HA3	2:B:2787:THR:HB	2.02	0.40
2:E:2094:LEU:HD23	2:E:2127:GLN:HE22	1.86	0.40
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.03	0.40
2:E:2823:ILE:HG12	2:E:2937:VAL:HG22	2.04	0.40
2:I:1595:LEU:HD23	2:I:1595:LEU:HA	1.97	0.40
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.40	0.40
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.39	0.40
2:G:4577:LEU:HG	2:G:4580:TYR:HE2	1.86	0.40
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	2.02	0.40
1:A:27:THR:HB	1:A:100:ASP:HB3	2.03	0.40
2:B:489:ASN:HA	2:B:492:ASP:HB2	2.03	0.40
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	2.03	0.40
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.40	0.40
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:794:GLY:H	2:G:798:GLY:HA3	1.86	0.40
2:G:3842:LEU:O	2:G:3929:SER:OG	2.40	0.40
2:G:4021:LYS:HG3	2:G:4142:ASN:HD22	1.86	0.40
2:B:479:GLN:HE21	2:B:536:ASN:ND2	2.19	0.40
2:B:794:GLY:H	2:B:798:GLY:HA3	1.86	0.40
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.03	0.40
2:B:2212:VAL:O	2:B:2216:GLY:N	2.48	0.40
2:B:2466:LEU:HD23	2:B:2469:ILE:HD12	2.02	0.40
2:B:3889:GLN:HE22	2:B:3963:ASN:HB3	1.86	0.40
2:E:2231:SER:HA	2:E:2234:ARG:HG2	2.03	0.40
2:I:489:ASN:HA	2:I:492:ASP:HB2	2.03	0.40
2:I:2094:LEU:HD23	2:I:2127:GLN:HE22	1.86	0.40
2:I:2212:VAL:O	2:I:2216:GLY:N	2.48	0.40
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	2.03	0.40
2:B:776:LEU:HG	2:B:848:HIS:HA	2.03	0.40
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.03	0.40
2:E:3365:UNK:O	2:E:3369:UNK:N	2.55	0.40
2:I:2823:ILE:HG12	2:I:2937:VAL:HG22	2.03	0.40
2:I:3365:UNK:O	2:I:3369:UNK:N	2.55	0.40
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.04	0.40
2:G:1078:GLU:HG3	2:G:1237:TRP:HE1	1.85	0.40
2:G:2231:SER:HA	2:G:2234:ARG:HG2	2.03	0.40
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.86	0.40
1:J:92:PRO:HD3	2:I:627:PRO:HB2	2.03	0.40
2:B:2290:LEU:HG	2:B:2291:GLN:H	1.86	0.40
2:B:2517:UNK:O	2:B:2521:UNK:N	2.55	0.40
2:B:2823:ILE:HG12	2:B:2937:VAL:HG22	2.04	0.40
2:I:794:GLY:H	2:I:798:GLY:HA3	1.86	0.40
2:G:3365:UNK:O	2:G:3369:UNK:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	F	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	H	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	J	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
2	B	3235/4676 (69%)	2894 (90%)	336 (10%)	5 (0%)	47	80
2	E	3235/4676 (69%)	2896 (90%)	334 (10%)	5 (0%)	47	80
2	G	3235/4676 (69%)	2894 (90%)	336 (10%)	5 (0%)	47	80
2	I	3235/4676 (69%)	2895 (90%)	335 (10%)	5 (0%)	47	80
All	All	13360/19136 (70%)	11959 (90%)	1381 (10%)	20 (0%)	54	85

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	E	1708	ARG
2	I	1708	ARG
2	G	1708	ARG
2	B	1932	PRO
2	E	1932	PRO
2	I	1932	PRO
2	G	1932	PRO
2	B	1840	PRO
2	B	4641	PRO
2	B	4958	CYS
2	E	1840	PRO
2	E	4641	PRO
2	E	4958	CYS
2	I	1840	PRO
2	I	4641	PRO
2	I	4958	CYS
2	G	1840	PRO
2	G	4641	PRO
2	G	4958	CYS

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%)	2475 (99%)	18 (1%)	84 90
2	E	2493/3202 (78%)	2475 (99%)	18 (1%)	84 90
2	G	2493/3202 (78%)	2475 (99%)	18 (1%)	84 90
2	I	2493/3202 (78%)	2475 (99%)	18 (1%)	84 90
All	All	10324/13164 (78%)	10252 (99%)	72 (1%)	84 90

All (72) 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	978	THR
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1703	LEU
2	B	1964	ARG
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	B	4137	ARG
2	B	4995	LEU
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	978	THR
2	E	1076	ARG
2	E	1141	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	1600	LEU
2	E	1676	LEU
2	E	1703	LEU
2	E	1964	ARG
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	E	4137	ARG
2	E	4995	LEU
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	978	THR
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1703	LEU
2	I	1964	ARG
2	I	3787	LYS
2	I	3805	LEU
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4137	ARG
2	I	4995	LEU
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	978	THR
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1703	LEU
2	G	1964	ARG
2	G	3787	LYS
2	G	3805	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4137	ARG
2	G	4995	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS
1	A	87	HIS
1	H	87	HIS
1	J	87	HIS
2	B	23	GLN
2	B	57	ASN
2	B	111	HIS
2	B	113	HIS
2	B	203	ASN
2	B	224	HIS
2	B	273	HIS
2	B	379	HIS
2	B	405	HIS
2	B	413	GLN
2	B	479	GLN
2	B	765	GLN
2	B	1158	ASN
2	B	1719	HIS
2	B	1760	HIS
2	B	1775	HIS
2	B	2005	GLN
2	B	2127	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3994	HIS
2	B	4034	ASN
2	B	4054	ASN
2	B	4120	ASN
2	B	4142	ASN
2	B	4553	ASN
2	B	4984	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	23	GLN
2	E	57	ASN
2	E	111	HIS
2	E	113	HIS
2	E	203	ASN
2	E	224	HIS
2	E	273	HIS
2	E	379	HIS
2	E	405	HIS
2	E	413	GLN
2	E	479	GLN
2	E	765	GLN
2	E	1158	ASN
2	E	1719	HIS
2	E	1760	HIS
2	E	1775	HIS
2	E	2005	GLN
2	E	2127	GLN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3994	HIS
2	E	4034	ASN
2	E	4054	ASN
2	E	4120	ASN
2	E	4142	ASN
2	E	4553	ASN
2	E	4984	ASN
2	I	23	GLN
2	I	57	ASN
2	I	111	HIS
2	I	113	HIS
2	I	203	ASN
2	I	224	HIS
2	I	273	HIS
2	I	379	HIS
2	I	405	HIS
2	I	413	GLN
2	I	479	GLN
2	I	765	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	1158	ASN
2	I	1719	HIS
2	I	1760	HIS
2	I	1775	HIS
2	I	2005	GLN
2	I	2127	GLN
2	I	3781	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3994	HIS
2	I	4034	ASN
2	I	4054	ASN
2	I	4120	ASN
2	I	4142	ASN
2	I	4553	ASN
2	I	4984	ASN
2	G	23	GLN
2	G	57	ASN
2	G	111	HIS
2	G	113	HIS
2	G	203	ASN
2	G	224	HIS
2	G	273	HIS
2	G	379	HIS
2	G	405	HIS
2	G	413	GLN
2	G	479	GLN
2	G	765	GLN
2	G	1158	ASN
2	G	1719	HIS
2	G	1760	HIS
2	G	1775	HIS
2	G	2005	GLN
2	G	2127	GLN
2	G	3781	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3994	HIS
2	G	4034	ASN
2	G	4054	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	4120	ASN
2	G	4142	ASN
2	G	4553	ASN
2	G	4984	ASN

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 monosaccharides 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	B	12
2	G	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	44.23
1	G	3613:UNK	C	3639:THR	N	43.95
1	I	3613:UNK	C	3639:THR	N	43.88
1	E	3613:UNK	C	3639:THR	N	43.84
1	E	3163:UNK	C	3170:UNK	N	16.60
1	I	3163:UNK	C	3170:UNK	N	16.60
1	G	3163:UNK	C	3170:UNK	N	16.59
1	B	3163:UNK	C	3170:UNK	N	16.55
1	B	3468:UNK	C	3511:UNK	N	15.45
1	G	3468:UNK	C	3511:UNK	N	15.42
1	E	3468:UNK	C	3511:UNK	N	15.40
1	I	3468:UNK	C	3511:UNK	N	15.40
1	B	3063:UNK	C	3134:UNK	N	14.93
1	E	3063:UNK	C	3134:UNK	N	14.90
1	I	3063:UNK	C	3134:UNK	N	14.90
1	G	3063:UNK	C	3134:UNK	N	14.90
1	I	2703:UNK	C	2734:ASN	N	14.22
1	E	2703:UNK	C	2734:ASN	N	14.16
1	G	2703:UNK	C	2734:ASN	N	14.10
1	B	2703:UNK	C	2734:ASN	N	13.86
1	E	3236:UNK	C	3241:UNK	N	13.47
1	I	3236:UNK	C	3241:UNK	N	13.47
1	B	3236:UNK	C	3241:UNK	N	13.46
1	G	3236:UNK	C	3241:UNK	N	13.46
1	I	1564:UNK	C	1573:MET	N	12.78
1	G	1564:UNK	C	1573:MET	N	12.68
1	E	1564:UNK	C	1573:MET	N	12.67
1	B	1564:UNK	C	1573:MET	N	12.65
1	B	2976:UNK	C	2995:UNK	N	12.08
1	E	2976:UNK	C	2995:UNK	N	12.07
1	I	2976:UNK	C	2995:UNK	N	12.07
1	G	2976:UNK	C	2995:UNK	N	12.07
1	E	3254:UNK	C	3261:UNK	N	8.41
1	I	3254:UNK	C	3261:UNK	N	8.41
1	G	3254:UNK	C	3261:UNK	N	8.40
1	B	3254:UNK	C	3261:UNK	N	8.34

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	1297:UNK	C	1430:UNK	N	5.95
1	B	1297:UNK	C	1430:UNK	N	5.94
1	E	1297:UNK	C	1430:UNK	N	5.94
1	G	1297:UNK	C	1430:UNK	N	5.94
1	B	2479:LEU	C	2487:UNK	N	3.52
1	B	2939:ARG	C	2942:UNK	N	3.51
1	E	2939:ARG	C	2942:UNK	N	3.44
1	I	2939:ARG	C	2942:UNK	N	3.43
1	G	2939:ARG	C	2942:UNK	N	3.41
1	G	2479:LEU	C	2487:UNK	N	3.26
1	E	2479:LEU	C	2487:UNK	N	3.22
1	I	2479:LEU	C	2487:UNK	N	3.21

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8375. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.