



wwPDB EM Map/Model Validation Report ⓘ

Oct 17, 2016 – 03:00 PM EDT

PDB ID : 5TB3
EMDB ID: : EMD-8394
Title : Structure of rabbit RyR1 (EGTA-only dataset, class 3)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on : 2016-09-11
Resolution : 4.70 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

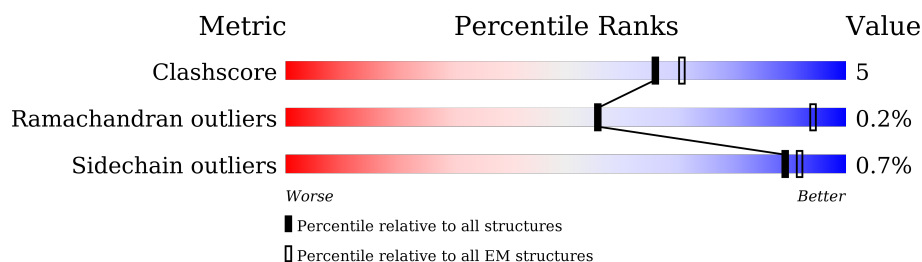
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	108	81% 18% .
1	F	108	81% 18% .
1	H	108	81% 18% .
1	J	108	81% 18% .
2	B	4416	84% 11% 5%
2	E	4416	84% 11% 5%
2	G	4416	84% 11% 5%
2	I	4416	84% 11% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 121312 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	4196	Total	C	N	O	S	0	0
			29509	18692	5230	5430	157		
2	E	4196	Total	C	N	O	S	0	0
			29509	18692	5230	5430	157		
2	I	4196	Total	C	N	O	S	0	0
			29509	18692	5230	5430	157		
2	G	4196	Total	C	N	O	S	0	0
			29509	18692	5230	5430	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	

3 Residue-property plots


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

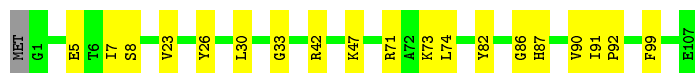
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 




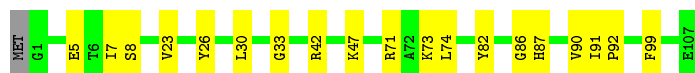
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A: 




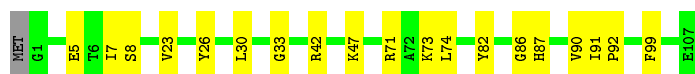
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 




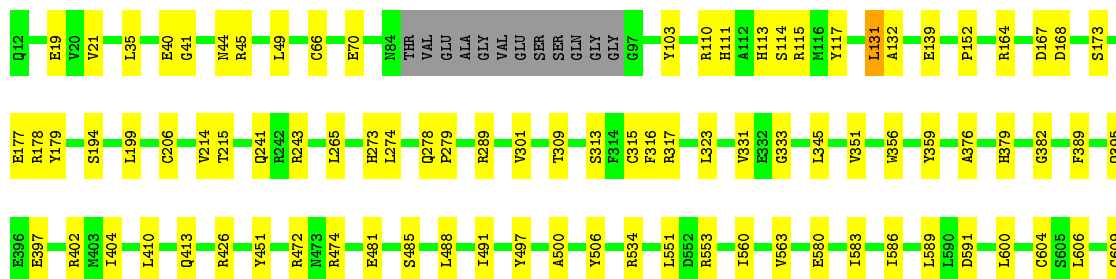
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 

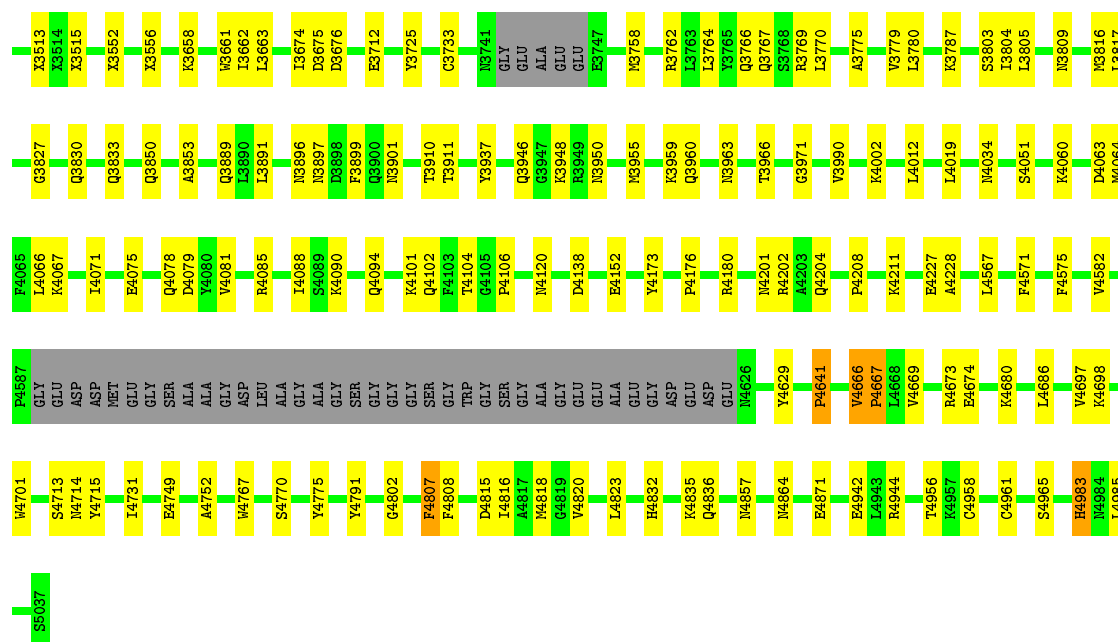


- Molecule 2: Ryanodine receptor 1

Chain B: 

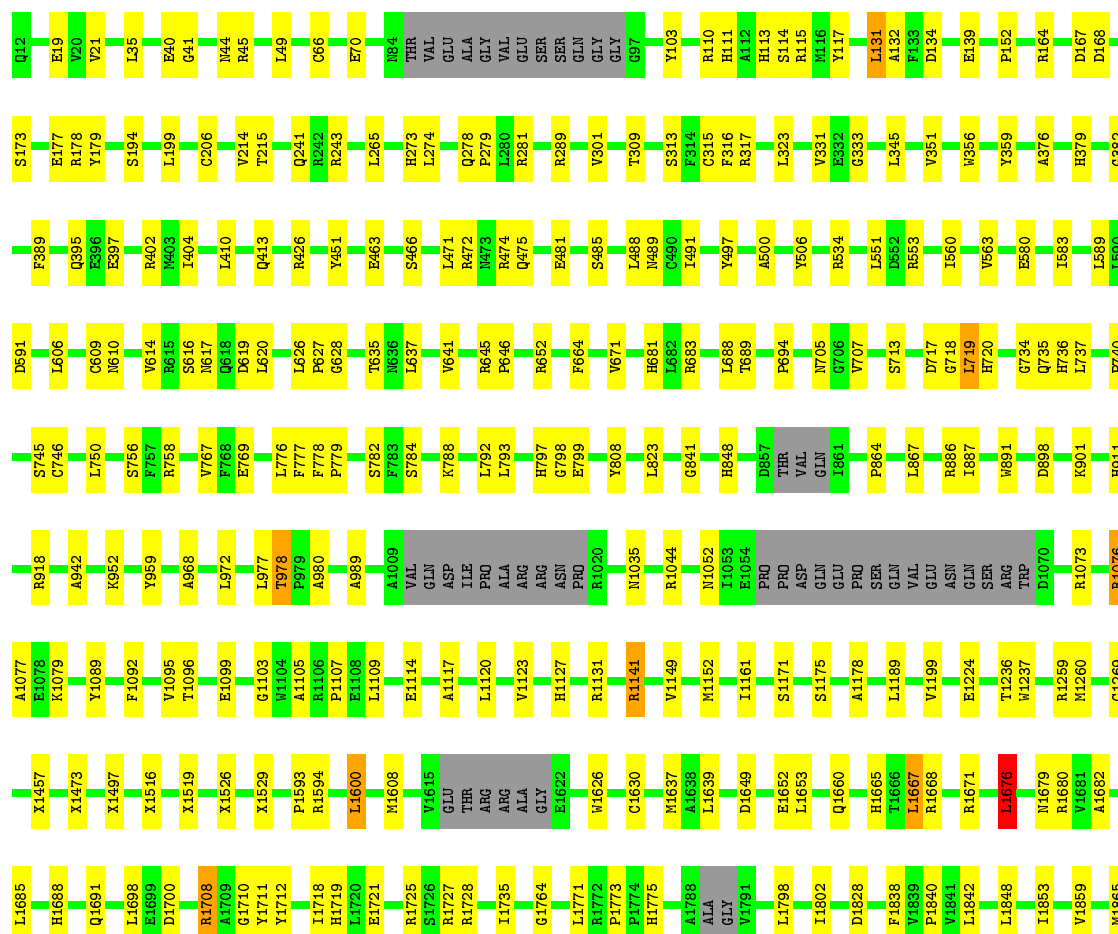


ASP	R4180	K3959	L3764	E2876	P2748	G2327	LYS	R1964	M1865	L1685	C1269	Y1089	A942	S756	H610
GLU	N4626	Q3960	Y3765	N2884	L2751	R2330	GLU	R1964	E1874	H1688	X1457	F1092	K952	R757	V614
N4201	N3963	Q3766	Q3767	L2894	L2751	F2337	LYS	Q1973	GLU	Q1691	X1473	F1092	Y959	R758	R615
R4202	T3966	S3768	S3769	L2894	I2755	F2337	PRO	R1976	GLU	Q1691	X1497	V1095	A968	V767	S616
Q4204	T3966	R3769	L3770	H2902	F2758	N2342	GLU	Y1977	GLU	Q1698	X1516	T1096	A968	P768	N617
A3775	G3971	A3775	A3775	R2920	T2762	G2343	LEU	T1991	GLU	L1698	X1516	E1099	L972	E769	N618
V3990	V3990	V3779	L3780	L2927	K2770	R2359	PRO	T1995	GLU	E1699	X1516	E1099	L972	L776	D619
K4002	K4002	L3780	L3780	L2927	K2770	R2359	ALA	T1995	GLU	D1700	X1516	E1099	L972	F777	L626
L4012	L4012	K3787	K3787	L2930	W2775	P2395	GLU	R1996	GLU	R1708	X1526	W1104	T978	F778	P627
L4019	L4019	S3803	S3803	X3361	P2793	VAL	GLU	E1997	GLU	G1710	X1526	W1104	T978	P779	G628
L3804	L3804	L3804	L3804	X3362	E2803	ARG	GLU	Q2003	GLU	Y1711	X1529	E1108	A989	S782	T635
L3805	L3805	L3805	L3805	X3365	E2803	ASP	GLU	Q2004	GLU	Y1712	P1593	E1108	A989	S784	L637
N3809	N3809	N3809	N3809	X3366	R2806	ARG	GLU	Q2005	GLU	I1718	R1594	E1108	A989	S784	T635
M3816	M3816	M3816	M3816	X3366	W2807	ARG	GLU	Q2006	GLU	H1719	L1600	E1108	A989	S784	L637
L3817	L3817	L3817	L3817	X3369	W2807	ARG	ASP	N2007	ASP	L1720	L1600	E1108	A989	S784	L637
Q3830	Q3830	Q3830	Q3830	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
Q3833	Q3833	Q3833	Q3833	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
Q3850	Q3850	Q3850	Q3850	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
A3853	A3853	A3853	A3853	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
I4071	I4071	I4071	I4071	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
E4075	E4075	E4075	E4075	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
Q4078	Q4078	Q4078	Q4078	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
Y4080	Y4080	Y4080	Y4080	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
V4081	V4081	V4081	V4081	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
R4085	R4085	R4085	R4085	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
I4088	I4088	I4088	I4088	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
K4101	K4101	K4101	K4101	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
Q4102	Q4102	Q4102	Q4102	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
F4103	F4103	F4103	F4103	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
T4104	T4104	T4104	T4104	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
G4105	G4105	G4105	G4105	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
P4106	P4106	P4106	P4106	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
Y3937	Y3937	Y3937	Y3937	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
Q3946	Q3946	Q3946	Q3946	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
G3947	G3947	G3947	G3947	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
K3948	K3948	K3948	K3948	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
R3949	R3949	R3949	R3949	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
N3950	N3950	N3950	N3950	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
M3955	M3955	M3955	M3955	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
P4176	P4176	P4176	P4176	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
N4815	N4815	N4815	N4815	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
I4816	I4816	I4816	I4816	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
A4817	A4817	A4817	A4817	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
N4818	N4818	N4818	N4818	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
G4819	G4819	G4819	G4819	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
V4820	V4820	V4820	V4820	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
L4823	L4823	L4823	L4823	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
H4832	H4832	H4832	H4832	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
K4835	K4835	K4835	K4835	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
Q4836	Q4836	Q4836	Q4836	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637
N4857	N4857	N4857	N4857	X3514	E2811	GLU	GLU	P2022	GLU	E1721	L1600	E1108	A989	S784	L637

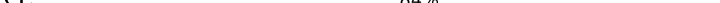


• Molecule 2: Ryanodine receptor 1

Chain I: 84% 11% 5%





Chain G:  84% 11% 5%






4 Experimental information

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 ($e^-/\text{\AA}^2$)	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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.32	0/834	0.53	0/1123
1	F	0.32	0/834	0.53	0/1123
1	H	0.32	0/834	0.53	0/1123
1	J	0.32	0/834	0.53	0/1123
2	B	0.30	0/25438	0.54	8/34548 (0.0%)
2	E	0.30	0/25438	0.54	8/34548 (0.0%)
2	G	0.30	0/25438	0.54	8/34548 (0.0%)
2	I	0.30	0/25438	0.54	8/34548 (0.0%)
All	All	0.30	0/105088	0.54	32/142684 (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	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	13
2	E	0	13
2	G	0	13
2	I	0	13
All	All	0	56

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	131	LEU	CA-CB-CG	7.74	133.11	115.30
2	B	131	LEU	CA-CB-CG	7.73	133.09	115.30
2	I	131	LEU	CA-CB-CG	7.73	133.08	115.30
2	G	131	LEU	CA-CB-CG	7.73	133.08	115.30
2	E	1600	LEU	CA-CB-CG	7.38	132.27	115.30
2	B	1600	LEU	CA-CB-CG	7.37	132.24	115.30
2	G	1600	LEU	CA-CB-CG	7.36	132.23	115.30
2	I	1600	LEU	CA-CB-CG	7.35	132.20	115.30
2	E	1676	LEU	CA-CB-CG	6.49	130.24	115.30
2	B	1676	LEU	CA-CB-CG	6.49	130.22	115.30
2	G	1676	LEU	CA-CB-CG	6.48	130.20	115.30
2	I	1676	LEU	CA-CB-CG	6.48	130.19	115.30
2	E	4985	LEU	CA-CB-CG	6.27	129.73	115.30
2	G	4985	LEU	CA-CB-CG	6.27	129.73	115.30
2	I	4985	LEU	CA-CB-CG	6.27	129.71	115.30
2	B	4985	LEU	CA-CB-CG	6.26	129.71	115.30
2	B	977	LEU	CA-CB-CG	5.85	128.76	115.30
2	G	977	LEU	CA-CB-CG	5.85	128.75	115.30
2	E	977	LEU	CA-CB-CG	5.84	128.72	115.30
2	I	977	LEU	CA-CB-CG	5.83	128.70	115.30
2	I	2290	LEU	CA-CB-CG	5.72	128.47	115.30
2	B	2290	LEU	CA-CB-CG	5.72	128.45	115.30
2	E	2290	LEU	CA-CB-CG	5.71	128.44	115.30
2	G	2290	LEU	CA-CB-CG	5.71	128.42	115.30
2	B	1667	LEU	CA-CB-CG	5.48	127.90	115.30
2	I	1667	LEU	CA-CB-CG	5.47	127.89	115.30
2	G	1667	LEU	CA-CB-CG	5.47	127.89	115.30
2	E	1667	LEU	CA-CB-CG	5.46	127.85	115.30
2	I	688	LEU	CA-CB-CG	5.18	127.21	115.30
2	B	688	LEU	CA-CB-CG	5.18	127.20	115.30
2	E	688	LEU	CA-CB-CG	5.17	127.20	115.30
2	G	688	LEU	CA-CB-CG	5.16	127.16	115.30

There are no chirality outliers.

All (56) 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	1828	ASP	Peptide
2	B	2291	GLN	Peptide
2	B	2343	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4641	PRO	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1828	ASP	Peptide
2	E	2291	GLN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4641	PRO	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1828	ASP	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4641	PRO	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1828	ASP	Peptide
2	I	2291	GLN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4641	PRO	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	Peptide

5.2 Too-close contacts ⓘ

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	11	0
1	F	818	0	824	11	0
1	H	818	0	824	11	0
1	J	818	0	824	11	0
2	B	29509	0	24752	277	0
2	E	29509	0	24753	269	0
2	G	29509	0	24753	269	0
2	I	29509	0	24753	276	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
All	All	121312	0	102307	1111	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1111) 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:4983:HIS:H	2:B:4983:HIS:CD2	2.10	0.70
2:E:4983:HIS:H	2:E:4983:HIS:CD2	2.10	0.70
2:G:4983:HIS:H	2:G:4983:HIS:CD2	2.10	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.10	0.67
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.61	0.65
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.61	0.65
2:E:111:HIS:HD2	2:E:114:SER:H	1.45	0.64
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.61	0.64
2:B:111:HIS:HD2	2:B:114:SER:H	1.45	0.64
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.61	0.64
2:E:4958:CYS:SG	2:E:4961:CYS:HB2	2.38	0.64
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.80	0.63
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.79	0.63
2:I:4958:CYS:SG	2:I:4961:CYS:HB2	2.38	0.63
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.63	0.63
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.63	0.63
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.81	0.63
2:G:4958:CYS:SG	2:G:4961:CYS:HB2	2.38	0.63
2:B:4958:CYS:SG	2:B:4961:CYS:HB2	2.38	0.63
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.81	0.62
2:G:111:HIS:HD2	2:G:114:SER:H	1.45	0.62
2:I:379:HIS:HD2	2:I:382:GLY:H	1.47	0.62
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.81	0.62
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.63	0.62
2:G:1259:ARG:HH12	2:G:1593:PRO:HA	1.64	0.62
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.80	0.62
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.63	0.62
2:I:4958:CYS:SG	2:I:4961:CYS:CB	2.88	0.62
2:I:111:HIS:HD2	2:I:114:SER:H	1.45	0.62
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.82	0.62
2:I:1259:ARG:HH12	2:I:1593:PRO:HA	1.64	0.62
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.81	0.61
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.81	0.61
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.81	0.61
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.82	0.61
2:B:4958:CYS:SG	2:B:4961:CYS:CB	2.88	0.61
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.82	0.61
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.82	0.61
2:B:379:HIS:HD2	2:B:382:GLY:H	1.47	0.61
2:E:1259:ARG:HH12	2:E:1593:PRO:HA	1.64	0.61
2:E:4958:CYS:SG	2:E:4961:CYS:CB	2.88	0.61
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.80	0.61
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.81	0.61
2:B:1259:ARG:HH12	2:B:1593:PRO:HA	1.64	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.81	0.61
2:E:379:HIS:HD2	2:E:382:GLY:H	1.47	0.61
2:G:379:HIS:HD2	2:G:382:GLY:H	1.47	0.61
2:G:4958:CYS:SG	2:G:4961:CYS:CB	2.88	0.60
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.35	0.60
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.35	0.60
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.35	0.60
2:B:173:SER:HB3	2:B:178:ARG:H	1.67	0.60
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.84	0.60
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.84	0.60
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.35	0.60
2:I:173:SER:HB3	2:I:178:ARG:H	1.67	0.60
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.84	0.59
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.35	0.59
2:G:173:SER:HB3	2:G:178:ARG:H	1.67	0.59
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.84	0.59
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.35	0.59
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.36	0.59
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.36	0.59
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.36	0.59
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.36	0.59
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.85	0.59
2:G:4176:PRO:O	2:G:4202:ARG:NH1	2.35	0.59
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.85	0.59
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.85	0.59
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.36	0.59
2:B:609:CYS:SG	2:B:610:ASN:N	2.75	0.59
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.35	0.59
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.84	0.59
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.85	0.59
2:E:609:CYS:SG	2:E:610:ASN:N	2.75	0.59
2:I:4176:PRO:O	2:I:4202:ARG:NH1	2.35	0.59
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.36	0.59
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.84	0.59
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.36	0.59
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.36	0.59
2:I:241:GLN:O	2:I:289:ARG:NH1	2.34	0.59
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.36	0.59
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.36	0.59
2:E:4176:PRO:O	2:E:4202:ARG:NH1	2.35	0.59
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.35	0.59
2:B:4176:PRO:O	2:B:4202:ARG:NH1	2.35	0.59
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.85	0.59
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.36	0.59
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.36	0.59
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.84	0.59
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.36	0.59
2:G:609:CYS:SG	2:G:610:ASN:N	2.75	0.59
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.36	0.58
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.84	0.58
2:G:3733:CYS:HA	2:G:3766:GLN:HG3	1.85	0.58
2:I:609:CYS:SG	2:I:610:ASN:N	2.75	0.58
2:E:173:SER:HB3	2:E:178:ARG:H	1.67	0.58
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.36	0.58
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.85	0.58
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.84	0.58
2:I:3733:CYS:HA	2:I:3766:GLN:HG3	1.85	0.58
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.85	0.58
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.36	0.58
2:B:3733:CYS:HA	2:B:3766:GLN:HG3	1.85	0.58
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.86	0.58
2:G:241:GLN:O	2:G:289:ARG:NH1	2.34	0.58
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.37	0.58
2:E:3733:CYS:HA	2:E:3766:GLN:HG3	1.84	0.58
2:E:4567:LEU:HA	2:E:4816:ILE:HD12	1.85	0.58
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.86	0.58
2:I:4567:LEU:HA	2:I:4816:ILE:HD12	1.85	0.58
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.85	0.58
2:B:4567:LEU:HA	2:B:4816:ILE:HD12	1.85	0.57
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.85	0.57
2:B:614:VAL:HG22	2:B:616:SER:H	1.69	0.57
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.85	0.57
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.38	0.57
2:G:614:VAL:HG22	2:G:616:SER:H	1.69	0.57
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.37	0.57
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.36	0.57
2:G:4567:LEU:HA	2:G:4816:ILE:HD12	1.85	0.57
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.37	0.57
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.37	0.57
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.37	0.57
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.36	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.86	0.57
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.38	0.57
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.38	0.57
2:I:614:VAL:HG22	2:I:616:SER:H	1.69	0.57
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.36	0.57
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.87	0.57
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.37	0.57
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.78	0.57
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.87	0.57
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.85	0.57
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.78	0.57
2:I:4983:HIS:N	2:I:4983:HIS:CD2	2.73	0.57
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.78	0.57
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.38	0.56
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.37	0.56
2:I:359:TYR:HA	2:I:376:ALA:HA	1.87	0.56
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.87	0.56
2:B:359:TYR:HA	2:B:376:ALA:HA	1.87	0.56
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.78	0.56
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.87	0.56
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.87	0.56
2:B:241:GLN:O	2:B:289:ARG:NH1	2.34	0.56
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.87	0.56
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.85	0.56
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.38	0.56
2:B:4983:HIS:N	2:B:4983:HIS:CD2	2.73	0.56
2:E:614:VAL:HG22	2:E:616:SER:H	1.69	0.56
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.38	0.56
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.37	0.56
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.70	0.56
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.87	0.56
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.78	0.56
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.38	0.56
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.38	0.56
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.70	0.56
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.87	0.56
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.87	0.56
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.88	0.56
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.88	0.56
2:G:3767:GLN:NE2	2:G:3804:ILE:O	2.39	0.56
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.37	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.89	0.55
2:B:3767:GLN:NE2	2:B:3804:ILE:O	2.39	0.55
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.70	0.55
2:G:359:TYR:HA	2:G:376:ALA:HA	1.87	0.55
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.87	0.55
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.78	0.55
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.87	0.55
2:E:3767:GLN:NE2	2:E:3804:ILE:O	2.39	0.55
2:G:4983:HIS:N	2:G:4983:HIS:CD2	2.73	0.55
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.87	0.55
2:I:3767:GLN:NE2	2:I:3804:ILE:O	2.39	0.55
2:E:359:TYR:HA	2:E:376:ALA:HA	1.88	0.55
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.88	0.55
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.70	0.55
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.89	0.55
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.89	0.55
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.89	0.55
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.89	0.55
2:E:241:GLN:O	2:E:289:ARG:NH1	2.34	0.55
2:E:978:THR:HB	2:E:980:ALA:H	1.72	0.55
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.89	0.55
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.89	0.55
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.89	0.55
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.88	0.55
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.89	0.55
2:B:978:THR:HB	2:B:980:ALA:H	1.72	0.54
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.89	0.54
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.78	0.54
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.41	0.54
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.89	0.54
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.90	0.54
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.41	0.54
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.73	0.54
2:E:132:ALA:HA	2:E:194:SER:HB2	1.90	0.54
2:E:451:TYR:O	2:E:474:ARG:NH1	2.41	0.54
2:B:132:ALA:HA	2:B:194:SER:HB2	1.90	0.54
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.90	0.54
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.73	0.54
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.78	0.54
2:E:315:CYS:SG	2:E:316:PHE:N	2.81	0.54
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:87:HIS:H	1:F:91:ILE:HB	1.73	0.54
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.89	0.54
2:B:2342:ASN:N	2:B:2342:ASN:OD1	2.41	0.54
2:B:315:CYS:SG	2:B:316:PHE:N	2.81	0.54
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.73	0.54
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.41	0.54
2:B:3675:ASP:OD1	2:B:3769:ARG:NH2	2.39	0.54
2:G:132:ALA:HA	2:G:194:SER:HB2	1.90	0.54
2:I:132:ALA:HA	2:I:194:SER:HB2	1.90	0.54
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.73	0.53
2:G:315:CYS:SG	2:G:316:PHE:N	2.81	0.53
2:G:3675:ASP:OD1	2:G:3769:ARG:NH2	2.39	0.53
2:I:978:THR:HB	2:I:980:ALA:H	1.72	0.53
2:B:313:SER:HB3	2:B:351:VAL:HB	1.90	0.53
2:G:978:THR:HB	2:G:980:ALA:H	1.72	0.53
2:I:2342:ASN:N	2:I:2342:ASN:OD1	2.41	0.53
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.90	0.53
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.90	0.53
1:H:87:HIS:H	1:H:91:ILE:HB	1.73	0.53
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.91	0.53
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.89	0.53
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.90	0.53
2:B:2420:HIS:ND1	2:B:2493:UNK:O	2.37	0.53
1:J:87:HIS:H	1:J:91:ILE:HB	1.73	0.53
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.90	0.53
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.91	0.53
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.91	0.53
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.41	0.53
2:I:645:ARG:HH11	2:I:778:PHE:HE1	1.57	0.53
1:A:87:HIS:H	1:A:91:ILE:HB	1.73	0.53
2:G:451:TYR:O	2:G:474:ARG:NH1	2.41	0.53
2:G:645:ARG:HH11	2:G:778:PHE:HE1	1.57	0.53
2:I:313:SER:HB3	2:I:351:VAL:HB	1.90	0.53
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.91	0.53
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.74	0.53
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.89	0.52
2:I:4075:GLU:HA	2:I:4078:GLN:HB2	1.91	0.52
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.91	0.52
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.91	0.52
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.74	0.52
2:B:2452:ARG:HH12	2:I:177:GLU:HG3	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2420:HIS:ND1	2:I:2493:UNK:O	2.37	0.52
2:I:315:CYS:SG	2:I:316:PHE:N	2.81	0.52
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.90	0.52
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.43	0.52
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.92	0.52
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.90	0.52
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.74	0.52
2:B:683:ARG:NH1	2:B:707:VAL:O	2.40	0.52
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.74	0.52
2:G:4075:GLU:HA	2:G:4078:GLN:HB2	1.91	0.52
2:G:776:LEU:HG	2:G:848:HIS:HA	1.91	0.52
2:B:645:ARG:HH11	2:B:778:PHE:HE1	1.57	0.52
2:B:776:LEU:HG	2:B:848:HIS:HA	1.91	0.52
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.92	0.52
2:E:776:LEU:HG	2:E:848:HIS:HA	1.91	0.52
2:I:4063:ASP:O	2:I:4067:LYS:NZ	2.37	0.52
2:I:4791:TYR:OH	2:I:4815:ASP:O	2.28	0.52
2:B:4063:ASP:O	2:B:4067:LYS:NZ	2.37	0.52
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.91	0.52
2:E:4791:TYR:OH	2:E:4815:ASP:O	2.28	0.52
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.74	0.52
2:I:776:LEU:HG	2:I:848:HIS:HA	1.91	0.52
2:E:313:SER:HB3	2:E:351:VAL:HB	1.90	0.52
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.43	0.52
2:G:313:SER:HB3	2:G:351:VAL:HB	1.91	0.52
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.92	0.52
2:B:4791:TYR:OH	2:B:4815:ASP:O	2.28	0.52
2:G:2342:ASN:N	2:G:2342:ASN:OD1	2.41	0.52
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.91	0.52
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.37	0.51
2:E:645:ARG:HH11	2:E:778:PHE:HE1	1.57	0.51
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.90	0.51
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.43	0.51
2:B:1685:LEU:HD22	2:B:1718:ILE:HG21	1.92	0.51
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.44	0.51
2:G:4791:TYR:OH	2:G:4815:ASP:O	2.28	0.51
2:G:683:ARG:NH1	2:G:707:VAL:O	2.40	0.51
2:I:1865:MET:SD	2:I:1865:MET:N	2.84	0.51
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.43	0.51
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.92	0.51
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.93	0.51
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.74	0.51
2:B:451:TYR:O	2:B:474:ARG:NH1	2.41	0.51
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.92	0.51
2:B:689:THR:H	2:B:778:PHE:HE2	1.59	0.51
2:B:898:ASP:HB3	2:B:901:LYS:HB2	1.93	0.51
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.43	0.51
2:E:4075:GLU:HA	2:E:4078:GLN:HB2	1.91	0.51
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.92	0.51
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.93	0.51
2:E:1865:MET:SD	2:E:1865:MET:N	2.84	0.51
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.74	0.51
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.92	0.51
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.43	0.51
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.93	0.51
2:E:4983:HIS:N	2:E:4983:HIS:CD2	2.73	0.51
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.41	0.51
2:I:111:HIS:CD2	2:I:114:SER:H	2.28	0.51
2:I:1685:LEU:HD22	2:I:1718:ILE:HG21	1.92	0.51
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.93	0.51
2:B:4820:VAL:HB	2:B:4823:LEU:HD23	1.93	0.51
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.41	0.51
2:G:4820:VAL:HB	2:G:4823:LEU:HD23	1.93	0.51
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.93	0.51
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.92	0.51
2:I:451:TYR:O	2:I:474:ARG:NH1	2.41	0.51
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.93	0.51
2:B:111:HIS:CD2	2:B:114:SER:H	2.28	0.50
2:B:1865:MET:SD	2:B:1865:MET:N	2.84	0.50
2:B:4075:GLU:HA	2:B:4078:GLN:HB2	1.91	0.50
2:E:1516:UNK:N	2:E:1529:UNK:O	2.45	0.50
2:E:1991:THR:O	2:E:1995:THR:OG1	2.29	0.50
2:G:111:HIS:CD2	2:G:114:SER:H	2.28	0.50
2:G:1516:UNK:N	2:G:1529:UNK:O	2.44	0.50
2:B:1516:UNK:N	2:B:1529:UNK:O	2.45	0.50
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.43	0.50
2:B:2868:SER:O	2:B:2872:GLN:N	2.44	0.50
2:E:4820:VAL:HB	2:E:4823:LEU:HD23	1.93	0.50
2:E:689:THR:H	2:E:778:PHE:HE2	1.59	0.50
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.93	0.50
2:G:898:ASP:HB3	2:G:901:LYS:HB2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4820:VAL:HB	2:I:4823:LEU:HD23	1.93	0.50
2:E:1457:UNK:N	2:E:1497:UNK:O	2.44	0.50
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.92	0.50
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.92	0.50
2:I:580:GLU:HG3	2:I:620:LEU:HD22	1.94	0.50
2:I:689:THR:H	2:I:778:PHE:HE2	1.59	0.50
2:I:898:ASP:HB3	2:I:901:LYS:HB2	1.93	0.50
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.45	0.50
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.92	0.50
2:G:1457:UNK:N	2:G:1497:UNK:O	2.44	0.50
2:G:1865:MET:SD	2:G:1865:MET:N	2.84	0.50
2:G:265:LEU:HD12	2:G:279:PRO:HB2	1.94	0.50
2:G:580:GLU:HG3	2:G:620:LEU:HD22	1.94	0.50
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.92	0.50
2:B:3733:CYS:HB2	2:B:3803:SER:HB3	1.94	0.50
2:E:41:GLY:O	2:E:45:ARG:NH1	2.45	0.50
2:E:911:HIS:O	2:E:918:ARG:NH2	2.45	0.50
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.93	0.50
2:G:1991:THR:O	2:G:1995:THR:OG1	2.29	0.50
2:I:243:ARG:NH1	2:I:301:VAL:O	2.38	0.50
2:E:214:VAL:HG12	2:E:274:LEU:HD12	1.93	0.50
2:E:265:LEU:HD12	2:E:279:PRO:HB2	1.94	0.50
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.92	0.50
2:G:214:VAL:HG12	2:G:274:LEU:HD12	1.93	0.50
2:G:41:GLY:O	2:G:45:ARG:NH1	2.45	0.50
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.93	0.50
2:I:214:VAL:HG12	2:I:274:LEU:HD12	1.93	0.50
2:I:3675:ASP:OD1	2:I:3769:ARG:NH2	2.39	0.50
2:I:41:GLY:O	2:I:45:ARG:NH1	2.45	0.50
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.41	0.50
2:E:4571:PHE:O	2:E:4575:PHE:N	2.45	0.50
2:G:1685:LEU:HD22	2:G:1718:ILE:HG21	1.92	0.50
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.77	0.50
2:I:1457:UNK:N	2:I:1497:UNK:O	2.44	0.50
2:I:1516:UNK:N	2:I:1529:UNK:O	2.45	0.50
2:I:1991:THR:O	2:I:1995:THR:OG1	2.29	0.50
2:I:683:ARG:NH1	2:I:707:VAL:O	2.40	0.50
2:B:214:VAL:HG12	2:B:274:LEU:HD12	1.93	0.50
2:B:265:LEU:HD12	2:B:279:PRO:HB2	1.94	0.50
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.94	0.50
2:E:2868:SER:O	2:E:2872:GLN:N	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4832:HIS:NE2	2:E:4942:GLU:OE2	2.45	0.50
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.77	0.50
2:G:911:HIS:O	2:G:918:ARG:NH2	2.45	0.50
2:I:265:LEU:HD12	2:I:279:PRO:HB2	1.94	0.50
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.94	0.49
2:B:1457:UNK:N	2:B:1497:UNK:O	2.44	0.49
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.94	0.49
2:B:41:GLY:O	2:B:45:ARG:NH1	2.45	0.49
2:E:3733:CYS:HB2	2:E:3803:SER:HB3	1.94	0.49
2:G:689:THR:H	2:G:778:PHE:HE2	1.59	0.49
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.93	0.49
2:B:1991:THR:O	2:B:1995:THR:OG1	2.29	0.49
2:B:4571:PHE:O	2:B:4575:PHE:N	2.45	0.49
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.45	0.49
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.45	0.49
2:I:4832:HIS:NE2	2:I:4942:GLU:OE2	2.45	0.49
2:B:1973:GLN:O	2:B:1977:TYR:N	2.40	0.49
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.94	0.49
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.46	0.49
2:G:4063:ASP:O	2:G:4067:LYS:NZ	2.37	0.49
2:B:4832:HIS:NE2	2:B:4942:GLU:OE2	2.45	0.49
2:G:4571:PHE:O	2:G:4575:PHE:N	2.45	0.49
2:B:1171:SER:OG	2:B:1175:SER:N	2.43	0.49
2:B:2876:GLU:OE1	2:B:2920:ARG:NH2	2.46	0.49
2:B:911:HIS:O	2:B:918:ARG:NH2	2.45	0.49
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.77	0.49
2:E:1685:LEU:HD22	2:E:1718:ILE:HG21	1.93	0.49
2:E:2876:GLU:OE1	2:E:2920:ARG:NH2	2.46	0.49
2:G:2868:SER:O	2:G:2872:GLN:N	2.44	0.49
2:I:3733:CYS:HB2	2:I:3803:SER:HB3	1.94	0.49
2:B:243:ARG:NH1	2:B:301:VAL:O	2.38	0.49
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.94	0.49
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.45	0.49
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.77	0.49
2:G:4832:HIS:NE2	2:G:4942:GLU:OE2	2.45	0.49
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.95	0.49
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.95	0.49
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.46	0.49
2:E:898:ASP:HB3	2:E:901:LYS:HB2	1.93	0.49
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.46	0.49
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:580:GLU:HG3	2:B:620:LEU:HD22	1.94	0.49
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.95	0.49
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.95	0.49
2:I:4571:PHE:O	2:I:4575:PHE:N	2.45	0.49
2:E:111:HIS:CD2	2:E:114:SER:H	2.28	0.48
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.46	0.48
2:E:4063:ASP:O	2:E:4067:LYS:NZ	2.37	0.48
2:I:2758:PHE:O	2:I:2762:THR:N	2.43	0.48
2:I:911:HIS:O	2:I:918:ARG:NH2	2.45	0.48
2:G:2876:GLU:OE1	2:G:2920:ARG:NH2	2.46	0.48
1:J:5:GLU:HB2	1:J:73:LYS:HB3	1.95	0.48
2:E:580:GLU:HG3	2:E:620:LEU:HD22	1.94	0.48
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.46	0.48
2:G:3733:CYS:HB2	2:G:3803:SER:HB3	1.94	0.48
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.94	0.48
2:I:3755:GLU:O	2:I:3762:ARG:NH2	2.44	0.48
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.95	0.48
1:A:5:GLU:HB2	1:A:73:LYS:HB3	1.95	0.48
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.46	0.48
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.96	0.48
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.96	0.48
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.94	0.48
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	1.96	0.48
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	1.96	0.48
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	1.96	0.48
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.95	0.48
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	1.96	0.48
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.96	0.48
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	1.96	0.48
2:B:792:LEU:HB3	2:B:798:GLY:HA2	1.95	0.48
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.41	0.48
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	1.96	0.48
1:F:5:GLU:HB2	1:F:73:LYS:HB3	1.95	0.48
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.96	0.48
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.96	0.48
1:H:5:GLU:HB2	1:H:73:LYS:HB3	1.95	0.48
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.42	0.48
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.46	0.48
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.79	0.48
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.79	0.48
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.94	0.48
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.46	0.48
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.95	0.48
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.79	0.48
2:E:243:ARG:NH1	2:E:301:VAL:O	2.38	0.48
2:G:2103:VAL:O	2:G:2107:GLN:N	2.43	0.48
2:E:177:GLU:HG3	2:G:2452:ARG:HH12	1.79	0.48
2:G:243:ARG:NH1	2:G:301:VAL:O	2.38	0.48
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.79	0.48
2:E:4582:VAL:HG23	2:E:4629:TYR:HA	1.96	0.48
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.47	0.48
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.95	0.48
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.47	0.48
2:B:345:LEU:HD23	2:B:389:PHE:HB3	1.96	0.47
2:B:4942:GLU:HA	2:E:4944:ARG:HH22	1.78	0.47
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.95	0.47
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.96	0.47
2:B:756:SER:HB3	2:B:767:VAL:HG22	1.96	0.47
2:I:1171:SER:OG	2:I:1175:SER:N	2.43	0.47
2:I:2868:SER:O	2:I:2872:GLN:N	2.44	0.47
2:I:2876:GLU:OE1	2:I:2920:ARG:NH2	2.46	0.47
2:B:177:GLU:HG3	2:E:2452:ARG:HH12	1.79	0.47
2:E:606:LEU:O	2:E:617:ASN:ND2	2.47	0.47
2:G:756:SER:HB3	2:G:767:VAL:HG22	1.96	0.47
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.97	0.47
2:E:3675:ASP:OD1	2:E:3769:ARG:NH2	2.39	0.47
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.96	0.47
2:G:345:LEU:HD23	2:G:389:PHE:HB3	1.96	0.47
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.79	0.47
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.79	0.47
2:B:4582:VAL:HG23	2:B:4629:TYR:HA	1.96	0.47
2:G:792:LEU:HB3	2:G:798:GLY:HA2	1.95	0.47
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.97	0.47
2:B:4673:ARG:HH22	2:B:4698:LYS:HE3	1.80	0.47
2:E:331:VAL:HG12	2:E:333:GLY:H	1.79	0.47
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.80	0.47
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.97	0.47
2:G:606:LEU:O	2:G:617:ASN:ND2	2.48	0.47
2:I:756:SER:HB3	2:I:767:VAL:HG22	1.96	0.47
2:B:2758:PHE:O	2:B:2762:THR:N	2.43	0.47
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:331:VAL:HG12	2:G:333:GLY:H	1.79	0.47
2:I:331:VAL:HG12	2:I:333:GLY:H	1.79	0.47
2:I:345:LEU:HD23	2:I:389:PHE:HB3	1.96	0.47
2:B:331:VAL:HG12	2:B:333:GLY:H	1.79	0.47
2:B:606:LEU:O	2:B:617:ASN:ND2	2.47	0.47
2:E:345:LEU:HD23	2:E:389:PHE:HB3	1.96	0.47
2:E:4673:ARG:HH22	2:E:4698:LYS:HE3	1.80	0.47
2:E:792:LEU:HB3	2:E:798:GLY:HA2	1.95	0.47
2:I:606:LEU:O	2:I:617:ASN:ND2	2.47	0.47
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.50	0.47
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.50	0.47
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.79	0.47
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.80	0.47
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.50	0.47
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.50	0.47
2:I:4673:ARG:HH22	2:I:4698:LYS:HE3	1.80	0.47
2:I:792:LEU:HB3	2:I:798:GLY:HA2	1.95	0.47
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	1.96	0.47
2:G:4152:GLU:OE2	2:G:4180:ARG:NH1	2.48	0.47
2:E:756:SER:HB3	2:E:767:VAL:HG22	1.96	0.47
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	1.96	0.47
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.97	0.46
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.47	0.46
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.98	0.46
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	1.98	0.46
2:E:2758:PHE:O	2:E:2762:THR:N	2.43	0.46
2:E:4152:GLU:OE2	2:E:4180:ARG:NH1	2.48	0.46
2:E:4767:TRP:HE3	2:E:4770:SER:HB2	1.80	0.46
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	1.98	0.46
2:G:1171:SER:OG	2:G:1175:SER:N	2.43	0.46
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.98	0.46
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.79	0.46
2:I:1976:ARG:NH1	2:I:1997:GLU:OE2	2.49	0.46
2:I:2103:VAL:O	2:I:2107:GLN:N	2.43	0.46
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.47	0.46
2:B:1976:ARG:NH1	2:B:1997:GLU:OE2	2.49	0.46
2:B:4101:LYS:HE3	2:I:4731:ILE:HA	1.97	0.46
2:E:1976:ARG:NH1	2:E:1997:GLU:OE2	2.49	0.46
2:E:683:ARG:NH1	2:E:707:VAL:O	2.40	0.46
2:B:792:LEU:HD22	2:B:799:GLU:H	1.81	0.46
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:792:LEU:HD22	2:E:799:GLU:H	1.81	0.46
1:F:82:TYR:O	1:F:86:GLY:N	2.46	0.46
2:G:4582:VAL:HG23	2:G:4629:TYR:HA	1.96	0.46
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	1.98	0.46
2:I:1965:TYR:OH	2:I:2027:ILE:O	2.29	0.46
2:I:4582:VAL:HG23	2:I:4629:TYR:HA	1.96	0.46
2:B:1099:GLU:OE2	2:B:1127:HIS:ND1	2.35	0.46
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.98	0.46
2:G:1976:ARG:NH1	2:G:1997:GLU:OE2	2.49	0.46
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.97	0.46
2:I:164:ARG:N	2:I:167:ASP:OD2	2.49	0.46
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.96	0.46
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.80	0.46
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.81	0.46
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.98	0.46
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.98	0.46
2:E:70:GLU:HG3	2:E:117:TYR:HE1	1.80	0.46
2:G:1973:GLN:O	2:G:1977:TYR:N	2.40	0.46
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.96	0.46
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	1.98	0.46
2:I:792:LEU:HD22	2:I:799:GLU:H	1.81	0.46
2:B:70:GLU:HG3	2:B:117:TYR:HE1	1.80	0.46
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.81	0.46
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	1.98	0.46
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.98	0.46
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.98	0.46
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.98	0.46
2:G:4673:ARG:HH22	2:G:4698:LYS:HE3	1.80	0.46
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	1.98	0.46
2:B:164:ARG:N	2:B:167:ASP:OD2	2.49	0.46
2:B:2894:LEU:HD11	2:B:2902:HIS:HB2	1.98	0.46
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.80	0.46
2:B:4152:GLU:OE2	2:B:4180:ARG:NH1	2.48	0.46
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.98	0.46
2:G:3897:ASN:O	2:G:3901:ASN:ND2	2.49	0.46
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.80	0.46
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	1.98	0.46
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.97	0.46
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.37	0.46
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.99	0.46
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:164:ARG:N	2:G:167:ASP:OD2	2.49	0.46
2:I:1077:ALA:HB3	2:I:1189:LEU:HD11	1.98	0.46
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.97	0.46
2:I:4767:TRP:HE3	2:I:4770:SER:HB2	1.80	0.46
2:B:4767:TRP:HE3	2:B:4770:SER:HB2	1.80	0.45
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.97	0.45
2:E:3362:UNK:O	2:E:3366:UNK:N	2.49	0.45
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.81	0.45
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.98	0.45
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.97	0.45
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.81	0.45
2:I:70:GLU:HG3	2:I:117:TYR:HE1	1.80	0.45
2:I:3362:UNK:O	2:I:3366:UNK:N	2.49	0.45
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	1.98	0.45
2:B:215:THR:HG22	2:B:273:HIS:HA	1.99	0.45
2:B:3897:ASN:O	2:B:3901:ASN:ND2	2.49	0.45
2:E:164:ARG:N	2:E:167:ASP:OD2	2.49	0.45
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.98	0.45
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.81	0.45
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.98	0.45
2:I:3897:ASN:O	2:I:3901:ASN:ND2	2.49	0.45
2:I:4081:VAL:HB	2:I:4088:ILE:HD12	1.98	0.45
2:I:4152:GLU:OE2	2:I:4180:ARG:NH1	2.48	0.45
2:B:626:LEU:HG	2:B:628:GLY:H	1.82	0.45
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.98	0.45
2:E:1735:ILE:HG23	2:E:1771:LEU:HD23	1.98	0.45
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.98	0.45
2:G:3362:UNK:O	2:G:3366:UNK:N	2.49	0.45
1:H:30:LEU:HD23	1:H:33:GLY:HA3	1.99	0.45
2:I:1099:GLU:OE2	2:I:1127:HIS:ND1	2.35	0.45
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.98	0.45
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.98	0.45
2:I:278:GLN:N	2:I:315:CYS:SG	2.90	0.45
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	1.98	0.45
2:B:3362:UNK:O	2:B:3366:UNK:N	2.49	0.45
2:B:4697:VAL:O	2:B:4701:TRP:N	2.49	0.45
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.97	0.45
2:E:2103:VAL:O	2:E:2107:GLN:N	2.43	0.45
2:E:4835:LYS:HG3	2:E:4836:GLN:HG3	1.98	0.45
2:E:626:LEU:HG	2:E:628:GLY:H	1.82	0.45
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1105:ALA:N	2:E:1189:LEU:O	2.50	0.45
2:E:1973:GLN:O	2:E:1977:TYR:N	2.40	0.45
2:E:3897:ASN:O	2:E:3901:ASN:ND2	2.49	0.45
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.97	0.45
2:G:1077:ALA:HB3	2:G:1189:LEU:HD11	1.98	0.45
2:G:1105:ALA:N	2:G:1189:LEU:O	2.50	0.45
2:G:1838:PHE:HB3	2:G:1842:LEU:HD11	1.99	0.45
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.98	0.45
2:I:2894:LEU:HD11	2:I:2902:HIS:HB2	1.98	0.45
2:I:463:GLU:O	2:I:466:SER:OG	2.30	0.45
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	1.98	0.45
2:B:4081:VAL:HB	2:B:4088:ILE:HD12	1.98	0.45
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.99	0.45
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	1.98	0.45
2:E:278:GLN:N	2:E:315:CYS:SG	2.90	0.45
2:E:4081:VAL:HB	2:E:4088:ILE:HD12	1.98	0.45
2:G:2758:PHE:O	2:G:2762:THR:N	2.43	0.45
2:G:395:GLN:HG3	2:G:397:GLU:H	1.82	0.45
2:G:4767:TRP:HE3	2:G:4770:SER:HB2	1.80	0.45
2:G:792:LEU:HD22	2:G:799:GLU:H	1.81	0.45
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.98	0.45
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.98	0.45
2:B:823:LEU:HD23	2:B:1626:TRP:HB3	1.99	0.45
2:B:1838:PHE:HB3	2:B:1842:LEU:HD11	1.99	0.45
2:E:1838:PHE:HB3	2:E:1842:LEU:HD11	1.99	0.45
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.98	0.45
2:E:21:VAL:HG12	2:E:66:CYS:HA	1.99	0.45
2:G:168:ASP:HB3	2:G:199:LEU:HD22	1.99	0.45
2:G:4081:VAL:HB	2:G:4088:ILE:HD12	1.98	0.45
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	1.98	0.45
2:B:21:VAL:HG12	2:B:66:CYS:HA	1.99	0.45
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.80	0.45
2:B:4956:THR:O	2:B:4965:SER:N	2.48	0.45
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	1.98	0.45
2:E:823:LEU:HD23	2:E:1626:TRP:HB3	1.99	0.45
2:E:215:THR:HG22	2:E:273:HIS:HA	1.99	0.45
2:G:70:GLU:HG3	2:G:117:TYR:HE1	1.80	0.45
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.98	0.45
2:G:4835:LYS:HG3	2:G:4836:GLN:HG3	1.98	0.45
2:I:1114:GLU:HG3	2:I:1117:ALA:HB2	1.99	0.45
2:I:215:THR:HG22	2:I:273:HIS:HA	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.99	0.45
2:B:1105:ALA:N	2:B:1189:LEU:O	2.50	0.45
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	1.99	0.45
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.50	0.45
2:E:168:ASP:HB3	2:E:199:LEU:HD22	1.99	0.45
2:E:4201:ASN:ND2	2:E:4204:GLN:OE1	2.49	0.45
2:G:1269:CYS:HA	2:G:1473:UNK:HA	1.99	0.45
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.50	0.45
2:G:4201:ASN:ND2	2:G:4204:GLN:OE1	2.49	0.45
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.52	0.45
2:B:1077:ALA:HB3	2:B:1189:LEU:HD11	1.98	0.45
2:B:1114:GLU:HG3	2:B:1117:ALA:HB2	1.99	0.45
2:B:1269:CYS:HA	2:B:1473:UNK:HA	1.99	0.45
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.99	0.45
2:B:4201:ASN:ND2	2:B:4204:GLN:OE1	2.49	0.45
2:B:4835:LYS:HG3	2:B:4836:GLN:HG3	1.98	0.45
1:F:30:LEU:HD23	1:F:33:GLY:HA3	1.99	0.45
2:G:2121:PHE:O	2:G:3725:TYR:OH	2.35	0.45
2:G:3990:VAL:HG13	2:G:4051:SER:HB2	1.99	0.45
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.99	0.45
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	1.99	0.45
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.98	0.45
2:B:2257:LEU:O	2:B:2261:SER:N	2.50	0.44
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.83	0.44
2:B:3755:GLU:O	2:B:3762:ARG:NH2	2.44	0.44
2:E:1077:ALA:HB3	2:E:1189:LEU:HD11	1.98	0.44
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.99	0.44
2:G:278:GLN:N	2:G:315:CYS:SG	2.90	0.44
2:I:1735:ILE:HG23	2:I:1771:LEU:HD23	1.98	0.44
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	1.98	0.44
2:I:3992:PHE:O	2:I:3996:PHE:N	2.40	0.44
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.99	0.44
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.98	0.44
2:E:3758:MET:HE2	2:E:3762:ARG:HH21	1.82	0.44
2:G:21:VAL:HG12	2:G:66:CYS:HA	1.99	0.44
2:G:3365:UNK:O	2:G:3369:UNK:N	2.50	0.44
2:I:1269:CYS:HA	2:I:1473:UNK:HA	1.99	0.44
2:I:1838:PHE:HB3	2:I:1842:LEU:HD11	1.99	0.44
2:I:4835:LYS:HG3	2:I:4836:GLN:HG3	1.98	0.44
2:I:4956:THR:O	2:I:4965:SER:N	2.48	0.44
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:82:TYR:O	1:J:86:GLY:N	2.46	0.44
2:B:168:ASP:HB3	2:B:199:LEU:HD22	1.99	0.44
2:B:3990:VAL:HG13	2:B:4051:SER:HB2	1.99	0.44
2:E:1114:GLU:HG3	2:E:1117:ALA:HB2	1.99	0.44
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.52	0.44
2:E:395:GLN:HG3	2:E:397:GLU:H	1.82	0.44
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.50	0.44
2:E:4697:VAL:O	2:E:4701:TRP:N	2.49	0.44
2:E:4802:GLY:HA2	2:E:4808:PHE:HB2	1.99	0.44
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.99	0.44
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.98	0.44
2:G:4697:VAL:O	2:G:4701:TRP:N	2.49	0.44
2:I:1973:GLN:O	2:I:1977:TYR:N	2.40	0.44
2:I:309:THR:O	2:I:313:SER:OG	2.35	0.44
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.50	0.44
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.99	0.44
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.91	0.44
2:B:3758:MET:HE2	2:B:3762:ARG:HH21	1.83	0.44
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.99	0.44
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.82	0.44
2:E:2894:LEU:HD11	2:E:2902:HIS:HB2	1.98	0.44
2:G:823:LEU:HD23	2:G:1626:TRP:HB3	1.99	0.44
2:G:2894:LEU:HD11	2:G:2902:HIS:HB2	1.98	0.44
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.99	0.44
2:I:21:VAL:HG12	2:I:66:CYS:HA	1.99	0.44
2:I:4201:ASN:ND2	2:I:4204:GLN:OE1	2.50	0.44
2:I:652:ARG:HD2	2:I:750:LEU:HB3	1.99	0.44
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	1.98	0.44
2:B:3764:LEU:HD21	2:B:3809:ASN:HD21	1.82	0.44
2:E:2257:LEU:O	2:E:2261:SER:N	2.50	0.44
2:E:3365:UNK:O	2:E:3369:UNK:N	2.50	0.44
2:G:1114:GLU:HG3	2:G:1117:ALA:HB2	1.99	0.44
2:G:1735:ILE:HG23	2:G:1771:LEU:HD23	1.98	0.44
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	2.00	0.44
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	1.98	0.44
2:G:4667:PRO:O	2:G:4714:ASN:ND2	2.48	0.44
2:G:626:LEU:HG	2:G:628:GLY:H	1.82	0.44
2:I:1708:ARG:HG2	2:I:1711:TYR:CE2	2.53	0.44
2:I:168:ASP:HB3	2:I:199:LEU:HD22	1.99	0.44
2:I:3990:VAL:HG13	2:I:4051:SER:HB2	1.99	0.44
2:B:1708:ARG:HG2	2:B:1711:TYR:CE2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.98	0.44
2:B:179:TYR:OH	2:E:2359:ARG:NH1	2.42	0.44
2:B:309:THR:O	2:B:313:SER:OG	2.35	0.44
2:B:395:GLN:HG3	2:B:397:GLU:H	1.82	0.44
2:B:652:ARG:HD2	2:B:750:LEU:HB3	1.99	0.44
2:E:1269:CYS:HA	2:E:1473:UNK:HA	1.99	0.44
2:E:864:PRO:HD2	2:E:867:LEU:HD12	1.99	0.44
2:G:2257:LEU:O	2:G:2261:SER:N	2.50	0.44
2:G:864:PRO:HD2	2:G:867:LEU:HD12	1.99	0.44
2:I:2121:PHE:O	2:I:3725:TYR:OH	2.35	0.44
2:I:2517:UNK:O	2:I:2521:UNK:N	2.51	0.44
2:I:3764:LEU:HD21	2:I:3809:ASN:HD21	1.82	0.44
2:I:4075:GLU:O	2:I:4079:ASP:N	2.51	0.44
2:I:4208:PRO:HA	2:I:4211:LYS:HB3	2.00	0.44
2:I:626:LEU:HG	2:I:628:GLY:H	1.82	0.44
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.99	0.44
2:B:719:LEU:HD22	2:B:735:GLN:HG2	2.00	0.44
2:E:3990:VAL:HG13	2:E:4051:SER:HB2	1.99	0.44
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.83	0.44
2:G:3758:MET:HE2	2:G:3762:ARG:HH21	1.83	0.44
2:G:719:LEU:HD22	2:G:735:GLN:HG2	2.00	0.44
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.91	0.44
2:I:4826:ILE:O	2:I:4829:SER:OG	2.29	0.44
2:I:864:PRO:HD2	2:I:867:LEU:HD12	1.99	0.44
1:J:30:LEU:HD23	1:J:33:GLY:HA3	1.99	0.44
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.52	0.44
2:B:404:ILE:HG21	2:B:481:GLU:HG3	2.00	0.44
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	1.99	0.44
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	1.99	0.44
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.91	0.44
2:G:4208:PRO:HA	2:G:4211:LYS:HB3	2.00	0.44
2:I:1105:ALA:N	2:I:1189:LEU:O	2.50	0.44
2:I:823:LEU:HD23	2:I:1626:TRP:HB3	1.99	0.44
2:I:2257:LEU:O	2:I:2261:SER:N	2.50	0.44
2:I:3365:UNK:O	2:I:3369:UNK:N	2.50	0.44
2:I:3729:MET:O	2:I:3732:SER:OG	2.32	0.44
2:B:3365:UNK:O	2:B:3369:UNK:N	2.50	0.44
2:B:356:TRP:O	2:B:379:HIS:N	2.51	0.44
2:B:4667:PRO:O	2:B:4714:ASN:ND2	2.48	0.44
2:B:4802:GLY:HA2	2:B:4808:PHE:HB2	1.99	0.44
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2517:UNK:O	2:E:2521:UNK:N	2.51	0.44
2:E:3959:LYS:O	2:E:3963:ASN:ND2	2.51	0.44
2:E:4075:GLU:O	2:E:4079:ASP:N	2.50	0.44
2:E:4942:GLU:HA	2:G:4944:ARG:HH22	1.83	0.44
2:G:2517:UNK:O	2:G:2521:UNK:N	2.51	0.44
2:G:215:THR:HG22	2:G:273:HIS:HA	1.99	0.44
2:G:3755:GLU:O	2:G:3762:ARG:NH2	2.44	0.44
2:G:3764:LEU:HD21	2:G:3809:ASN:HD21	1.83	0.44
2:G:3959:LYS:O	2:G:3963:ASN:ND2	2.51	0.44
2:G:4075:GLU:O	2:G:4079:ASP:N	2.51	0.44
2:I:4802:GLY:HA2	2:I:4808:PHE:HB2	1.99	0.44
2:I:404:ILE:HG21	2:I:481:GLU:HG3	2.00	0.44
1:A:30:LEU:HD23	1:A:33:GLY:HA3	1.99	0.43
2:B:3552:UNK:O	2:B:3556:UNK:N	2.51	0.43
2:B:560:ILE:HA	2:B:563:VAL:HG12	2.00	0.43
2:B:864:PRO:HD2	2:B:867:LEU:HD12	1.99	0.43
2:E:1171:SER:OG	2:E:1175:SER:N	2.43	0.43
2:E:1708:ARG:HG2	2:E:1711:TYR:CE2	2.53	0.43
2:E:4956:THR:O	2:E:4965:SER:N	2.48	0.43
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.41	0.43
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.52	0.43
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.98	0.43
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.83	0.43
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.83	0.43
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.99	0.43
2:I:4697:VAL:O	2:I:4701:TRP:N	2.49	0.43
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.91	0.43
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.83	0.43
2:G:3963:ASN:O	2:G:3966:THR:OG1	2.33	0.43
2:I:3552:UNK:O	2:I:3556:UNK:N	2.51	0.43
2:I:4667:PRO:O	2:I:4714:ASN:ND2	2.48	0.43
2:I:560:ILE:HA	2:I:563:VAL:HG12	2.00	0.43
2:I:719:LEU:HD22	2:I:735:GLN:HG2	2.00	0.43
1:A:26:TYR:OH	1:A:42:ARG:NH2	2.52	0.43
2:B:4208:PRO:HA	2:B:4211:LYS:HB3	2.00	0.43
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	2.00	0.43
2:E:3948:LYS:HG2	2:E:4012:LEU:HD22	2.01	0.43
2:E:652:ARG:HD2	2:E:750:LEU:HB3	1.99	0.43
2:G:1708:ARG:HG2	2:G:1711:TYR:CE2	2.53	0.43
1:H:82:TYR:O	1:H:86:GLY:N	2.46	0.43
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1131:ARG:NH1	2:I:1178:ALA:O	2.52	0.43
2:I:3927:GLN:O	2:I:3931:SER:N	2.51	0.43
2:I:4066:LEU:HD11	2:I:4173:TYR:CG	2.53	0.43
2:B:1131:ARG:NH1	2:B:1178:ALA:O	2.52	0.43
2:B:2517:UNK:O	2:B:2521:UNK:N	2.51	0.43
2:B:278:GLN:N	2:B:315:CYS:SG	2.90	0.43
2:B:4075:GLU:O	2:B:4079:ASP:N	2.51	0.43
2:E:3552:UNK:O	2:E:3556:UNK:N	2.51	0.43
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.52	0.43
2:G:404:ILE:HG21	2:G:481:GLU:HG3	2.00	0.43
2:G:4956:THR:O	2:G:4965:SER:N	2.48	0.43
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.84	0.43
2:I:3758:MET:HE2	2:I:3762:ARG:HH21	1.83	0.43
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	2.00	0.43
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	2.00	0.43
2:E:2121:PHE:O	2:E:3725:TYR:OH	2.35	0.43
2:E:404:ILE:HG21	2:E:481:GLU:HG3	2.00	0.43
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	2.00	0.43
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	2.01	0.43
2:G:309:THR:O	2:G:313:SER:OG	2.35	0.43
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.52	0.43
2:B:3674:ILE:HB	2:B:3769:ARG:HH21	1.84	0.43
2:B:3948:LYS:HG2	2:B:4012:LEU:HD22	2.01	0.43
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.99	0.43
2:E:793:LEU:HB2	2:E:797:HIS:H	1.84	0.43
1:F:26:TYR:OH	1:F:42:ARG:NH2	2.52	0.43
2:G:4802:GLY:HA2	2:G:4808:PHE:HB2	1.99	0.43
2:G:4976:GLU:O	2:G:4979:THR:OG1	2.35	0.43
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	2.00	0.43
2:I:3963:ASN:O	2:I:3966:THR:OG1	2.33	0.43
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.84	0.43
2:B:4944:ARG:HH22	2:I:4942:GLU:HA	1.83	0.43
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.99	0.43
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.99	0.43
2:I:395:GLN:HG3	2:I:397:GLU:H	1.82	0.43
2:I:734:GLY:O	2:I:736:HIS:ND1	2.52	0.43
2:E:356:TRP:O	2:E:379:HIS:N	2.51	0.43
2:I:3765:TYR:OH	2:I:4755:GLU:O	2.34	0.43
2:I:681:HIS:HB3	2:I:784:SER:HB3	2.01	0.43
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.83	0.43
2:B:4066:LEU:HD11	2:B:4173:TYR:CG	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:591:ASP:O	2:B:1594:ARG:NH2	2.52	0.43
2:B:750:LEU:HD21	2:B:777:PHE:HE2	1.84	0.43
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	2.00	0.43
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.84	0.43
2:G:1131:ARG:NH1	2:G:1178:ALA:O	2.52	0.43
2:G:3674:ILE:HB	2:G:3769:ARG:HH21	1.84	0.43
2:G:4066:LEU:HD11	2:G:4173:TYR:CG	2.53	0.43
2:G:652:ARG:HD2	2:G:750:LEU:HB3	1.99	0.43
2:G:750:LEU:HD21	2:G:777:PHE:HE2	1.84	0.43
2:I:3959:LYS:O	2:I:3963:ASN:ND2	2.51	0.43
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	2.00	0.43
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	2.00	0.43
2:B:4857:ASN:HB2	2:E:4807:PHE:HZ	1.84	0.43
2:E:719:LEU:HD22	2:E:735:GLN:HG2	2.00	0.43
2:E:750:LEU:HD21	2:E:777:PHE:HE2	1.84	0.43
2:G:3676:ASP:N	2:G:3676:ASP:OD1	2.52	0.43
2:G:356:TRP:O	2:G:379:HIS:N	2.51	0.43
2:G:3948:LYS:HG2	2:G:4012:LEU:HD22	2.01	0.43
2:I:4944:ARG:HH22	2:G:4942:GLU:HA	1.83	0.43
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.52	0.43
2:I:2452:ARG:HH12	2:G:177:GLU:HG3	1.84	0.43
2:B:3959:LYS:O	2:B:3963:ASN:ND2	2.51	0.42
2:B:734:GLY:O	2:B:736:HIS:ND1	2.52	0.42
2:E:1131:ARG:NH1	2:E:1178:ALA:O	2.52	0.42
2:E:309:THR:O	2:E:313:SER:OG	2.35	0.42
2:E:3361:UNK:O	2:E:3365:UNK:N	2.52	0.42
2:E:4208:PRO:HA	2:E:4211:LYS:HB3	2.00	0.42
2:E:4713:SER:HG	2:E:4775:TYR:HH	1.67	0.42
2:E:591:ASP:O	2:E:1594:ARG:NH2	2.52	0.42
2:G:591:ASP:O	2:G:1594:ARG:NH2	2.52	0.42
2:G:1954:ARG:HE	2:G:2041:HIS:HD2	1.67	0.42
2:I:2022:PRO:HB2	2:I:2024:PRO:HD2	2.01	0.42
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.84	0.42
2:E:1954:ARG:HE	2:E:2041:HIS:HD2	1.67	0.42
2:G:3552:UNK:O	2:G:3556:UNK:N	2.51	0.42
2:G:793:LEU:HB2	2:G:797:HIS:H	1.84	0.42
2:I:1954:ARG:HE	2:I:2041:HIS:HD2	1.68	0.42
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	2.00	0.42
2:I:356:TRP:O	2:I:379:HIS:N	2.51	0.42
2:I:3948:LYS:HG2	2:I:4012:LEU:HD22	2.01	0.42
2:I:793:LEU:HB2	2:I:797:HIS:H	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:600:LEU:O	2:B:604:CYS:N	2.50	0.42
2:B:793:LEU:HB2	2:B:797:HIS:H	1.84	0.42
2:E:1089:TYR:N	2:E:1224:GLU:O	2.52	0.42
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.83	0.42
2:E:3764:LEU:HD21	2:E:3809:ASN:HD21	1.83	0.42
2:G:3992:PHE:O	2:G:3996:PHE:N	2.40	0.42
2:G:600:LEU:O	2:G:604:CYS:N	2.50	0.42
2:I:3674:ILE:HB	2:I:3769:ARG:HH21	1.84	0.42
2:I:591:ASP:O	2:I:1594:ARG:NH2	2.52	0.42
2:I:750:LEU:HD21	2:I:777:PHE:HE2	1.84	0.42
2:B:681:HIS:HB3	2:B:784:SER:HB3	2.01	0.42
2:E:4066:LEU:HD11	2:E:4173:TYR:CG	2.53	0.42
2:E:560:ILE:HA	2:E:563:VAL:HG12	2.00	0.42
1:H:26:TYR:OH	1:H:42:ARG:NH2	2.52	0.42
2:I:3361:UNK:O	2:I:3365:UNK:N	2.52	0.42
2:B:1089:TYR:N	2:B:1224:GLU:O	2.52	0.42
2:B:4978:HIS:CE1	2:B:4983:HIS:NE2	2.87	0.42
2:E:2022:PRO:HB2	2:E:2024:PRO:HD2	2.01	0.42
2:E:734:GLY:O	2:E:736:HIS:ND1	2.52	0.42
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	2.00	0.42
2:G:3361:UNK:O	2:G:3365:UNK:N	2.52	0.42
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.01	0.42
2:I:1089:TYR:N	2:I:1224:GLU:O	2.52	0.42
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	2.02	0.42
2:B:2265:LEU:HD22	2:B:2330:ARG:HB3	2.02	0.42
2:B:3361:UNK:O	2:B:3365:UNK:N	2.52	0.42
2:B:4060:LYS:NZ	2:B:4064:MET:SD	2.93	0.42
2:E:1099:GLU:OE2	2:E:1127:HIS:ND1	2.35	0.42
2:E:2272:PRO:HA	2:E:2275:VAL:HG12	2.02	0.42
2:E:3805:LEU:H	2:E:3805:LEU:HG	1.77	0.42
2:G:3927:GLN:O	2:G:3931:SER:N	2.51	0.42
2:G:560:ILE:HA	2:G:563:VAL:HG12	2.00	0.42
1:A:82:TYR:O	1:A:86:GLY:N	2.46	0.42
2:B:1954:ARG:HE	2:B:2041:HIS:HD2	1.67	0.42
2:B:3676:ASP:N	2:B:3676:ASP:OD1	2.52	0.42
2:B:3927:GLN:O	2:B:3931:SER:N	2.51	0.42
2:G:35:LEU:HD13	2:G:49:LEU:HD13	2.01	0.42
2:I:2265:LEU:HD22	2:I:2330:ARG:HB3	2.02	0.42
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.85	0.42
2:E:3674:ILE:HB	2:E:3769:ARG:HH21	1.84	0.42
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.37	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.01	0.42
2:G:1099:GLU:OE2	2:G:1127:HIS:ND1	2.35	0.42
2:G:1089:TYR:N	2:G:1224:GLU:O	2.52	0.42
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	2.02	0.42
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.85	0.42
1:J:26:TYR:OH	1:J:42:ARG:NH2	2.52	0.42
2:B:1679:ASN:HA	2:B:1682:ALA:HB3	2.02	0.42
2:B:4056:GLU:O	2:B:4060:LYS:N	2.51	0.42
2:B:35:LEU:HD13	2:B:49:LEU:HD13	2.01	0.42
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	2.02	0.42
2:E:4060:LYS:NZ	2:E:4064:MET:SD	2.93	0.42
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	2.02	0.42
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	2.02	0.42
2:B:2022:PRO:HB2	2:B:2024:PRO:HD2	2.01	0.42
2:G:2272:PRO:HA	2:G:2275:VAL:HG12	2.02	0.42
2:I:1679:ASN:HA	2:I:1682:ALA:HB3	2.02	0.42
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	2.02	0.41
2:G:40:GLU:HB3	2:G:44:ASN:HB3	2.02	0.41
2:B:4071:ILE:HD11	2:B:4102:GLN:HE21	1.85	0.41
2:E:3963:ASN:O	2:E:3966:THR:OG1	2.33	0.41
2:E:40:GLU:HB3	2:E:44:ASN:HB3	2.02	0.41
2:G:2867:LEU:HB3	2:G:2871:LEU:HB2	2.02	0.41
2:I:317:ARG:HE	2:I:323:LEU:HD22	1.86	0.41
2:I:4060:LYS:NZ	2:I:4064:MET:SD	2.93	0.41
2:I:4071:ILE:HD11	2:I:4102:GLN:HE21	1.85	0.41
2:I:35:LEU:HD13	2:I:49:LEU:HD13	2.01	0.41
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	2.02	0.41
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.86	0.41
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	2.02	0.41
2:I:2196:ASN:OD1	2:I:2199:ARG:NH1	2.41	0.41
2:B:2272:PRO:HA	2:B:2275:VAL:HG12	2.02	0.41
2:B:2466:LEU:HD23	2:B:2469:ILE:HD12	2.02	0.41
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	2.02	0.41
2:B:2867:LEU:HB3	2:B:2871:LEU:HB2	2.03	0.41
2:B:4138:ASP:N	2:B:4138:ASP:OD1	2.53	0.41
2:E:2265:LEU:HD22	2:E:2330:ARG:HB3	2.02	0.41
2:E:4071:ILE:HD11	2:E:4102:GLN:HE21	1.85	0.41
2:E:940:GLY:O	2:E:1052:ASN:N	2.53	0.41
2:G:1141:ARG:HD2	2:G:1141:ARG:H	1.86	0.41
2:G:2466:LEU:HD23	2:G:2469:ILE:HD12	2.02	0.41
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2359:ARG:NH1	2:I:179:TYR:OH	2.41	0.41
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	2.02	0.41
2:E:2867:LEU:HB3	2:E:2871:LEU:HB2	2.02	0.41
2:G:317:ARG:HE	2:G:323:LEU:HD22	1.86	0.41
2:G:4060:LYS:NZ	2:G:4064:MET:SD	2.93	0.41
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.86	0.41
2:I:2867:LEU:HB3	2:I:2871:LEU:HB2	2.02	0.41
2:B:2121:PHE:O	2:B:3725:TYR:OH	2.35	0.41
2:B:3770:LEU:HD21	2:B:3775:ALA:HB3	2.03	0.41
2:E:1141:ARG:HD2	2:E:1141:ARG:H	1.86	0.41
2:E:2871:LEU:HD22	2:E:2927:LEU:HD22	2.02	0.41
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	2.02	0.41
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.39	0.41
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.39	0.41
2:E:2466:LEU:HD23	2:E:2469:ILE:HD12	2.02	0.41
2:E:4731:ILE:HA	2:G:4101:LYS:HE3	2.02	0.41
2:G:1679:ASN:HA	2:G:1682:ALA:HB3	2.02	0.41
2:G:2265:LEU:HD22	2:G:2330:ARG:HB3	2.02	0.41
2:G:4071:ILE:HD11	2:G:4102:GLN:HE21	1.85	0.41
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	2.03	0.41
2:I:3827:GLY:HA2	2:I:3830:GLN:HE21	1.86	0.41
2:B:317:ARG:HE	2:B:323:LEU:HD22	1.86	0.41
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	2.02	0.41
2:E:3770:LEU:HD21	2:E:3775:ALA:HB3	2.03	0.41
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.85	0.41
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.36	0.41
2:G:583:ILE:HA	2:G:586:ILE:HD12	2.03	0.41
2:I:3891:LEU:HB3	2:I:3899:PHE:HE2	1.86	0.41
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.37	0.41
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.52	0.41
2:B:2793:PRO:HG3	2:B:2855:TYR:CZ	2.56	0.41
2:B:3963:ASN:O	2:B:3966:THR:OG1	2.33	0.41
2:B:113:HIS:CE1	2:B:402:ARG:HB3	2.56	0.41
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	2.03	0.41
2:B:4807:PHE:HZ	2:I:4857:ASN:HB2	1.86	0.41
2:E:1154:ASP:O	2:E:1158:ASN:N	2.54	0.41
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.52	0.41
2:E:35:LEU:HD13	2:E:49:LEU:HD13	2.01	0.41
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	2.02	0.41
2:G:134:ASP:OD1	2:G:134:ASP:N	2.54	0.41
2:G:4138:ASP:N	2:G:4138:ASP:OD1	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4236:SER:OG	2:G:4675:LYS:NZ	2.53	0.41
2:G:485:SER:HA	2:G:488:LEU:HB2	2.03	0.41
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	2.02	0.41
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.78	0.41
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.03	0.41
2:B:2103:VAL:O	2:B:2107:GLN:N	2.43	0.41
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.85	0.41
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	2.02	0.41
2:B:583:ILE:HA	2:B:586:ILE:HD12	2.03	0.41
2:E:1096:THR:HG23	2:E:1199:VAL:HG22	2.03	0.41
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.39	0.41
2:G:1096:THR:HG23	2:G:1199:VAL:HG22	2.03	0.41
2:G:2793:PRO:HG3	2:G:2855:TYR:CZ	2.56	0.41
2:G:3891:LEU:HB3	2:G:3899:PHE:HE2	1.86	0.41
2:G:4063:ASP:OD1	2:G:4169:SER:OG	2.37	0.41
2:I:2871:LEU:HD22	2:I:2927:LEU:HD22	2.03	0.41
2:I:3770:LEU:HD21	2:I:3775:ALA:HB3	2.03	0.41
2:I:4837:LEU:HA	2:I:4837:LEU:HD13	1.96	0.41
2:B:1154:ASP:O	2:B:1158:ASN:N	2.54	0.41
2:E:134:ASP:N	2:E:134:ASP:OD1	2.54	0.41
2:E:2793:PRO:HG3	2:E:2855:TYR:CZ	2.56	0.41
2:E:4090:LYS:O	2:E:4094:GLN:N	2.49	0.41
2:G:4978:HIS:CE1	2:G:4983:HIS:NE2	2.87	0.41
2:I:2272:PRO:HA	2:I:2275:VAL:HG12	2.02	0.41
2:I:40:GLU:HB3	2:I:44:ASN:HB3	2.03	0.41
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	2.03	0.41
2:I:485:SER:O	2:I:489:ASN:N	2.43	0.41
2:I:485:SER:HA	2:I:488:LEU:HB2	2.03	0.41
2:B:40:GLU:HB3	2:B:44:ASN:HB3	2.02	0.40
2:B:767:VAL:HG12	2:B:769:GLU:HG3	2.03	0.40
2:E:3827:GLY:HA2	2:E:3830:GLN:HE21	1.86	0.40
2:E:485:SER:HA	2:E:488:LEU:HB2	2.03	0.40
2:G:2318:TYR:HA	2:G:2319:PRO:HD3	1.95	0.40
2:G:3827:GLY:HA2	2:G:3830:GLN:HE21	1.86	0.40
2:G:113:HIS:CE1	2:G:402:ARG:HB3	2.56	0.40
2:I:1973:GLN:HA	2:I:1976:ARG:HB3	2.03	0.40
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	2.03	0.40
2:I:471:LEU:O	2:I:475:GLN:N	2.53	0.40
2:B:3891:LEU:HB3	2:B:3899:PHE:HE2	1.86	0.40
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	2.03	0.40
2:B:4731:ILE:HA	2:E:4101:LYS:HE3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:940:GLY:O	2:B:1052:ASN:N	2.53	0.40
2:E:317:ARG:HE	2:E:323:LEU:HD22	1.85	0.40
2:E:3513:UNK:O	2:E:3515:UNK:N	2.55	0.40
2:E:4667:PRO:O	2:E:4714:ASN:ND2	2.48	0.40
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	2.02	0.40
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	2.03	0.40
2:G:734:GLY:O	2:G:736:HIS:ND1	2.52	0.40
2:B:1096:THR:HG23	2:B:1199:VAL:HG22	2.03	0.40
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	2.02	0.40
2:E:3891:LEU:HB3	2:E:3899:PHE:HE2	1.86	0.40
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	2.03	0.40
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	2.03	0.40
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.39	0.40
2:G:3513:UNK:O	2:G:3515:UNK:N	2.55	0.40
2:I:2231:SER:HA	2:I:2234:ARG:HG2	2.04	0.40
2:I:2793:PRO:HG3	2:I:2855:TYR:CZ	2.56	0.40
2:B:2231:SER:HA	2:B:2234:ARG:HG2	2.04	0.40
2:B:2587:UNK:O	2:B:2591:UNK:N	2.54	0.40
2:B:2871:LEU:HD22	2:B:2927:LEU:HD22	2.02	0.40
2:B:3514:UNK:O	2:B:3518:UNK:N	2.55	0.40
2:B:4987:ASN:O	2:B:4991:PHE:N	2.55	0.40
2:E:113:HIS:CE1	2:E:402:ARG:HB3	2.56	0.40
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	2.04	0.40
2:E:550:LYS:HA	2:E:550:LYS:HD3	1.93	0.40
2:G:3842:LEU:O	2:G:3929:SER:OG	2.40	0.40
2:G:463:GLU:O	2:G:466:SER:OG	2.30	0.40
2:G:946:ALA:HA	2:G:949:ASN:HB2	2.03	0.40
2:I:134:ASP:OD1	2:I:134:ASP:N	2.54	0.40
2:I:1236:THR:OG1	2:I:1608:MET:SD	2.78	0.40
2:B:1973:GLN:HA	2:B:1976:ARG:HB3	2.03	0.40
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	2.04	0.40
2:B:2742:THR:OG1	2:B:2811:GLU:OE1	2.34	0.40
2:B:485:SER:HA	2:B:488:LEU:HB2	2.03	0.40
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.49	0.40
2:E:4138:ASP:N	2:E:4138:ASP:OD1	2.53	0.40
2:E:4857:ASN:HB2	2:G:4807:PHE:HZ	1.86	0.40
2:I:1096:THR:HG23	2:I:1199:VAL:HG22	2.03	0.40
2:I:2025:GLU:HA	2:I:2028:ARG:NE	2.37	0.40
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.49	0.40
2:I:113:HIS:CE1	2:I:402:ARG:HB3	2.56	0.40
2:I:4138:ASP:N	2:I:4138:ASP:OD1	2.53	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:767:VAL:HG12	2:I:769:GLU:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	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	3237/4416 (73%)	2887 (89%)	344 (11%)	6 (0%)	52	86
2	E	3237/4416 (73%)	2887 (89%)	344 (11%)	6 (0%)	52	86
2	G	3237/4416 (73%)	2887 (89%)	344 (11%)	6 (0%)	52	86
2	I	3237/4416 (73%)	2890 (89%)	341 (10%)	6 (0%)	52	86
All	All	13368/18096 (74%)	11931 (89%)	1413 (11%)	24 (0%)	56	86

All (24) 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	B	4641	PRO
2	E	1932	PRO
2	E	4641	PRO
2	I	1932	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	4641	PRO
2	G	1932	PRO
2	G	4641	PRO
2	B	1840	PRO
2	B	2291	GLN
2	E	2291	GLN
2	I	1840	PRO
2	I	2291	GLN
2	G	1840	PRO
2	G	2291	GLN
2	E	1840	PRO
2	B	4667	PRO
2	E	4667	PRO
2	I	4667	PRO
2	G	4667	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2475 (99%)	18 (1%)	88	94
2	E	2493/3022 (82%)	2475 (99%)	18 (1%)	88	94
2	G	2493/3022 (82%)	2475 (99%)	18 (1%)	88	94
2	I	2493/3022 (82%)	2475 (99%)	18 (1%)	88	94
All	All	10324/12444 (83%)	10252 (99%)	72 (1%)	89	94

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	719	LEU
2	B	978	THR
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	3663	LEU
2	B	3787	LYS
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4818	MET
2	B	4983	HIS
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	719	LEU
2	E	978	THR
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3663	LEU
2	E	3787	LYS
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4818	MET
2	E	4983	HIS
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	719	LEU
2	I	978	THR
2	I	1076	ARG
2	I	1141	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	3663	LEU
2	I	3787	LYS
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4818	MET
2	I	4983	HIS
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	719	LEU
2	G	978	THR
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
2	G	3663	LEU
2	G	3787	LYS
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4818	MET
2	G	4983	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) 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	71	GLN
2	B	111	HIS
2	B	113	HIS
2	B	273	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	379	HIS
2	B	413	GLN
2	B	479	GLN
2	B	520	ASN
2	B	1598	GLN
2	B	1679	ASN
2	B	1688	HIS
2	B	1691	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	2127	GLN
2	B	3766	GLN
2	B	3809	ASN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	4034	ASN
2	B	4054	ASN
2	B	4102	GLN
2	B	4120	ASN
2	B	4553	ASN
2	B	4946	GLN
2	E	57	ASN
2	E	71	GLN
2	E	111	HIS
2	E	113	HIS
2	E	273	HIS
2	E	379	HIS
2	E	413	GLN
2	E	479	GLN
2	E	520	ASN
2	E	797	HIS
2	E	1598	GLN
2	E	1679	ASN
2	E	1688	HIS
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	2127	GLN
2	E	3766	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	3809	ASN
2	E	3830	GLN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	4034	ASN
2	E	4054	ASN
2	E	4102	GLN
2	E	4120	ASN
2	E	4553	ASN
2	E	4946	GLN
2	I	57	ASN
2	I	71	GLN
2	I	111	HIS
2	I	113	HIS
2	I	273	HIS
2	I	379	HIS
2	I	413	GLN
2	I	479	GLN
2	I	520	ASN
2	I	797	HIS
2	I	1598	GLN
2	I	1679	ASN
2	I	1688	HIS
2	I	1691	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	2127	GLN
2	I	3766	GLN
2	I	3809	ASN
2	I	3830	GLN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	4034	ASN
2	I	4054	ASN
2	I	4102	GLN
2	I	4120	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	4553	ASN
2	I	4946	GLN
2	G	57	ASN
2	G	71	GLN
2	G	111	HIS
2	G	113	HIS
2	G	273	HIS
2	G	379	HIS
2	G	413	GLN
2	G	479	GLN
2	G	520	ASN
2	G	797	HIS
2	G	1598	GLN
2	G	1679	ASN
2	G	1688	HIS
2	G	1691	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	2127	GLN
2	G	3766	GLN
2	G	3809	ASN
2	G	3830	GLN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	4034	ASN
2	G	4054	ASN
2	G	4102	GLN
2	G	4120	ASN
2	G	4553	ASN
2	G	4946	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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	14
2	B	14
2	I	14
2	E	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.38
1	E	4345:UNK	C	4540:PHE	N	73.38
1	I	4345:UNK	C	4540:PHE	N	73.38
1	G	4345:UNK	C	4540:PHE	N	73.38
1	B	3613:UNK	C	3639:THR	N	48.21
1	E	3613:UNK	C	3639:THR	N	48.21
1	I	3613:UNK	C	3639:THR	N	48.21
1	G	3613:UNK	C	3639:THR	N	48.21
1	B	4253:GLU	C	4320:UNK	N	27.50

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	4253:GLU	C	4320:UNK	N	27.50
1	I	4253:GLU	C	4320:UNK	N	27.50
1	G	4253:GLU	C	4320:UNK	N	27.50
1	B	3163:UNK	C	3170:UNK	N	16.06
1	E	3163:UNK	C	3170:UNK	N	16.06
1	I	3163:UNK	C	3170:UNK	N	16.06
1	G	3163:UNK	C	3170:UNK	N	16.06
1	B	3063:UNK	C	3134:UNK	N	14.88
1	E	3063:UNK	C	3134:UNK	N	14.88
1	I	3063:UNK	C	3134:UNK	N	14.88
1	G	3063:UNK	C	3134:UNK	N	14.88
1	B	3468:UNK	C	3511:UNK	N	14.29
1	E	3468:UNK	C	3511:UNK	N	14.29
1	I	3468:UNK	C	3511:UNK	N	14.29
1	G	3468:UNK	C	3511:UNK	N	14.29
1	B	2703:UNK	C	2734:ASN	N	13.58
1	E	2703:UNK	C	2734:ASN	N	13.58
1	I	2703:UNK	C	2734:ASN	N	13.58
1	G	2703:UNK	C	2734:ASN	N	13.58
1	B	3236:UNK	C	3241:UNK	N	13.52
1	E	3236:UNK	C	3241:UNK	N	13.52
1	I	3236:UNK	C	3241:UNK	N	13.52
1	G	3236:UNK	C	3241:UNK	N	13.52
1	B	1564:UNK	C	1573:MET	N	12.58
1	E	1564:UNK	C	1573:MET	N	12.58
1	I	1564:UNK	C	1573:MET	N	12.58
1	G	1564:UNK	C	1573:MET	N	12.58
1	B	2976:UNK	C	2995:UNK	N	12.37
1	E	2976:UNK	C	2995:UNK	N	12.37
1	I	2976:UNK	C	2995:UNK	N	12.37
1	G	2976:UNK	C	2995:UNK	N	12.37
1	B	3254:UNK	C	3261:UNK	N	8.09
1	E	3254:UNK	C	3261:UNK	N	8.09
1	I	3254:UNK	C	3261:UNK	N	8.09
1	G	3254:UNK	C	3261:UNK	N	8.09
1	B	1297:UNK	C	1430:UNK	N	5.89
1	I	1297:UNK	C	1430:UNK	N	5.89
1	E	1297:UNK	C	1430:UNK	N	5.88
1	G	1297:UNK	C	1430:UNK	N	5.88
1	B	2479:LEU	C	2487:UNK	N	3.66
1	E	2479:LEU	C	2487:UNK	N	3.66
1	I	2479:LEU	C	2487:UNK	N	3.66

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	2479:LEU	C	2487:UNK	N	3.66
1	B	2939:ARG	C	2942:UNK	N	3.38
1	E	2939:ARG	C	2942:UNK	N	3.38
1	I	2939:ARG	C	2942:UNK	N	3.38
1	G	2939:ARG	C	2942:UNK	N	3.38