



wwPDB EM Map/Model Validation Report ⓘ

Oct 17, 2016 – 04:44 PM EDT

PDB ID : 5TB2
EMDB ID: : EMD-8393
Title : Structure of rabbit RyR1 (EGTA-only dataset, class 2)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-11
Resolution : 4.60 Å(reported)

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

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

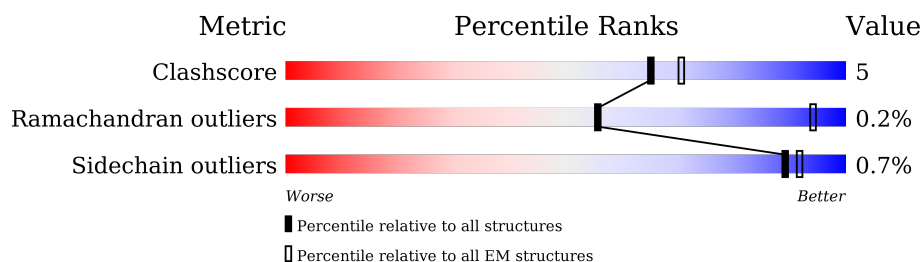
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	108	
1	F	108	
1	H	108	
1	J	108	
2	B	4416	
2	E	4416	
2	G	4416	
2	I	4416	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 121272 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a protein called Ryanodine receptor 1.

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



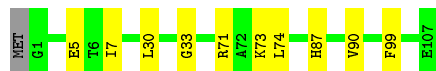
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 




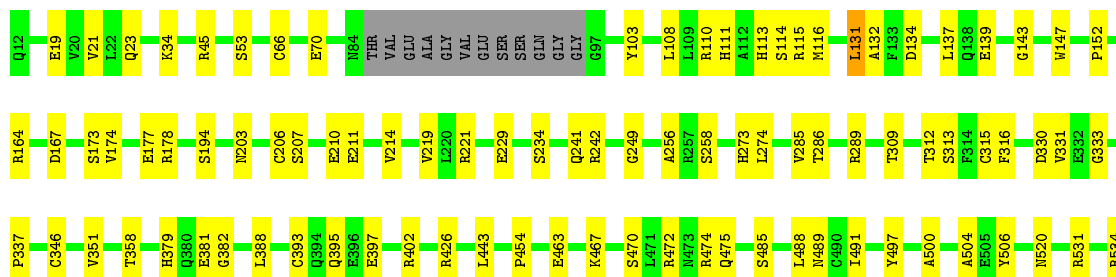
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 



- Molecule 2: Ryanodine receptor 1

Chain B: 

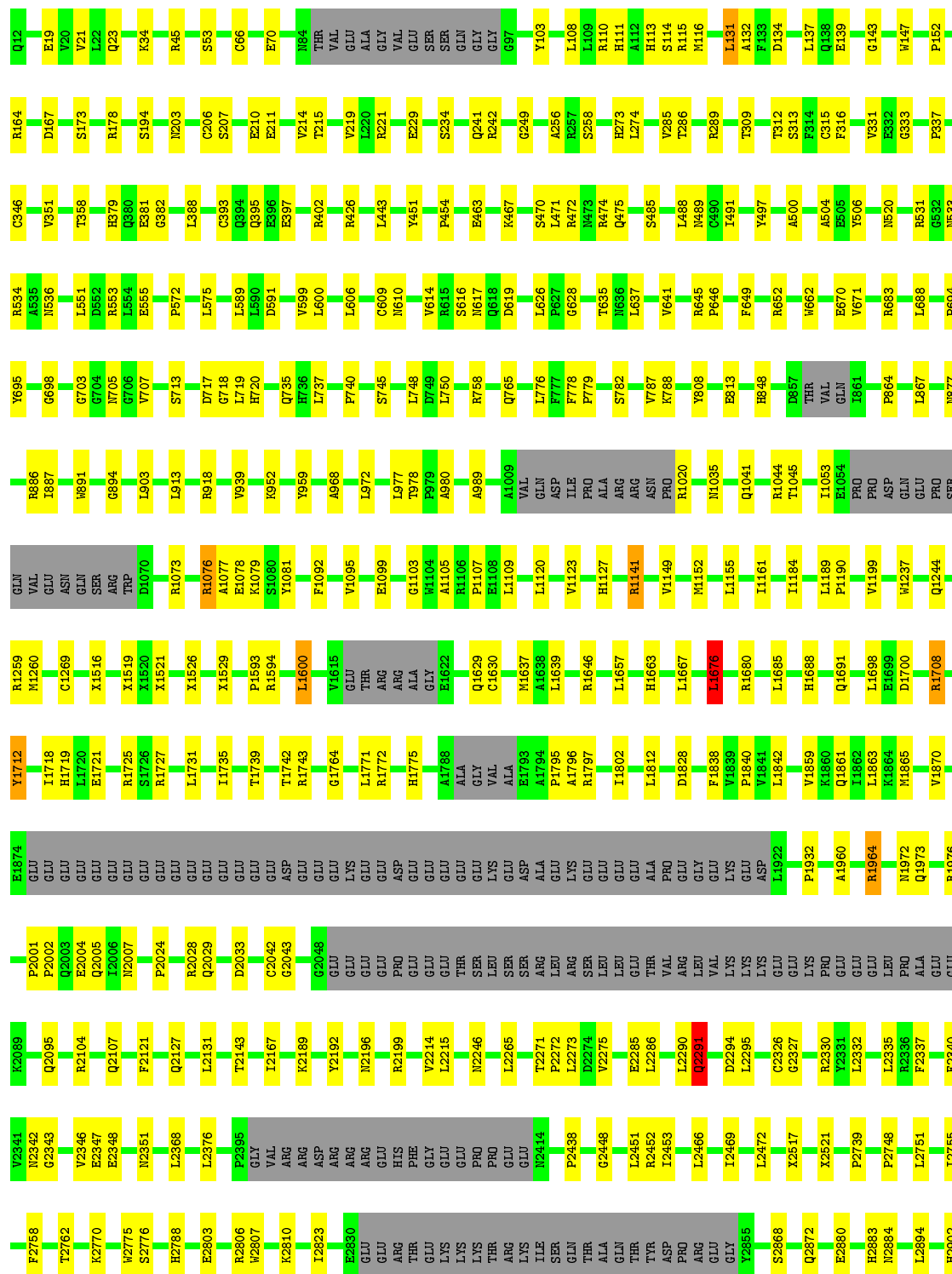


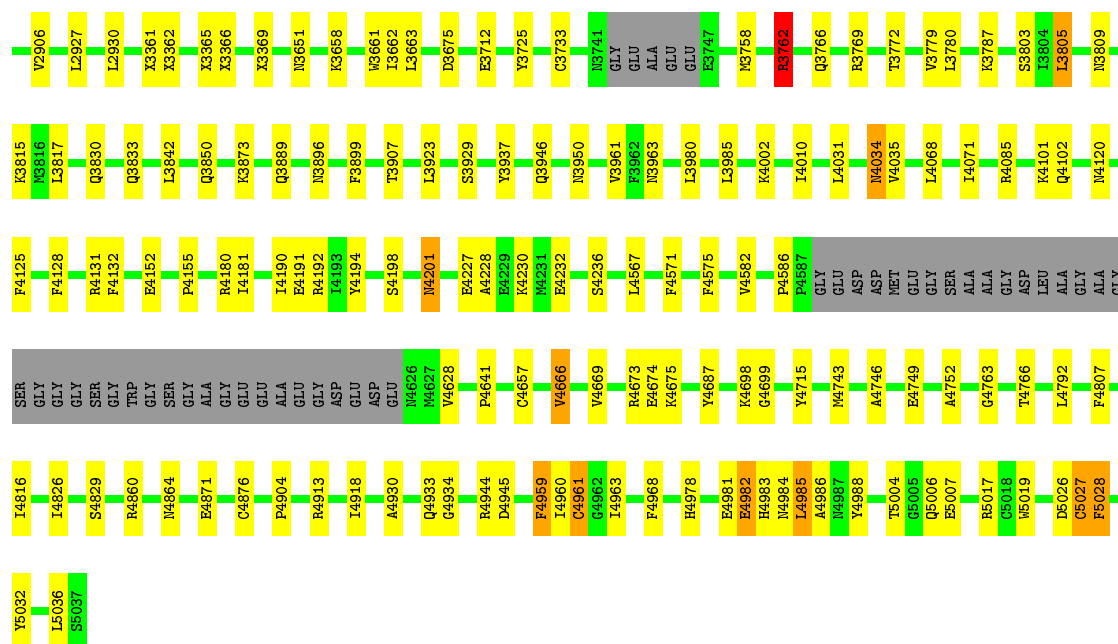
I4816	SER	F4128	M3816	V2346	K2089	Q1973	V1870	Y1711	R1269	VAL	W931	G703	L551
R4860	GLY	R4131	L3817	E2347	R2104	R1976	E1874	Y1712	M1260	GLU	G704	D552	D552
N4864	GLY	F4132	Q3830	E2348	Q2107	P2001	GLU	I1718	C1269	ASN	N705	R553	R553
E4871	GLY	E4152	Q3833	N2351	F2121	Q2002	GLU	L1720	R1719	SER	G706	L554	L554
C4876	TRP	P4155	L3842	L2368	L2121	Q2003	GLU	E1721	X1516	ARG	V707	E555	E555
Y4888	GLY	R4180	Q3850	L2376	L2131	E2004	GLU	R1725	X1519	TRP	S713	P572	P572
I4897	ALA	I4181	P2395	L2006	T2143	Q2005	GLU	R1727	X1521	GLU	D717	L575	L575
I4901	GLY	K3873	GLY	L2007	L2143	N2007	GLU	R1731	X1526	GLU	G718	L719	L719
P4904	GLY	K3873	VAL	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L720	H720	L589
R4913	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	Y859	L590	L590
I4918	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	A727	D591	D591
A4930	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	A968	L599	L599
Q4933	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
C4934	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
R4944	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
D4945	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
F4959	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
I4960	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
A4961	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
F4968	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
H4978	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
E4981	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
E4982	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
H4983	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
N4984	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
L4985	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
A4986	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
H4987	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
E4988	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
T5004	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
G5005	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
Q5006	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
E5007	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
Y5014	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
R5017	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
C5018	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
W5019	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
D5026	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
C5027	GLY	K3873	ARG	N2007	L2143	Q2007	GLU	L1731	X1526	GLU	L972	L600	L600
R1269	VAL	W931	G703	L551	D552	R553	L554	E555	P572	L575	L719	L720	L589
M1260	GLU	G704	D552	R553	L554	E555	P572	L575	L719	L720	L589	L590	L590
C1269	GLU	G706	L554	E555	P572	L575	L719	L720	L589	L590	D591	D591	D591
X1516	TRP	S713	P572	L575	L719	L720	L589	L590	D591	D591	L599	L599	L599
X1519	GLU	D717	L575	L719	L720	L589	L590	D591	D591	D591	L599	L599	L599
X1521	GLU	G718	L575	L719	L720	L589	L590	D591	D591	D591	L599	L599	L599
X1526	GLU	L719	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
X1529	GLU	H720	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
P1593	GLU	Y859	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
R1594	GLU	A968	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
L1600	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
V1615	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
THR	THR	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
ARG	ARG	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
ALA	ALA	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
GLY	GLY	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
E1622	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
Q1639	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
C1630	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
M1637	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
A1638	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
L1639	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
H1641	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
P1642	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
R1646	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
L1676	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
R1680	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
L1685	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
H1688	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
Q1691	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
L1698	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
E1699	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
D1700	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
L1707	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
R1708	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
A1709	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
G1710	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
M1865	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
Y1711	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
Y1712	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
I1718	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
H1719	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
L1720	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
E1721	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
R1725	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
S1726	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
R1727	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
L1731	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
I1735	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
T1739	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
T1742	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
R1743	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
G1764	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
L1771	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
R1772	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
H1775	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
A1784	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
A1788	GLU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
ALA	ALA	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
GLY	GLY	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
VAL	VAL	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
ALA	ALA	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
LEU	LEU	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
SER	SER	L972	L589	L590	D591	D591	L599	L599	L599	L599	L599	L599	L599
THR	THR	L972	L589	L590	D591	D591	L599	L599	L599	L599</			



• Molecule 2: Ryanodine receptor 1

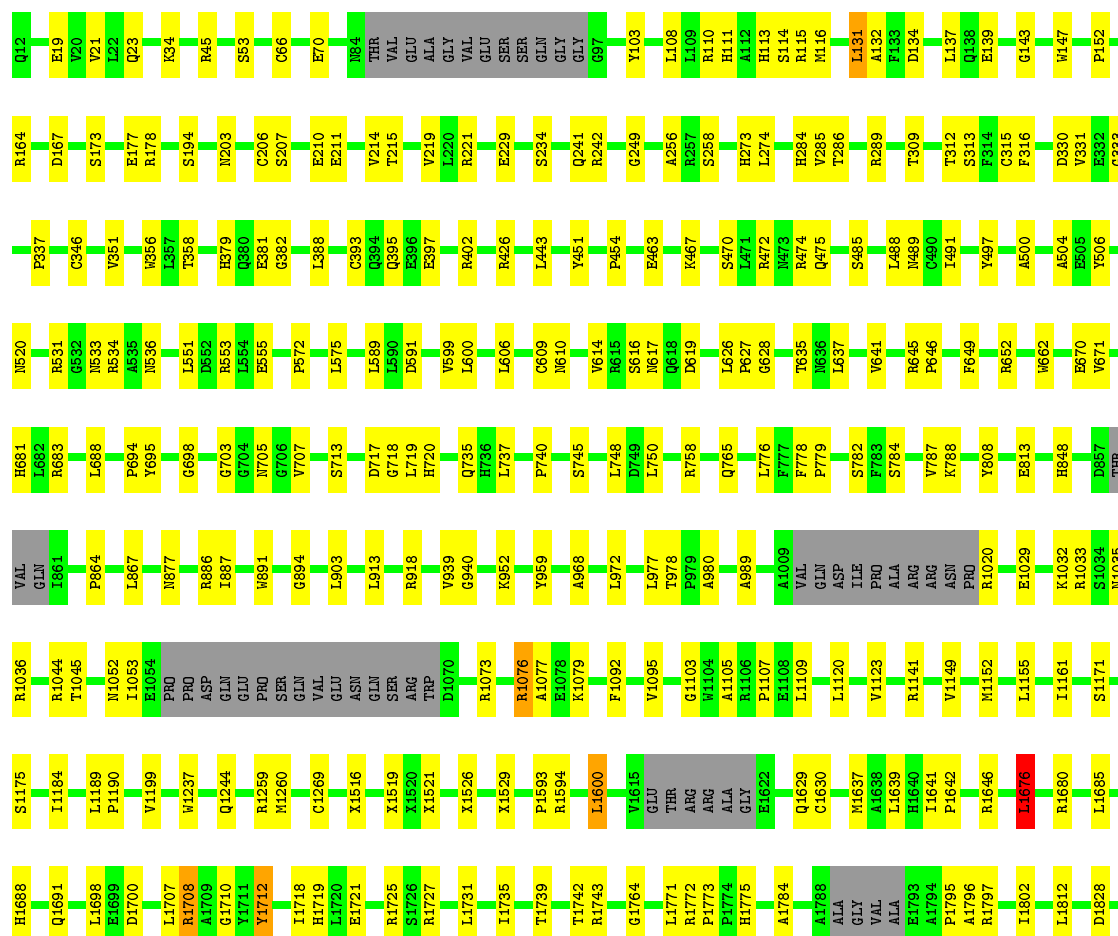
Chain I: 84% 11% 5%





• Molecule 2: Ryanodine receptor 1

Chain E: 84% 11% 5%



Y4888	P4155	Q3833	L2930	K2770	G2343	Q2095	P2002	GIJ	L1720	H1260	ASP	R886	6698
Y4897	R4180	L3842	X3362	W2776	V2346	R2104	Q2003	GIJ	E1721	C1269	GLN	1887	E703
I4901	I4190	Q3850	X3365	H2788	E2347	Q2107	E2004	GIJ	R1725	X1516	PRO	W891	G704
P4904	E4191	X3873	X3366	E2803	E2348	Q2121	Q2005	GIJ	S1726	G894	SER	G894	W705
R4913	R4192	X3889	X3369	W2806	R2351	Q2127	Q2006	GIJ	R1727	X1519	GLN	L903	G706
A4930	I4193	Q3896	Q3651	W2807	L2376	L2131	Q2007	GIJ	L1731	X1520	VAL	L903	Y707
A4930	S4198	Q3896	Q3658	K2810	P2395	T2143	P2024	GIJ	L1735	X1521	GLU	L913	S713
Q4933	W4201	F3899	Q3661	I2823	GLY	T2167	P2028	GIJ	T1739	X1526	ASN	R918	D717
G4934	E4227	T3907	I3662	E2830	VAL	I2167	Q2029	GIJ	T1742	X1529	GLN	Y939	G718
R4944	A4228	T3907	I3663	GLU	ARG	K2189	R2028	GIJ	R1743	P1593	ARG	6940	L719
D4945	E4229	L3923	D8675	GLU	ASP	Y2192	Q2043	ASP	G1764	R1594	TRP	Y959	H720
F4959	I4230	S3929	E3712	GLU	ARG	Y2196	G2048	GIJ	L1771	L1600	R1076	Y959	G734
C4961	W4231	Y3937	E3725	ARG	ARG	R2199	GLU	GLU	R1772	Y1615	A1077	A968	Q735
G4962	E4232	Y3937	Y3725	LYS	HIS	R2199	GLU	GLU	P1774	THR	K1078	P740	H736
I4963	S4236	Q3946	C3733	LYS	PHE	Y2214	GLU	ASP	H1775	ALA	F1092	L972	W737
F4968	E4239	Q3950	E3741	LYS	GLY	L2215	GLU	GLU	A1784	GLY	Y1095	L977	L748
H4978	L4567	Y3961	GLY	ARG	GLU	N2246	THR	GLU	A1788	E1622	G1103	T978	D749
E4981	F4571	I3962	GLU	LYS	PRO	N2265	GLU	GLU	ALA	Q1629	Y1104	P979	L750
H4982	F4575	I3963	GLU	ILE	GLU	L2265	LEU	GLU	VAL	C1630	A1105	A980	R758
H4984	Y4582	I3985	E3747	GLN	GLU	T2271	SER	LYS	ALA	M1637	A1106	A989	Q765
L4985	P4586	I3985	Y3758	THR	GLU	T2272	ARG	ASP	E1793	A1638	E1108	Y1009	L776
A4986	Y4587	K4002	Y3762	THR	GLU	T2273	LEU	ALA	A1794	L1639	L1109	VAL	F777
Y4988	GLY	L4031	Q3766	ASP	PRO	T2275	SER	LYS	A1796	L1646	L1120	ILE	F778
T5004	ASP	L4034	Q3769	PRO	ARG	E2285	GLU	GLU	R1797	L1676	Y1123	PRO	P779
D5005	ASP	Y4035	Y3769	GLY	GLU	L2286	LEU	GLU	I1802	R1141	R1141	ALA	S782
E5007	GLY	L4068	Y3772	GLY	GLU	L2290	VAL	ALA	L1812	R1680	V1149	ARG	V787
Y5014	SER	L4071	Y3779	ARG	GLU	L2291	VAL	VAL	D1828	L1685	M1152	ASN	K788
R5017	ALA	R4085	L3780	GLY	GLU	L2326	VAL	GLY	F1838	H1688	L1155	PRO	Y808
G5018	GLY	Y3787	Y3803	E2880	Y2521	C2326	LYS	LYS	Y1839	Q1691	L1161	ARG	E813
Y5019	ASP	Q3787	L3805	Y2883	Y2521	G2327	GLU	ASP	V1841	L1698	I1184	K1032	H848
D5026	LEU	Q4102	S3803	H2884	P2739	G2330	LYS	L1922	L1842	E1699	L1189	R1033	D857
C5027	ALA	Y4120	I3804	I2884	P2748	Y2331	PRO	P1932	V1859	D1700	L1189	R1035	THR
F5028	GLY	F4125	L3805	L2894	P2748	L2332	GLU	K1936	K1860	L1707	P1190	R1036	VAL
Y5032	GLY	F4128	Y3809	H2902	L2751	L2335	LEU	C1940	Q1861	R1708	V1199	T1045	L861
L5036	GLY	F4132	Y3815	Y2906	L2751	L2336	PRO	Y1711	L1863	G1710	V1199	R1052	P864
S5037	GLY	F4132	Y3816	Y2906	P2758	F2337	ALA	A1960	K1864	Y1712	H1237	L1053	L867
	SER	E4152	L3817	L2927	P2758	F2340	GLU	R1964	Y1712	I1718	Q1244	E1054	
	TRP	Q3830	Q3830	L2927	T2762	N2342	GLU	P2001	E1874	H1719	R1259	PRO	N877

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	0.31	0/834	0.52	0/1123
1	F	0.31	0/834	0.52	0/1123
1	H	0.31	0/834	0.52	0/1123
1	J	0.31	0/834	0.52	0/1123
2	B	0.31	0/25428	0.55	9/34534 (0.0%)
2	E	0.31	0/25428	0.55	8/34534 (0.0%)
2	G	0.31	0/25428	0.55	8/34534 (0.0%)
2	I	0.31	0/25428	0.55	8/34534 (0.0%)
All	All	0.31	0/105048	0.55	33/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	17
2	E	0	17
2	G	0	16
2	I	0	16
All	All	0	66

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	131	LEU	CA-CB-CG	8.36	134.52	115.30
2	G	131	LEU	CA-CB-CG	8.35	134.51	115.30
2	B	131	LEU	CA-CB-CG	8.34	134.48	115.30
2	E	131	LEU	CA-CB-CG	8.33	134.46	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1676	LEU	CA-CB-CG	6.33	129.86	115.30
2	G	1676	LEU	CA-CB-CG	6.33	129.86	115.30
2	B	1676	LEU	CA-CB-CG	6.32	129.84	115.30
2	E	1676	LEU	CA-CB-CG	6.32	129.84	115.30
2	E	1600	LEU	CA-CB-CG	6.29	129.77	115.30
2	B	1600	LEU	CA-CB-CG	6.29	129.75	115.30
2	I	1600	LEU	CA-CB-CG	6.29	129.76	115.30
2	B	4985	LEU	CA-CB-CG	6.28	129.75	115.30
2	E	4985	LEU	CA-CB-CG	6.28	129.74	115.30
2	G	4985	LEU	CA-CB-CG	6.28	129.74	115.30
2	G	1600	LEU	CA-CB-CG	6.28	129.74	115.30
2	I	4985	LEU	CA-CB-CG	6.27	129.73	115.30
2	G	977	LEU	CA-CB-CG	5.57	128.11	115.30
2	E	977	LEU	CA-CB-CG	5.56	128.08	115.30
2	B	977	LEU	CA-CB-CG	5.55	128.08	115.30
2	I	977	LEU	CA-CB-CG	5.54	128.04	115.30
2	I	3663	LEU	CA-CB-CG	5.22	127.30	115.30
2	E	3663	LEU	CA-CB-CG	5.21	127.27	115.30
2	G	3663	LEU	CA-CB-CG	5.20	127.26	115.30
2	B	3663	LEU	CA-CB-CG	5.20	127.25	115.30
2	E	688	LEU	CA-CB-CG	5.08	126.99	115.30
2	I	2290	LEU	CA-CB-CG	5.08	126.98	115.30
2	G	688	LEU	CA-CB-CG	5.08	126.97	115.30
2	B	688	LEU	CA-CB-CG	5.07	126.97	115.30
2	B	2290	LEU	CA-CB-CG	5.07	126.96	115.30
2	I	688	LEU	CA-CB-CG	5.07	126.96	115.30
2	G	2290	LEU	CA-CB-CG	5.07	126.95	115.30
2	E	2290	LEU	CA-CB-CG	5.06	126.94	115.30
2	B	727	ALA	C-N-CA	-5.00	109.19	121.70

There are no chirality outliers.

All (66) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1712	TYR	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	2001	PRO	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	312	THR	Peptide
2	B	4031	LEU	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	1712	TYR	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	2001	PRO	Peptide
2	E	2291	GLN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	312	THR	Peptide
2	E	4031	LEU	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
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1712	TYR	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	2001	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	312	THR	Peptide
2	G	4031	LEU	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1712	TYR	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	2001	PRO	Peptide
2	I	2291	GLN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	312	THR	Peptide
2	I	4031	LEU	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	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	8	0
1	F	818	0	824	8	0
1	H	818	0	824	8	0
1	J	818	0	824	5	0
2	B	29499	0	24751	284	0
2	E	29499	0	24751	290	0
2	G	29499	0	24751	288	0
2	I	29499	0	24751	286	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	121272	0	102300	1147	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 (1147) 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:E:4190:ILE:CD1	2:E:5026:ASP:OD2	1.77	1.33
2:I:4190:ILE:CD1	2:I:5026:ASP:OD2	1.76	1.33
2:G:4190:ILE:CD1	2:G:5026:ASP:OD2	1.77	1.32
2:B:4190:ILE:CD1	2:B:5026:ASP:OD2	1.76	1.31
2:B:4190:ILE:HD11	2:B:5026:ASP:OD2	1.31	1.26
2:E:4190:ILE:HD11	2:E:5026:ASP:OD2	1.31	1.19
2:G:4190:ILE:HD11	2:G:5026:ASP:OD2	1.31	1.13
2:I:4190:ILE:HD11	2:I:5026:ASP:OD2	1.31	1.11
2:G:5028:PHE:HE1	2:G:5032:TYR:CE2	1.78	1.02
2:I:5028:PHE:HE1	2:I:5032:TYR:CE2	1.78	1.01
2:B:5028:PHE:HE1	2:B:5032:TYR:CE2	1.78	1.01
2:E:5028:PHE:HE1	2:E:5032:TYR:CE2	1.78	1.00
2:I:4968:PHE:CZ	2:I:4978:HIS:ND1	2.31	0.99
2:G:4968:PHE:CZ	2:G:4978:HIS:ND1	2.30	0.99
2:B:4968:PHE:CZ	2:B:4978:HIS:ND1	2.30	0.98
2:E:4968:PHE:CZ	2:E:4978:HIS:ND1	2.30	0.98
2:I:4190:ILE:HD11	2:I:5026:ASP:CG	1.92	0.90
2:B:4190:ILE:HD11	2:B:5026:ASP:CG	1.92	0.90
2:E:4190:ILE:HD11	2:E:5026:ASP:CG	1.92	0.89
2:G:4190:ILE:HD11	2:G:5026:ASP:CG	1.92	0.89
2:G:4968:PHE:CZ	2:G:4978:HIS:CE1	2.61	0.89
2:B:5028:PHE:CE1	2:B:5032:TYR:CD2	2.61	0.89
2:B:4968:PHE:CZ	2:B:4978:HIS:CE1	2.61	0.88
2:E:5028:PHE:CE1	2:E:5032:TYR:CD2	2.61	0.88
2:G:5028:PHE:CE1	2:G:5032:TYR:CD2	2.61	0.88
2:I:5028:PHE:CE1	2:I:5032:TYR:CD2	2.61	0.88
2:I:4968:PHE:CZ	2:I:4978:HIS:CE1	2.61	0.87
2:E:4968:PHE:CZ	2:E:4978:HIS:CE1	2.61	0.87
2:I:5028:PHE:CE1	2:I:5032:TYR:CE2	2.66	0.83
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.60	0.83
2:B:5028:PHE:CE1	2:B:5032:TYR:CE2	2.66	0.82
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.61	0.82
2:B:4190:ILE:CD1	2:B:5026:ASP:CG	2.49	0.81
2:E:4190:ILE:CD1	2:E:5026:ASP:CG	2.49	0.81
2:E:5028:PHE:CE1	2:E:5032:TYR:CE2	2.66	0.81
2:B:4968:PHE:HZ	2:B:4978:HIS:CE1	1.99	0.81
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.60	0.80
2:I:4190:ILE:HD13	2:I:5026:ASP:OD2	1.81	0.80
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.61	0.80
2:E:4190:ILE:HD13	2:E:5026:ASP:OD2	1.81	0.80
2:G:5028:PHE:CE1	2:G:5032:TYR:CE2	2.66	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4190:ILE:CD1	2:G:5026:ASP:CG	2.49	0.79
2:I:4190:ILE:CD1	2:I:5026:ASP:CG	2.49	0.79
2:B:5028:PHE:HE1	2:B:5032:TYR:CD2	2.01	0.78
2:G:5028:PHE:HE1	2:G:5032:TYR:CD2	2.01	0.78
2:I:4968:PHE:HZ	2:I:4978:HIS:CE1	1.99	0.78
2:I:5028:PHE:HE1	2:I:5032:TYR:CD2	2.01	0.78
2:G:4968:PHE:HZ	2:G:4978:HIS:CE1	1.99	0.78
2:E:4968:PHE:HZ	2:E:4978:HIS:CE1	1.99	0.77
2:E:5028:PHE:HE1	2:E:5032:TYR:CD2	2.01	0.76
2:G:5028:PHE:HE1	2:G:5032:TYR:HE2	1.33	0.76
2:I:4960:ILE:N	2:I:4960:ILE:HD13	2.01	0.75
2:B:5028:PHE:HE1	2:B:5032:TYR:HE2	1.33	0.75
2:B:4190:ILE:HD13	2:B:5026:ASP:OD2	1.81	0.75
2:G:4190:ILE:HD13	2:G:5026:ASP:OD2	1.81	0.74
2:I:5028:PHE:HE1	2:I:5032:TYR:HE2	1.33	0.74
2:B:4960:ILE:HD13	2:B:4960:ILE:N	2.01	0.74
2:G:4960:ILE:N	2:G:4960:ILE:HD13	2.01	0.74
2:E:4960:ILE:HD13	2:E:4960:ILE:N	2.01	0.73
2:E:5028:PHE:HE1	2:E:5032:TYR:HE2	1.33	0.72
2:I:4960:ILE:HG23	2:I:4988:TYR:HE2	1.56	0.71
2:G:4960:ILE:HG23	2:G:4988:TYR:HE2	1.56	0.70
2:I:4968:PHE:CE2	2:I:4978:HIS:ND1	2.60	0.70
2:G:4968:PHE:CE2	2:G:4978:HIS:ND1	2.59	0.70
2:B:4960:ILE:HG23	2:B:4988:TYR:HE2	1.56	0.70
2:E:4968:PHE:CE2	2:E:4978:HIS:ND1	2.59	0.69
2:E:379:HIS:HD2	2:E:382:GLY:H	1.41	0.69
2:E:4960:ILE:HG23	2:E:4988:TYR:HE2	1.56	0.69
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.57	0.69
2:B:4968:PHE:CE2	2:B:4978:HIS:ND1	2.59	0.69
2:B:379:HIS:HD2	2:B:382:GLY:H	1.41	0.68
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.57	0.68
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.57	0.68
2:I:379:HIS:HD2	2:I:382:GLY:H	1.41	0.68
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.57	0.68
2:G:379:HIS:HD2	2:G:382:GLY:H	1.41	0.67
2:B:4933:GLN:NE2	2:I:4933:GLN:OE1	2.29	0.65
2:B:173:SER:HB3	2:B:178:ARG:H	1.62	0.65
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.30	0.65
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.62	0.65
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.30	0.65
2:G:5028:PHE:CE1	2:G:5032:TYR:HD2	2.13	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.30	0.64
2:I:5028:PHE:CE1	2:I:5032:TYR:HD2	2.13	0.64
2:G:173:SER:HB3	2:G:178:ARG:H	1.62	0.64
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.62	0.64
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.62	0.64
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.31	0.64
2:E:5028:PHE:CE1	2:E:5032:TYR:HD2	2.13	0.64
2:I:173:SER:HB3	2:I:178:ARG:H	1.62	0.64
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.31	0.63
2:E:173:SER:HB3	2:E:178:ARG:H	1.62	0.63
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.80	0.63
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.31	0.63
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.31	0.63
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.62	0.63
2:B:5028:PHE:CE1	2:B:5032:TYR:HD2	2.13	0.63
2:I:4191:GLU:OE1	2:I:5006:GLN:NE2	2.32	0.63
2:G:4191:GLU:OE1	2:G:5006:GLN:NE2	2.32	0.62
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.80	0.62
2:B:4191:GLU:OE1	2:B:5006:GLN:NE2	2.32	0.62
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.65	0.62
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.82	0.62
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.65	0.62
2:E:4191:GLU:OE1	2:E:5006:GLN:NE2	2.32	0.62
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.80	0.62
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.65	0.61
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.82	0.61
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.82	0.61
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.65	0.61
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.30	0.61
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.82	0.61
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.80	0.61
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.82	0.61
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.83	0.61
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.83	0.61
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.83	0.61
2:B:2347:GLU:O	2:B:2351:ASN:N	2.34	0.61
2:E:2347:GLU:O	2:E:2351:ASN:N	2.34	0.61
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.82	0.60
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.83	0.60
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.35	0.60
2:G:2347:GLU:O	2:G:2351:ASN:N	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3675:ASP:OD1	2:B:3769:ARG:NH2	2.35	0.60
2:I:2347:GLU:O	2:I:2351:ASN:N	2.34	0.60
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.35	0.60
2:E:3675:ASP:OD1	2:E:3769:ARG:NH2	2.35	0.59
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.35	0.59
2:G:626:LEU:HG	2:G:628:GLY:H	1.66	0.59
2:B:2346:VAL:HG22	2:B:2348:GLU:H	1.67	0.59
2:E:626:LEU:HG	2:E:628:GLY:H	1.66	0.59
2:G:2346:VAL:HG22	2:G:2348:GLU:H	1.67	0.59
2:I:626:LEU:HG	2:I:628:GLY:H	1.66	0.59
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.35	0.59
2:E:2346:VAL:HG22	2:E:2348:GLU:H	1.67	0.59
2:G:3675:ASP:OD1	2:G:3769:ARG:NH2	2.35	0.59
2:G:111:HIS:HD2	2:G:114:SER:H	1.51	0.59
2:E:111:HIS:HD2	2:E:114:SER:H	1.51	0.59
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.84	0.59
2:B:111:HIS:HD2	2:B:114:SER:H	1.51	0.59
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.85	0.59
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.85	0.59
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.85	0.59
2:I:4944:ARG:NH2	2:G:4945:ASP:OD2	2.36	0.59
2:I:111:HIS:HD2	2:I:114:SER:H	1.51	0.59
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.85	0.59
2:B:626:LEU:HG	2:B:628:GLY:H	1.66	0.58
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.68	0.58
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.85	0.58
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.85	0.58
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.85	0.58
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.84	0.58
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.84	0.58
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.85	0.58
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.68	0.58
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.85	0.58
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.86	0.58
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.86	0.58
2:G:614:VAL:HG22	2:G:616:SER:H	1.69	0.58
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.84	0.58
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.68	0.58
2:I:315:CYS:SG	2:I:316:PHE:N	2.77	0.58
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.37	0.58
2:E:315:CYS:SG	2:E:316:PHE:N	2.77	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.85	0.57
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.86	0.57
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.85	0.57
2:I:2346:VAL:HG22	2:I:2348:GLU:H	1.67	0.57
2:I:3675:ASP:OD1	2:I:3769:ARG:NH2	2.35	0.57
2:I:614:VAL:HG22	2:I:616:SER:H	1.69	0.57
2:B:315:CYS:SG	2:B:316:PHE:N	2.77	0.57
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.37	0.57
2:G:315:CYS:SG	2:G:316:PHE:N	2.77	0.57
2:E:4933:GLN:OE1	2:G:4933:GLN:NE2	2.36	0.57
2:E:4232:GLU:OE1	2:E:5019:TRP:NE1	2.38	0.57
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.86	0.57
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.86	0.57
2:E:132:ALA:HA	2:E:194:SER:HB2	1.87	0.57
2:E:614:VAL:HG22	2:E:616:SER:H	1.69	0.57
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.86	0.57
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.37	0.57
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.68	0.57
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.86	0.57
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.37	0.57
2:G:4232:GLU:OE1	2:G:5019:TRP:NE1	2.38	0.57
2:G:4960:ILE:HG23	2:G:4988:TYR:CE2	2.40	0.57
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.87	0.57
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.87	0.57
2:I:132:ALA:HA	2:I:194:SER:HB2	1.87	0.57
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.86	0.56
2:B:132:ALA:HA	2:B:194:SER:HB2	1.87	0.56
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.87	0.56
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.38	0.56
2:B:4232:GLU:OE1	2:B:5019:TRP:NE1	2.38	0.56
2:I:4960:ILE:HG23	2:I:4988:TYR:CE2	2.40	0.56
2:B:4904:PRO:HB3	2:B:4913:ARG:HD3	1.87	0.56
2:B:614:VAL:HG22	2:B:616:SER:H	1.69	0.56
2:E:470:SER:O	2:E:474:ARG:NE	2.37	0.56
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.86	0.56
2:E:4904:PRO:HB3	2:E:4913:ARG:HD3	1.87	0.56
2:I:4232:GLU:OE1	2:I:5019:TRP:NE1	2.38	0.56
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.86	0.56
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.86	0.56
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.87	0.56
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.38	0.56
2:G:132:ALA:HA	2:G:194:SER:HB2	1.87	0.56
2:B:609:CYS:SG	2:B:610:ASN:N	2.79	0.56
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.79	0.56
2:G:609:CYS:SG	2:G:610:ASN:N	2.79	0.56
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.38	0.56
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.87	0.56
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.88	0.55
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.79	0.55
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.86	0.55
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.79	0.55
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.38	0.55
2:E:609:CYS:SG	2:E:610:ASN:N	2.79	0.55
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.40	0.55
2:E:4960:ILE:HG23	2:E:4988:TYR:CE2	2.40	0.55
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.88	0.55
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.86	0.55
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.79	0.55
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.86	0.55
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.89	0.55
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.89	0.55
2:I:4904:PRO:HB3	2:I:4913:ARG:HD3	1.87	0.55
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.89	0.55
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.40	0.55
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.40	0.55
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	1.89	0.55
2:G:4904:PRO:HB3	2:G:4913:ARG:HD3	1.87	0.55
2:I:609:CYS:SG	2:I:610:ASN:N	2.79	0.55
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.89	0.55
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.88	0.55
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.40	0.55
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.39	0.55
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.40	0.55
2:G:470:SER:O	2:G:474:ARG:NE	2.37	0.55
2:B:4933:GLN:OE1	2:E:4933:GLN:NE2	2.39	0.55
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.72	0.55
2:I:4933:GLN:NE2	2:G:4933:GLN:OE1	2.40	0.55
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.89	0.54
2:B:4960:ILE:HG23	2:B:4988:TYR:CE2	2.40	0.54
2:I:2452:ARG:NH1	2:G:174:VAL:O	2.40	0.54
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.39	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	1.89	0.54
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.39	0.54
2:B:606:LEU:O	2:B:617:ASN:ND2	2.41	0.54
2:I:214:VAL:HG12	2:I:274:LEU:HD12	1.89	0.54
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	1.89	0.54
2:E:214:VAL:HG12	2:E:274:LEU:HD12	1.89	0.54
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.90	0.54
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.89	0.54
2:G:4567:LEU:HD12	2:G:4816:ILE:HD12	1.90	0.54
2:E:520:ASN:ND2	2:E:555:GLU:OE2	2.41	0.54
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.41	0.54
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.72	0.54
2:B:520:ASN:ND2	2:B:555:GLU:OE2	2.41	0.54
2:E:4567:LEU:HD12	2:E:4816:ILE:HD12	1.90	0.54
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.90	0.54
2:G:520:ASN:ND2	2:G:555:GLU:OE2	2.41	0.54
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.89	0.54
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.72	0.54
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.90	0.54
2:B:331:VAL:HG12	2:B:333:GLY:H	1.73	0.54
2:B:4888:TYR:HA	2:I:4918:ILE:HD11	1.90	0.54
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.40	0.54
2:G:606:LEU:O	2:G:617:ASN:ND2	2.41	0.54
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.41	0.54
2:I:34:LYS:H	2:I:53:SER:HG	1.54	0.54
2:B:470:SER:O	2:B:474:ARG:NE	2.37	0.54
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.90	0.54
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.41	0.54
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.90	0.54
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.41	0.54
2:B:214:VAL:HG12	2:B:274:LEU:HD12	1.89	0.54
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.72	0.54
2:E:670:GLU:HG3	2:E:787:VAL:HG13	1.90	0.54
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.90	0.54
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.90	0.54
2:I:572:PRO:HA	2:I:575:LEU:HD13	1.90	0.54
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.90	0.53
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.90	0.53
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.90	0.53
2:E:331:VAL:HG12	2:E:333:GLY:H	1.73	0.53
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:606:LEU:O	2:I:617:ASN:ND2	2.41	0.53
2:B:4190:ILE:HD13	2:B:5026:ASP:CG	2.26	0.53
2:B:572:PRO:HA	2:B:575:LEU:HD13	1.90	0.53
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.90	0.53
2:E:2868:SER:O	2:E:2872:GLN:N	2.41	0.53
2:I:4152:GLU:OE1	2:I:4192:ARG:NH2	2.42	0.53
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	1.89	0.53
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.42	0.53
2:I:520:ASN:ND2	2:I:555:GLU:OE2	2.41	0.53
2:E:606:LEU:O	2:E:617:ASN:ND2	2.41	0.53
2:B:4152:GLU:OE1	2:B:4192:ARG:NH2	2.42	0.53
2:B:978:THR:HB	2:B:980:ALA:H	1.73	0.53
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.41	0.53
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.91	0.53
2:G:214:VAL:HG12	2:G:274:LEU:HD12	1.89	0.53
2:B:670:GLU:HG3	2:B:787:VAL:HG13	1.91	0.53
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.42	0.53
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.90	0.53
2:G:331:VAL:HG12	2:G:333:GLY:H	1.73	0.53
2:I:4567:LEU:HD12	2:I:4816:ILE:HD12	1.90	0.53
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.42	0.53
2:E:978:THR:HB	2:E:980:ALA:H	1.73	0.53
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.42	0.53
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.42	0.53
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.90	0.53
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.91	0.53
2:I:331:VAL:HG12	2:I:333:GLY:H	1.73	0.53
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.74	0.53
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.89	0.53
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.90	0.53
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.40	0.53
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.91	0.53
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.90	0.53
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.91	0.53
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.74	0.53
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.40	0.52
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.90	0.52
2:B:4567:LEU:HD12	2:B:4816:ILE:HD12	1.90	0.52
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.40	0.52
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.91	0.52
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.42	0.52
2:E:4152:GLU:OE1	2:E:4192:ARG:NH2	2.42	0.52
2:G:23:GLN:OE1	2:G:203:ASN:ND2	2.41	0.52
2:G:4190:ILE:HD13	2:G:5026:ASP:CG	2.26	0.52
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.42	0.52
2:E:23:GLN:OE1	2:E:203:ASN:ND2	2.41	0.52
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.41	0.52
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.91	0.52
2:G:4152:GLU:OE1	2:G:4192:ARG:NH2	2.42	0.52
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.42	0.52
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	1.91	0.52
2:E:572:PRO:HA	2:E:575:LEU:HD13	1.90	0.52
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.92	0.52
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.89	0.52
2:I:683:ARG:NH1	2:I:707:VAL:O	2.40	0.52
2:I:670:GLU:HG3	2:I:787:VAL:HG13	1.91	0.52
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.92	0.52
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.41	0.52
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.89	0.52
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.92	0.52
2:B:4945:ASP:OD2	2:E:4944:ARG:NH2	2.42	0.52
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.42	0.52
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.42	0.52
2:I:978:THR:HB	2:I:980:ALA:H	1.73	0.52
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.42	0.52
2:B:864:PRO:HD2	2:B:867:LEU:HD12	1.92	0.52
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.74	0.52
2:I:864:PRO:HD2	2:I:867:LEU:HD12	1.92	0.52
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.92	0.52
2:E:4190:ILE:HD13	2:E:5026:ASP:CG	2.26	0.52
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.92	0.52
2:E:256:ALA:HB1	2:E:286:THR:HG21	1.92	0.52
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.74	0.52
2:I:241:GLN:O	2:I:289:ARG:NH1	2.40	0.52
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.92	0.51
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	1.91	0.51
2:G:256:ALA:HB1	2:G:286:THR:HG21	1.92	0.51
2:G:978:THR:HB	2:G:980:ALA:H	1.73	0.51
2:I:470:SER:O	2:I:474:ARG:NE	2.37	0.51
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.92	0.51
2:G:111:HIS:CD2	2:G:114:SER:H	2.28	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:572:PRO:HA	2:G:575:LEU:HD13	1.90	0.51
2:I:23:GLN:OE1	2:I:203:ASN:ND2	2.41	0.51
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.93	0.51
2:E:34:LYS:H	2:E:53:SER:HG	1.55	0.51
2:G:2342:ASN:N	2:G:2342:ASN:OD1	2.43	0.51
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.93	0.51
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	1.91	0.51
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.91	0.51
2:G:864:PRO:HD2	2:G:867:LEU:HD12	1.92	0.51
2:I:256:ALA:HB1	2:I:286:THR:HG21	1.92	0.51
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.75	0.51
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.84	0.51
2:G:683:ARG:NH1	2:G:707:VAL:O	2.40	0.51
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.43	0.51
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.92	0.51
2:B:2342:ASN:N	2:B:2342:ASN:OD1	2.43	0.51
2:B:2868:SER:O	2:B:2872:GLN:N	2.41	0.51
2:B:256:ALA:HB1	2:B:286:THR:HG21	1.92	0.51
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.93	0.51
2:G:4236:SER:OG	2:G:4675:LYS:NZ	2.39	0.51
2:I:111:HIS:CD2	2:I:114:SER:H	2.28	0.51
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.92	0.51
2:B:485:SER:O	2:B:489:ASN:N	2.42	0.51
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.92	0.51
2:E:111:HIS:CD2	2:E:114:SER:H	2.28	0.51
2:E:221:ARG:NE	2:E:258:SER:OG	2.44	0.51
2:E:864:PRO:HD2	2:E:867:LEU:HD12	1.92	0.51
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.75	0.51
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	1.93	0.51
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.92	0.51
2:G:670:GLU:HG3	2:G:787:VAL:HG13	1.90	0.51
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.92	0.51
2:I:1796:ALA:HB1	2:I:1797:ARG:HH21	1.76	0.51
2:I:4190:ILE:HD13	2:I:5026:ASP:CG	2.26	0.51
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.84	0.51
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.93	0.51
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	1.93	0.51
2:B:34:LYS:H	2:B:53:SER:HG	1.55	0.51
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.84	0.51
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	1.91	0.51
2:G:1796:ALA:HB1	2:G:1797:ARG:HH21	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:309:THR:O	2:G:313:SER:OG	2.29	0.51
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.92	0.51
2:B:683:ARG:NH1	2:B:707:VAL:O	2.40	0.51
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	1.93	0.51
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.93	0.51
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.84	0.51
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.91	0.51
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.92	0.51
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.93	0.50
2:B:1796:ALA:HB1	2:B:1797:ARG:HH21	1.76	0.50
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	1.93	0.50
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.93	0.50
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.84	0.50
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.93	0.50
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.84	0.50
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.93	0.50
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.75	0.50
2:B:4236:SER:OG	2:B:4675:LYS:NZ	2.39	0.50
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.75	0.50
2:E:1796:ALA:HB1	2:E:1797:ARG:HH21	1.76	0.50
2:E:309:THR:O	2:E:313:SER:OG	2.29	0.50
2:G:3758:MET:HG3	2:G:3762:ARG:HD2	1.94	0.50
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.84	0.50
2:I:3758:MET:HG3	2:I:3762:ARG:HD2	1.94	0.50
2:I:395:GLN:HG3	2:I:397:GLU:H	1.77	0.50
2:E:4960:ILE:CG2	2:E:4988:TYR:CE2	2.95	0.50
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.94	0.50
2:G:34:LYS:H	2:G:53:SER:HG	1.55	0.50
2:I:2868:SER:O	2:I:2872:GLN:N	2.41	0.50
2:B:4960:ILE:CG2	2:B:4988:TYR:CE2	2.95	0.50
2:E:395:GLN:HG3	2:E:397:GLU:H	1.77	0.50
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.92	0.50
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.40	0.50
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.84	0.50
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.93	0.50
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.94	0.50
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.93	0.50
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.94	0.50
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.93	0.50
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.93	0.50
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.43	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.93	0.50
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.76	0.50
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.94	0.50
2:G:241:GLN:O	2:G:289:ARG:NH1	2.40	0.50
2:G:2868:SER:O	2:G:2872:GLN:N	2.41	0.50
2:I:309:THR:O	2:I:313:SER:OG	2.29	0.50
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	1.94	0.50
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.44	0.50
2:B:4198:SER:HB3	2:B:4201:ASN:HB2	1.94	0.50
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.43	0.50
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	1.94	0.50
2:G:4198:SER:HB3	2:G:4201:ASN:HB2	1.94	0.50
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.93	0.50
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.93	0.50
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	1.94	0.50
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.93	0.50
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.93	0.50
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.94	0.49
2:B:3758:MET:HG3	2:B:3762:ARG:HD2	1.94	0.49
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.44	0.49
2:G:395:GLN:HG3	2:G:397:GLU:H	1.77	0.49
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	1.94	0.49
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.93	0.49
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.93	0.49
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.94	0.49
2:E:3758:MET:HG3	2:E:3762:ARG:HD2	1.94	0.49
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.94	0.49
2:I:143:GLY:HA3	2:I:147:TRP:HE1	1.77	0.49
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.94	0.49
2:B:395:GLN:HG3	2:B:397:GLU:H	1.77	0.49
2:E:683:ARG:NH1	2:E:707:VAL:O	2.40	0.49
2:G:221:ARG:NE	2:G:258:SER:OG	2.44	0.49
2:G:662:TRP:HB2	2:G:748:LEU:HD23	1.94	0.49
2:B:309:THR:O	2:B:313:SER:OG	2.29	0.49
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.46	0.49
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.78	0.49
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.46	0.49
2:G:776:LEU:HG	2:G:848:HIS:HA	1.94	0.49
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.94	0.49
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.43	0.49
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.76	0.49
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.94	0.49
2:G:4960:ILE:CG2	2:G:4988:TYR:CE2	2.95	0.49
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.78	0.49
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.46	0.49
2:B:241:GLN:O	2:B:289:ARG:NH1	2.40	0.49
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.94	0.49
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.45	0.49
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.95	0.49
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.78	0.49
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.45	0.49
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.94	0.49
2:I:4960:ILE:CG2	2:I:4988:TYR:CE2	2.95	0.49
2:I:662:TRP:HB2	2:I:748:LEU:HD23	1.94	0.49
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.94	0.49
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.95	0.49
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.78	0.49
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.94	0.49
1:H:55:VAL:HA	2:G:1784:ALA:HA	1.94	0.49
2:G:2758:PHE:O	2:G:2762:THR:N	2.46	0.49
2:G:3733:CYS:HB2	2:G:3803:SER:HB3	1.95	0.49
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.40	0.49
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.95	0.49
2:I:776:LEU:HG	2:I:848:HIS:HA	1.94	0.49
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.93	0.49
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.94	0.49
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.48	0.49
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.46	0.49
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.95	0.49
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.94	0.49
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.43	0.49
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.40	0.49
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.95	0.49
2:G:143:GLY:HA3	2:G:147:TRP:HE1	1.76	0.49
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.95	0.48
2:B:111:HIS:CD2	2:B:114:SER:H	2.28	0.48
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.48	0.48
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.94	0.48
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.44	0.48
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.95	0.48
2:E:4945:ASP:OD2	2:G:4944:ARG:NH2	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4198:SER:HB3	2:I:4201:ASN:HB2	1.94	0.48
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.45	0.48
2:B:358:THR:HG21	2:B:382:GLY:HA2	1.95	0.48
2:E:4571:PHE:O	2:E:4575:PHE:N	2.47	0.48
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.85	0.48
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.96	0.48
2:E:358:THR:HG21	2:E:382:GLY:HA2	1.95	0.48
2:G:2880:GLU:O	2:G:2884:ASN:N	2.46	0.48
2:I:467:LYS:HA	2:I:470:SER:HB2	1.96	0.48
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.95	0.48
2:B:4571:PHE:O	2:B:4575:PHE:N	2.47	0.48
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.29	0.48
2:B:776:LEU:HG	2:B:848:HIS:HA	1.94	0.48
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.45	0.48
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.95	0.48
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.94	0.48
2:I:234:SER:O	2:I:242:ARG:NE	2.46	0.48
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.95	0.48
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.95	0.48
2:E:2880:GLU:O	2:E:2884:ASN:N	2.46	0.48
2:E:3733:CYS:HB2	2:E:3803:SER:HB3	1.95	0.48
2:E:662:TRP:HB2	2:E:748:LEU:HD23	1.94	0.48
2:E:776:LEU:HG	2:E:848:HIS:HA	1.94	0.48
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.78	0.48
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.78	0.48
2:I:485:SER:O	2:I:489:ASN:N	2.42	0.48
2:B:2758:PHE:O	2:B:2762:THR:N	2.46	0.48
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.48	0.48
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.43	0.48
1:F:55:VAL:HA	2:E:1784:ALA:HA	1.95	0.48
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.96	0.48
2:E:4586:PRO:HB3	2:E:4628:VAL:HG21	1.95	0.48
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.48	0.48
2:B:134:ASP:OD1	2:B:134:ASP:N	2.47	0.48
2:B:206:CYS:SG	2:B:207:SER:N	2.87	0.48
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.96	0.48
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.95	0.48
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.78	0.48
2:E:206:CYS:SG	2:E:207:SER:N	2.87	0.48
2:E:2758:PHE:O	2:E:2762:THR:N	2.46	0.48
2:G:467:LYS:HA	2:G:470:SER:HB2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:221:ARG:NE	2:I:258:SER:OG	2.44	0.48
2:I:358:THR:HG21	2:I:382:GLY:HA2	1.95	0.48
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.40	0.48
2:B:467:LYS:HA	2:B:470:SER:HB2	1.96	0.48
2:E:1838:PHE:HB3	2:E:1842:LEU:HD11	1.96	0.48
2:E:4198:SER:HB3	2:E:4201:ASN:HB2	1.94	0.48
2:E:467:LYS:HA	2:E:470:SER:HB2	1.95	0.48
2:G:234:SER:O	2:G:242:ARG:NE	2.46	0.48
2:G:4586:PRO:HB3	2:G:4628:VAL:HG21	1.96	0.48
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.95	0.48
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.95	0.48
2:I:4930:ALA:O	2:I:4934:GLY:N	2.47	0.48
2:B:3733:CYS:HB2	2:B:3803:SER:HB3	1.94	0.47
2:B:4930:ALA:O	2:B:4934:GLY:N	2.47	0.47
2:E:241:GLN:O	2:E:289:ARG:NH1	2.40	0.47
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.78	0.47
2:G:4930:ALA:O	2:G:4934:GLY:N	2.47	0.47
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.96	0.47
2:E:939:VAL:HG22	2:E:1053:ILE:HG23	1.96	0.47
2:E:234:SER:O	2:E:242:ARG:NE	2.46	0.47
2:I:1838:PHE:HB3	2:I:1842:LEU:HD11	1.96	0.47
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.43	0.47
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.30	0.47
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.96	0.47
2:E:134:ASP:N	2:E:134:ASP:OD1	2.47	0.47
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.96	0.47
2:I:3733:CYS:HB2	2:I:3803:SER:HB3	1.95	0.47
2:I:4068:LEU:HD13	2:I:4132:PHE:HE2	1.79	0.47
2:B:234:SER:O	2:B:242:ARG:NE	2.46	0.47
2:B:662:TRP:HB2	2:B:748:LEU:HD23	1.94	0.47
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.96	0.47
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.30	0.47
2:G:358:THR:HG21	2:G:382:GLY:HA2	1.95	0.47
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.96	0.47
2:B:939:VAL:HG22	2:B:1053:ILE:HG23	1.96	0.47
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.80	0.47
2:B:3889:GLN:HE22	2:B:3963:ASN:HB3	1.80	0.47
2:E:3889:GLN:HE22	2:E:3963:ASN:HB3	1.80	0.47
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.95	0.47
2:G:4571:PHE:O	2:G:4575:PHE:N	2.47	0.47
2:G:4180:ARG:NH1	2:G:4981:GLU:OE1	2.33	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:206:CYS:SG	2:G:207:SER:N	2.87	0.47
2:G:4068:LEU:HD13	2:G:4132:PHE:HE2	1.80	0.47
2:I:4571:PHE:O	2:I:4575:PHE:N	2.47	0.47
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.85	0.47
2:B:4068:LEU:HD13	2:B:4132:PHE:HE2	1.80	0.47
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.96	0.47
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.80	0.47
2:G:4239:GLU:OE2	2:G:5014:TYR:OH	2.28	0.47
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.29	0.47
2:I:939:VAL:HG22	2:I:1053:ILE:HG23	1.96	0.47
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.80	0.47
2:B:4586:PRO:HB3	2:B:4628:VAL:HG21	1.95	0.47
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.96	0.47
2:I:2452:ARG:HH12	2:G:177:GLU:HG3	1.79	0.47
2:I:2880:GLU:O	2:I:2884:ASN:N	2.46	0.47
2:I:3889:GLN:HE22	2:I:3963:ASN:HB3	1.80	0.47
2:I:4586:PRO:HB3	2:I:4628:VAL:HG21	1.95	0.47
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.80	0.47
2:G:1838:PHE:HB3	2:G:1842:LEU:HD11	1.96	0.47
2:G:485:SER:O	2:G:489:ASN:N	2.42	0.47
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.97	0.47
2:I:4180:ARG:NH1	2:I:4981:GLU:OE1	2.33	0.47
2:B:4944:ARG:NH2	2:I:4945:ASP:OD2	2.48	0.46
2:E:4918:ILE:HD11	2:G:4888:TYR:HA	1.97	0.46
2:G:134:ASP:OD1	2:G:134:ASP:N	2.47	0.46
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.80	0.46
2:I:206:CYS:SG	2:I:207:SER:N	2.87	0.46
2:B:2880:GLU:O	2:B:2884:ASN:N	2.46	0.46
2:E:4068:LEU:HD13	2:E:4132:PHE:HE2	1.79	0.46
2:G:2368:LEU:HD13	2:G:2376:LEU:HD23	1.97	0.46
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.97	0.46
2:I:2368:LEU:HD13	2:I:2376:LEU:HD23	1.97	0.46
2:I:2758:PHE:O	2:I:2762:THR:N	2.46	0.46
2:B:4034:ASN:ND2	2:B:4035:VAL:O	2.49	0.46
2:E:3766:GLN:HE22	2:E:3769:ARG:HH11	1.64	0.46
2:E:4180:ARG:NH1	2:E:4981:GLU:OE1	2.33	0.46
2:G:3766:GLN:HE22	2:G:3769:ARG:HH11	1.64	0.46
2:B:1838:PHE:HB3	2:B:1842:LEU:HD11	1.96	0.46
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	1.97	0.46
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.96	0.46
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.30	0.46
2:I:2466:LEU:HD23	2:I:2469:ILE:HD12	1.98	0.46
2:I:3766:GLN:HE22	2:I:3769:ARG:HH11	1.64	0.46
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	1.97	0.46
2:E:2368:LEU:HD13	2:E:2376:LEU:HD23	1.97	0.46
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.49	0.46
2:G:939:VAL:HG22	2:G:1053:ILE:HG23	1.96	0.46
2:I:211:GLU:OE2	2:I:3907:THR:OG1	2.34	0.46
2:B:1516:UNK:N	2:B:1529:UNK:O	2.49	0.46
2:E:2121:PHE:O	2:E:3725:TYR:OH	2.34	0.46
2:E:4034:ASN:ND2	2:E:4035:VAL:O	2.49	0.46
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.97	0.46
2:I:1516:UNK:N	2:I:1529:UNK:O	2.49	0.46
2:I:2272:PRO:HA	2:I:2275:VAL:HG12	1.98	0.46
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.49	0.46
2:B:2894:LEU:HD11	2:B:2902:HIS:HB2	1.98	0.46
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.97	0.46
2:B:4180:ARG:NH1	2:B:4981:GLU:OE1	2.33	0.46
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.97	0.46
2:E:485:SER:O	2:E:489:ASN:N	2.42	0.46
2:G:1516:UNK:N	2:G:1529:UNK:O	2.49	0.46
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.41	0.46
2:B:2368:LEU:HD13	2:B:2376:LEU:HD23	1.97	0.46
2:B:221:ARG:NE	2:B:258:SER:OG	2.44	0.46
2:E:1244:GLN:OE1	2:E:1646:ARG:NH1	2.49	0.46
2:I:4034:ASN:ND2	2:I:4035:VAL:O	2.49	0.46
2:I:4236:SER:OG	2:I:4675:LYS:NZ	2.39	0.46
2:B:3766:GLN:HE22	2:B:3769:ARG:HH11	1.64	0.46
2:E:4930:ALA:O	2:E:4934:GLY:N	2.47	0.46
2:G:4034:ASN:ND2	2:G:4035:VAL:O	2.49	0.46
2:I:2265:LEU:HD22	2:I:2330:ARG:HB3	1.97	0.46
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	1.97	0.45
2:B:1244:GLN:OE1	2:B:1646:ARG:NH1	2.49	0.45
2:B:2265:LEU:HD22	2:B:2330:ARG:HB3	1.97	0.45
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	1.97	0.45
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.85	0.45
2:G:2466:LEU:HD23	2:G:2469:ILE:HD12	1.98	0.45
2:I:1244:GLN:OE1	2:I:1646:ARG:NH1	2.49	0.45
2:B:2272:PRO:HA	2:B:2275:VAL:HG12	1.98	0.45
2:B:379:HIS:CD2	2:B:381:GLU:H	2.35	0.45
2:E:1516:UNK:N	2:E:1529:UNK:O	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1244:GLN:OE1	2:G:1646:ARG:NH1	2.49	0.45
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.30	0.45
2:E:2466:LEU:HD23	2:E:2469:ILE:HD12	1.98	0.45
2:E:2894:LEU:HD11	2:E:2902:HIS:HB2	1.98	0.45
2:E:379:HIS:CD2	2:E:381:GLU:H	2.35	0.45
2:E:652:ARG:HD2	2:E:750:LEU:HB3	1.98	0.45
2:G:3362:UNK:O	2:G:3366:UNK:N	2.50	0.45
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.97	0.45
1:H:5:GLU:HB2	1:H:73:LYS:HB3	1.99	0.45
2:I:2894:LEU:HD11	2:I:2902:HIS:HB2	1.98	0.45
2:B:211:GLU:OE2	2:B:3907:THR:OG1	2.34	0.45
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.49	0.45
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.97	0.45
2:E:2265:LEU:HD22	2:E:2330:ARG:HB3	1.97	0.45
2:E:3362:UNK:O	2:E:3366:UNK:N	2.50	0.45
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.49	0.45
2:G:2332:LEU:HD13	2:G:2335:LEU:HD12	1.99	0.45
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.97	0.45
2:E:2272:PRO:HA	2:E:2275:VAL:HG12	1.98	0.45
1:F:5:GLU:HB2	1:F:73:LYS:HB3	1.99	0.45
2:G:2265:LEU:HD22	2:G:2330:ARG:HB3	1.97	0.45
2:I:4181:ILE:HG13	2:I:4988:TYR:HE1	1.82	0.45
2:B:2332:LEU:HD13	2:B:2335:LEU:HD12	1.99	0.45
2:B:4181:ILE:HG13	2:B:4988:TYR:HE1	1.82	0.45
2:E:4181:ILE:HG13	2:E:4988:TYR:HE1	1.82	0.45
2:G:1735:ILE:HG23	2:G:1771:LEU:HD23	1.99	0.45
2:G:211:GLU:OE2	2:G:3907:THR:OG1	2.33	0.45
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.82	0.45
2:I:1735:ILE:HG23	2:I:1771:LEU:HD23	1.99	0.45
2:I:1865:MET:SD	2:I:1865:MET:N	2.90	0.45
1:J:5:GLU:HB2	1:J:73:LYS:HB3	1.99	0.45
2:B:1707:LEU:O	2:B:1710:GLY:N	2.33	0.45
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.99	0.45
2:B:2121:PHE:O	2:B:3725:TYR:OH	2.34	0.45
2:B:652:ARG:HD2	2:B:750:LEU:HB3	1.98	0.45
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.99	0.45
2:G:4230:LYS:HD2	2:G:4959:PHE:CD1	2.52	0.45
2:G:652:ARG:HD2	2:G:750:LEU:HB3	1.98	0.45
2:I:3362:UNK:O	2:I:3366:UNK:N	2.50	0.45
1:A:55:VAL:HA	2:B:1784:ALA:HA	1.98	0.45
2:I:788:LYS:HG2	2:I:1629:GLN:HA	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.35	0.45
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	1.99	0.45
2:E:3658:LYS:HA	2:E:3661:TRP:CE2	2.52	0.45
2:E:4763:GLY:O	2:E:4766:THR:OG1	2.29	0.45
2:E:4230:LYS:HD2	2:E:4959:PHE:CD1	2.52	0.45
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.43	0.45
2:G:379:HIS:CD2	2:G:381:GLU:H	2.35	0.45
2:G:4959:PHE:CD1	2:G:4959:PHE:O	2.70	0.45
2:I:134:ASP:OD1	2:I:134:ASP:N	2.47	0.45
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.82	0.45
2:I:4959:PHE:O	2:I:4959:PHE:CD1	2.70	0.45
2:I:5028:PHE:O	2:I:5028:PHE:CG	2.70	0.45
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.40	0.44
2:B:4230:LYS:HD2	2:B:4959:PHE:CD1	2.52	0.44
2:G:3842:LEU:O	2:G:3929:SER:OG	2.34	0.44
2:G:4181:ILE:HG13	2:G:4988:TYR:HE1	1.82	0.44
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.99	0.44
2:I:4230:LYS:HD2	2:I:4959:PHE:CD1	2.52	0.44
1:A:5:GLU:HB2	1:A:73:LYS:HB3	1.99	0.44
2:B:1865:MET:SD	2:B:1865:MET:N	2.90	0.44
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.82	0.44
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.43	0.44
2:B:3658:LYS:HA	2:B:3661:TRP:CE2	2.52	0.44
2:B:5028:PHE:CD1	2:B:5028:PHE:O	2.70	0.44
2:G:2894:LEU:HD11	2:G:2902:HIS:HB2	1.98	0.44
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.99	0.44
2:B:2466:LEU:HD23	2:B:2469:ILE:HD12	1.98	0.44
2:B:5028:PHE:O	2:B:5028:PHE:CG	2.70	0.44
2:B:788:LYS:HG2	2:B:1629:GLN:HA	1.99	0.44
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.82	0.44
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.82	0.44
2:E:4961:CYS:HB3	2:E:4983:HIS:CE1	2.53	0.44
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.35	0.44
2:G:1865:MET:SD	2:G:1865:MET:N	2.90	0.44
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.99	0.44
2:I:210:GLU:H	2:I:273:HIS:HE1	1.66	0.44
2:I:379:HIS:CD2	2:I:381:GLU:H	2.35	0.44
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.43	0.44
2:B:4961:CYS:HB3	2:B:4983:HIS:CE1	2.53	0.44
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.99	0.44
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4961:CYS:HB3	2:E:4983:HIS:HE1	1.82	0.44
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.99	0.44
2:G:5028:PHE:O	2:G:5028:PHE:CG	2.70	0.44
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.35	0.44
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.82	0.44
2:I:652:ARG:HD2	2:I:750:LEU:HB3	1.98	0.44
2:I:645:ARG:HH11	2:I:778:PHE:HE1	1.66	0.44
1:A:30:LEU:HD23	1:A:33:GLY:HA3	2.00	0.44
2:G:1676:LEU:HD23	2:G:2167:ILE:HG23	1.99	0.44
2:G:2272:PRO:HA	2:G:2275:VAL:HG12	1.98	0.44
2:G:695:TYR:OH	2:G:1073:ARG:NH1	2.44	0.44
2:I:3842:LEU:O	2:I:3929:SER:OG	2.34	0.44
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.82	0.44
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.85	0.44
2:E:2332:LEU:HD13	2:E:2335:LEU:HD12	1.99	0.44
2:G:4961:CYS:HB3	2:G:4983:HIS:HE1	1.82	0.44
2:I:4826:ILE:O	2:I:4829:SER:OG	2.29	0.44
2:I:5028:PHE:O	2:I:5028:PHE:CD1	2.70	0.44
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	1.99	0.44
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.83	0.44
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.99	0.44
2:E:1032:LYS:O	2:E:1036:ARG:N	2.47	0.44
2:E:1077:ALA:HB3	2:E:1189:LEU:HD11	2.00	0.44
2:E:210:GLU:H	2:E:273:HIS:HE1	1.66	0.44
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.83	0.44
2:E:4236:SER:OG	2:E:4675:LYS:NZ	2.39	0.44
2:G:4961:CYS:HB3	2:G:4983:HIS:CE1	2.53	0.44
2:I:4071:ILE:HD11	2:I:4102:GLN:HE21	1.83	0.44
1:J:30:LEU:HD23	1:J:33:GLY:HA3	2.00	0.44
2:B:1171:SER:OG	2:B:1175:SER:N	2.42	0.44
2:B:210:GLU:H	2:B:273:HIS:HE1	1.66	0.44
2:B:645:ARG:HH11	2:B:778:PHE:HE1	1.66	0.44
2:E:4959:PHE:CD1	2:E:4959:PHE:O	2.70	0.44
2:E:5028:PHE:O	2:E:5028:PHE:CD1	2.71	0.44
2:E:5028:PHE:CG	2:E:5028:PHE:O	2.70	0.44
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.82	0.44
2:G:788:LYS:HG2	2:G:1629:GLN:HA	1.99	0.44
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.82	0.44
2:B:1077:ALA:HB3	2:B:1189:LEU:HD11	2.00	0.44
2:B:177:GLU:HG3	2:E:2452:ARG:HH12	1.83	0.44
2:B:3362:UNK:O	2:B:3366:UNK:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3842:LEU:O	2:B:3929:SER:OG	2.35	0.44
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.35	0.44
2:E:3842:LEU:O	2:E:3929:SER:OG	2.35	0.44
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.40	0.44
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.82	0.43
2:B:219:VAL:HG13	2:B:285:VAL:HG21	2.00	0.43
2:B:4959:PHE:CD1	2:B:4959:PHE:O	2.70	0.43
2:B:4961:CYS:HB3	2:B:4983:HIS:HE1	1.82	0.43
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.99	0.43
2:E:219:VAL:HG13	2:E:285:VAL:HG21	2.00	0.43
2:G:210:GLU:H	2:G:273:HIS:HE1	1.66	0.43
2:G:3658:LYS:HA	2:G:3661:TRP:CE2	2.52	0.43
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.43	0.43
2:I:3658:LYS:HA	2:I:3661:TRP:CE2	2.52	0.43
2:I:3980:LEU:HD22	2:I:3985:LEU:HD22	2.00	0.43
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.36	0.43
2:I:4228:ALA:O	2:I:4232:GLU:N	2.51	0.43
2:I:719:LEU:HD22	2:I:735:GLN:HG2	2.00	0.43
2:E:1865:MET:N	2:E:1865:MET:SD	2.90	0.43
2:E:4228:ALA:O	2:E:4232:GLU:N	2.51	0.43
2:G:2024:PRO:O	2:G:2028:ARG:NE	2.46	0.43
2:G:2121:PHE:O	2:G:3725:TYR:OH	2.34	0.43
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	2.00	0.43
2:G:4071:ILE:HD11	2:G:4102:GLN:HE21	1.83	0.43
2:G:645:ARG:HH11	2:G:778:PHE:HE1	1.66	0.43
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.99	0.43
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	2.00	0.43
2:B:4071:ILE:HD11	2:B:4102:GLN:HE21	1.83	0.43
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.36	0.43
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.99	0.43
2:G:2143:THR:O	2:G:3651:ASN:ND2	2.44	0.43
2:G:471:LEU:O	2:G:475:GLN:N	2.52	0.43
2:I:1077:ALA:HB3	2:I:1189:LEU:HD11	2.00	0.43
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	1.99	0.43
2:I:2332:LEU:HD13	2:I:2335:LEU:HD12	1.99	0.43
2:B:3980:LEU:HD22	2:B:3985:LEU:HD22	2.00	0.43
1:F:30:LEU:HD23	1:F:33:GLY:HA3	2.00	0.43
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.83	0.43
2:B:1189:LEU:HD12	2:B:1190:PRO:HD2	2.00	0.43
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	1.99	0.43
2:E:765:GLN:NE2	2:E:1521:UNK:O	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:788:LYS:HG2	2:E:1629:GLN:HA	1.99	0.43
2:G:1189:LEU:HD12	2:G:1190:PRO:HD2	2.00	0.43
2:G:5028:PHE:O	2:G:5028:PHE:CD1	2.71	0.43
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.40	0.43
2:I:4961:CYS:HB3	2:I:4983:HIS:HE1	1.83	0.43
2:E:1735:ILE:HG23	2:E:1771:LEU:HD23	1.99	0.43
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.83	0.43
2:E:719:LEU:HD22	2:E:735:GLN:HG2	2.00	0.43
2:G:1707:LEU:O	2:G:1710:GLY:N	2.34	0.43
2:I:4961:CYS:HB3	2:I:4983:HIS:CE1	2.53	0.43
2:B:21:VAL:HG12	2:B:66:CYS:HA	2.00	0.43
2:B:3733:CYS:HA	2:B:3766:GLN:HB2	2.01	0.43
2:E:3980:LEU:HD22	2:E:3985:LEU:HD22	2.00	0.43
2:E:645:ARG:HH11	2:E:778:PHE:HE1	1.66	0.43
2:G:765:GLN:NE2	2:G:1521:UNK:O	2.52	0.43
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.83	0.43
2:G:454:PRO:HG2	2:G:531:ARG:HH12	1.84	0.43
2:B:1155:LEU:HD23	2:B:1184:ILE:HD12	2.01	0.43
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	2.01	0.43
2:E:1189:LEU:HD12	2:E:1190:PRO:HD2	2.00	0.43
2:E:454:PRO:HG2	2:E:531:ARG:HH12	1.84	0.43
2:G:1155:LEU:HD23	2:G:1184:ILE:HD12	2.00	0.43
2:G:3980:LEU:HD22	2:G:3985:LEU:HD22	2.00	0.43
1:H:30:LEU:HD23	1:H:33:GLY:HA3	2.00	0.43
2:I:500:ALA:HB1	2:I:504:ALA:HB2	2.00	0.43
2:B:1032:LYS:O	2:B:1036:ARG:N	2.47	0.43
2:E:1155:LEU:HD23	2:E:1184:ILE:HD12	2.00	0.43
2:G:1032:LYS:O	2:G:1036:ARG:N	2.47	0.43
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.36	0.43
2:G:719:LEU:HD22	2:G:735:GLN:HG2	2.00	0.43
2:I:1189:LEU:HD12	2:I:1190:PRO:HD2	2.00	0.43
2:I:3733:CYS:HA	2:I:3766:GLN:HB2	2.01	0.43
2:B:500:ALA:HB1	2:B:504:ALA:HB2	2.00	0.42
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.83	0.42
2:G:2883:HIS:NE2	2:G:2906:VAL:O	2.52	0.42
2:G:3733:CYS:HA	2:G:3766:GLN:HB2	2.01	0.42
2:G:4228:ALA:O	2:G:4232:GLU:N	2.51	0.42
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	2.01	0.42
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.29	0.42
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	2.01	0.42
2:E:500:ALA:HB1	2:E:504:ALA:HB2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:219:VAL:HG13	2:G:285:VAL:HG21	2.00	0.42
2:G:3805:LEU:HG	2:G:3805:LEU:H	1.69	0.42
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	2.01	0.42
2:I:2024:PRO:O	2:I:2028:ARG:NE	2.46	0.42
2:I:2029:GLN:O	2:I:2033:ASP:N	2.52	0.42
2:I:2121:PHE:O	2:I:3725:TYR:OH	2.34	0.42
2:I:21:VAL:HG12	2:I:66:CYS:HA	2.00	0.42
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.36	0.42
2:B:4228:ALA:O	2:B:4232:GLU:N	2.51	0.42
2:E:21:VAL:HG12	2:E:66:CYS:HA	2.00	0.42
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	2.00	0.42
2:G:1077:ALA:HB3	2:G:1189:LEU:HD11	2.00	0.42
2:I:219:VAL:HG13	2:I:285:VAL:HG21	2.00	0.42
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	2.00	0.42
2:I:765:GLN:NE2	2:I:1521:UNK:O	2.52	0.42
2:B:4978:HIS:HA	2:B:4982:GLU:HB2	2.02	0.42
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	2.01	0.42
2:E:2024:PRO:O	2:E:2028:ARG:NE	2.46	0.42
2:G:3365:UNK:O	2:G:3369:UNK:N	2.53	0.42
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	2.01	0.42
2:I:4101:LYS:HG3	2:G:4731:ILE:HA	2.01	0.42
2:B:1099:GLU:OE2	2:B:1127:HIS:ND1	2.35	0.42
2:B:454:PRO:HG2	2:B:531:ARG:HH12	1.84	0.42
2:E:4125:PHE:HA	2:E:4128:PHE:HB3	2.02	0.42
2:G:1863:LEU:HB3	2:G:1870:VAL:HG21	2.02	0.42
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	2.01	0.42
2:G:2214:VAL:HG23	2:G:2215:LEU:HD12	2.02	0.42
2:G:500:ALA:HB1	2:G:504:ALA:HB2	2.00	0.42
2:I:471:LEU:O	2:I:475:GLN:N	2.52	0.42
2:E:211:GLU:OE2	2:E:3907:THR:OG1	2.34	0.42
1:F:92:PRO:HD3	2:E:627:PRO:HB2	2.01	0.42
2:G:1259:ARG:HH12	2:G:1593:PRO:HA	1.85	0.42
2:G:4125:PHE:HA	2:G:4128:PHE:HB3	2.02	0.42
2:I:1863:LEU:HB3	2:I:1870:VAL:HG21	2.02	0.42
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.52	0.42
2:B:765:GLN:NE2	2:B:1521:UNK:O	2.52	0.42
2:E:2214:VAL:HG23	2:E:2215:LEU:HD12	2.02	0.42
2:G:164:ARG:N	2:G:167:ASP:OD2	2.53	0.42
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	2.01	0.42
2:G:313:SER:HB3	2:G:351:VAL:HB	2.02	0.42
2:I:1259:ARG:HH12	2:I:1593:PRO:HA	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:913:LEU:O	2:I:918:ARG:NH2	2.53	0.42
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.52	0.42
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.01	0.42
2:E:3733:CYS:HA	2:E:3766:GLN:HB2	2.01	0.42
2:E:4071:ILE:HD11	2:E:4102:GLN:HE21	1.83	0.42
2:G:21:VAL:HG12	2:G:66:CYS:HA	2.00	0.42
2:G:472:ARG:HA	2:G:475:GLN:HB2	2.02	0.42
2:I:2214:VAL:HG23	2:I:2215:LEU:HD12	2.02	0.42
2:I:2883:HIS:NE2	2:I:2906:VAL:O	2.52	0.42
2:B:164:ARG:N	2:B:167:ASP:OD2	2.53	0.42
2:B:719:LEU:HD22	2:B:735:GLN:HG2	2.00	0.42
2:B:913:LEU:O	2:B:918:ARG:NH2	2.53	0.42
2:E:2776:SER:O	2:E:2788:HIS:N	2.53	0.42
2:E:3365:UNK:O	2:E:3369:UNK:N	2.53	0.42
2:G:2776:SER:O	2:G:2788:HIS:N	2.53	0.42
2:I:1155:LEU:HD23	2:I:1184:ILE:HD12	2.01	0.42
2:I:3365:UNK:O	2:I:3369:UNK:N	2.53	0.42
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.55	0.42
2:B:1259:ARG:HH12	2:B:1593:PRO:HA	1.85	0.42
2:B:1863:LEU:HB3	2:B:1870:VAL:HG21	2.02	0.42
2:B:2029:GLN:O	2:B:2033:ASP:N	2.51	0.42
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.55	0.42
2:B:472:ARG:HA	2:B:475:GLN:HB2	2.02	0.42
2:G:451:TYR:O	2:G:474:ARG:NH1	2.53	0.42
2:I:2143:THR:O	2:I:3651:ASN:ND2	2.43	0.42
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.84	0.42
2:B:313:SER:HB3	2:B:351:VAL:HB	2.02	0.41
2:B:3365:UNK:O	2:B:3369:UNK:N	2.53	0.41
2:E:1259:ARG:HH12	2:E:1593:PRO:HA	1.85	0.41
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	2.01	0.41
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.52	0.41
2:G:4897:ILE:HG12	2:G:4901:ILE:HD13	2.02	0.41
2:I:2095:GLN:NE2	2:I:2127:GLN:O	2.53	0.41
2:I:472:ARG:HA	2:I:475:GLN:HB2	2.02	0.41
2:B:1972:ASN:O	2:B:1976:ARG:N	2.52	0.41
2:B:4897:ILE:HG12	2:B:4901:ILE:HD13	2.02	0.41
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.40	0.41
2:I:1041:GLN:O	2:I:1045:THR:OG1	2.31	0.41
2:I:2196:ASN:OD1	2:I:2199:ARG:NH1	2.43	0.41
2:B:4125:PHE:HA	2:B:4128:PHE:HB3	2.02	0.41
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:599:VAL:HG23	2:B:600:LEU:HD12	2.02	0.41
2:B:940:GLY:O	2:B:1052:ASN:N	2.54	0.41
2:E:1171:SER:OG	2:E:1175:SER:N	2.42	0.41
2:E:1863:LEU:HB3	2:E:1870:VAL:HG21	2.02	0.41
2:E:356:TRP:O	2:E:379:HIS:N	2.52	0.41
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.43	0.41
2:E:599:VAL:HG23	2:E:600:LEU:HD12	2.02	0.41
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.55	0.41
2:G:346:CYS:N	2:G:388:LEU:O	2.52	0.41
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.01	0.41
2:B:70:GLU:HB2	2:B:108:LEU:HD23	2.03	0.41
2:E:1641:ILE:HA	2:E:1642:PRO:HD3	1.93	0.41
2:E:2285:GLU:HG3	2:E:2286:LEU:HG	2.03	0.41
2:E:3923:LEU:HD13	2:E:3961:VAL:HG11	2.03	0.41
2:E:451:TYR:O	2:E:474:ARG:NH1	2.53	0.41
2:E:472:ARG:HA	2:E:475:GLN:HB2	2.02	0.41
2:E:4978:HIS:HA	2:E:4982:GLU:HB2	2.01	0.41
2:G:599:VAL:HG23	2:G:600:LEU:HD12	2.02	0.41
2:G:913:LEU:O	2:G:918:ARG:NH2	2.53	0.41
2:I:4125:PHE:HA	2:I:4128:PHE:HB3	2.02	0.41
2:B:591:ASP:O	2:B:1594:ARG:NH2	2.54	0.41
2:E:164:ARG:N	2:E:167:ASP:OD2	2.53	0.41
2:E:177:GLU:HG3	2:G:2452:ARG:HH12	1.86	0.41
2:E:346:CYS:N	2:E:388:LEU:O	2.52	0.41
2:E:591:ASP:O	2:E:1594:ARG:NH2	2.54	0.41
2:E:913:LEU:O	2:E:918:ARG:NH2	2.53	0.41
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.84	0.41
2:G:1936:LYS:O	2:G:1940:CYS:N	2.49	0.41
2:G:698:GLY:HA2	2:G:703:GLY:HA2	2.03	0.41
2:I:116:MET:HB2	2:I:137:LEU:HD12	2.03	0.41
2:I:2776:SER:O	2:I:2788:HIS:N	2.53	0.41
2:I:599:VAL:HG23	2:I:600:LEU:HD12	2.02	0.41
2:I:698:GLY:HA2	2:I:703:GLY:HA2	2.03	0.41
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.53	0.41
2:B:2214:VAL:HG23	2:B:2215:LEU:HD12	2.02	0.41
2:B:3694:LYS:HA	2:B:3695:PRO:HD3	1.95	0.41
2:B:346:CYS:N	2:B:388:LEU:O	2.52	0.41
2:B:4918:ILE:HD11	2:E:4888:TYR:HA	2.03	0.41
2:B:4961:CYS:O	2:B:4961:CYS:SG	2.79	0.41
2:E:284:HIS:N	2:E:289:ARG:O	2.42	0.41
2:E:2883:HIS:NE2	2:E:2906:VAL:O	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.55	0.41
2:G:116:MET:HB2	2:G:137:LEU:HD12	2.03	0.41
2:G:2285:GLU:HG3	2:G:2286:LEU:HG	2.03	0.41
2:G:3923:LEU:HD13	2:G:3961:VAL:HG11	2.03	0.41
2:G:4236:SER:HG	2:G:4675:LYS:HZ1	1.64	0.41
2:G:4978:HIS:HA	2:G:4982:GLU:HB2	2.01	0.41
2:I:1973:GLN:HA	2:I:1976:ARG:HB3	2.03	0.41
2:I:3361:UNK:O	2:I:3365:UNK:N	2.54	0.41
2:I:70:GLU:HB2	2:I:108:LEU:HD23	2.03	0.41
2:B:2285:GLU:HG3	2:B:2286:LEU:HG	2.03	0.41
2:B:3361:UNK:O	2:B:3365:UNK:N	2.54	0.41
2:E:1739:THR:H	2:E:1742:THR:HB	1.86	0.41
2:E:940:GLY:O	2:E:1052:ASN:N	2.54	0.41
2:G:591:ASP:O	2:G:1594:ARG:NH2	2.53	0.41
2:G:2095:GLN:NE2	2:G:2127:GLN:O	2.53	0.41
2:G:2517:UNK:O	2:G:2521:UNK:N	2.54	0.41
2:I:1739:THR:H	2:I:1742:THR:HB	1.86	0.41
2:I:2517:UNK:O	2:I:2521:UNK:N	2.54	0.41
2:I:3923:LEU:HD13	2:I:3961:VAL:HG11	2.03	0.41
2:I:591:ASP:O	2:I:1594:ARG:NH2	2.54	0.41
2:B:2143:THR:O	2:B:3651:ASN:ND2	2.43	0.41
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	2.03	0.41
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.86	0.41
2:E:1972:ASN:O	2:E:1976:ARG:N	2.52	0.41
2:E:4984:ASN:C	2:E:4986:ALA:H	2.24	0.41
2:E:70:GLU:HB2	2:E:108:LEU:HD23	2.03	0.41
2:G:4961:CYS:SG	2:G:4961:CYS:O	2.79	0.41
2:G:70:GLU:HB2	2:G:108:LEU:HD23	2.03	0.41
2:G:894:GLY:HA3	2:G:903:LEU:HD22	2.03	0.41
2:I:313:SER:HB3	2:I:351:VAL:HB	2.02	0.41
2:I:451:TYR:O	2:I:474:ARG:NH1	2.53	0.41
2:I:4961:CYS:O	2:I:4961:CYS:SG	2.79	0.41
2:I:5004:THR:H	2:I:5007:GLU:HB2	1.86	0.41
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.84	0.41
2:B:116:MET:HB2	2:B:137:LEU:HD12	2.03	0.41
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.85	0.41
2:E:4960:ILE:CG2	2:E:4988:TYR:OH	2.69	0.41
2:E:4963:ILE:HD13	2:E:5027:CYS:SG	2.61	0.41
2:E:649:PHE:HB3	2:E:776:LEU:HD13	2.03	0.41
2:G:2029:GLN:O	2:G:2033:ASP:N	2.51	0.41
2:I:1972:ASN:O	2:I:1976:ARG:N	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4657:CYS:HB3	2:I:4792:LEU:HD11	2.03	0.41
2:I:4960:ILE:CG2	2:I:4988:TYR:OH	2.69	0.41
2:I:4978:HIS:HA	2:I:4982:GLU:HB2	2.02	0.41
2:B:2517:UNK:O	2:B:2521:UNK:N	2.54	0.41
2:B:330:ASP:OD1	2:B:330:ASP:N	2.54	0.41
2:B:5004:THR:H	2:B:5007:GLU:HB2	1.86	0.41
2:B:670:GLU:H	2:B:740:PRO:HB3	1.86	0.41
2:E:3361:UNK:O	2:E:3365:UNK:N	2.54	0.41
2:E:4897:ILE:HG12	2:E:4901:ILE:HD13	2.02	0.41
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.86	0.41
2:G:1739:THR:H	2:G:1742:THR:HB	1.86	0.41
2:G:330:ASP:OD1	2:G:330:ASP:N	2.54	0.41
2:G:4984:ASN:C	2:G:4986:ALA:H	2.24	0.41
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.52	0.41
2:G:670:GLU:H	2:G:740:PRO:HB3	1.86	0.41
2:G:940:GLY:O	2:G:1052:ASN:N	2.54	0.41
2:I:1657:LEU:HA	2:I:1657:LEU:HD13	1.94	0.41
2:I:4984:ASN:C	2:I:4986:ALA:H	2.24	0.41
2:I:670:GLU:H	2:I:740:PRO:HB3	1.86	0.41
2:B:2883:HIS:NE2	2:B:2906:VAL:O	2.52	0.41
2:B:4960:ILE:CG2	2:B:4988:TYR:OH	2.69	0.41
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.52	0.41
2:E:2143:THR:O	2:E:3651:ASN:ND2	2.43	0.41
2:E:313:SER:HB3	2:E:351:VAL:HB	2.02	0.41
2:E:813:GLU:OE2	2:E:1020:ARG:N	2.54	0.41
2:G:1141:ARG:HD2	2:G:1141:ARG:H	1.86	0.41
2:G:215:THR:HG22	2:G:273:HIS:HA	2.03	0.41
2:I:1663:HIS:O	2:I:1667:LEU:N	2.53	0.41
2:I:164:ARG:N	2:I:167:ASP:OD2	2.53	0.41
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.86	0.41
2:I:2285:GLU:HG3	2:I:2286:LEU:HG	2.03	0.41
2:B:1029:GLU:HB3	2:B:1033:ARG:HH12	1.86	0.40
2:B:1739:THR:H	2:B:1742:THR:HB	1.86	0.40
2:B:4010:ILE:HD12	2:B:4131:ARG:HD2	2.03	0.40
2:B:113:HIS:CE1	2:B:402:ARG:HB3	2.56	0.40
2:B:4239:GLU:OE2	2:B:5014:TYR:OH	2.28	0.40
2:E:1973:GLN:HA	2:E:1976:ARG:HB3	2.03	0.40
2:E:4010:ILE:HD12	2:E:4131:ARG:HD2	2.03	0.40
2:E:4961:CYS:O	2:E:4961:CYS:SG	2.79	0.40
2:E:5004:THR:H	2:E:5007:GLU:HB2	1.86	0.40
2:G:3361:UNK:O	2:G:3365:UNK:N	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1099:GLU:OE2	2:I:1127:HIS:ND1	2.35	0.40
2:I:215:THR:HG22	2:I:273:HIS:HA	2.03	0.40
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.86	0.40
2:B:2448:GLY:HA2	2:B:2451:LEU:HD12	2.04	0.40
2:B:698:GLY:HA2	2:B:703:GLY:HA2	2.03	0.40
2:E:116:MET:HB2	2:E:137:LEU:HD12	2.03	0.40
2:E:1707:LEU:O	2:E:1710:GLY:N	2.33	0.40
2:E:215:THR:HG22	2:E:273:HIS:HA	2.03	0.40
2:E:4148:THR:HG21	2:E:4178:LEU:HD21	2.04	0.40
2:E:670:GLU:H	2:E:740:PRO:HB3	1.86	0.40
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.04	0.40
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.85	0.40
2:G:734:GLY:O	2:G:736:HIS:ND1	2.52	0.40
2:I:4963:ILE:HD13	2:I:5027:CYS:SG	2.61	0.40
2:B:1641:ILE:HA	2:B:1642:PRO:HD3	1.93	0.40
2:B:1973:GLN:HA	2:B:1976:ARG:HB3	2.03	0.40
2:B:2776:SER:O	2:B:2788:HIS:N	2.53	0.40
2:E:2517:UNK:O	2:E:2521:UNK:N	2.54	0.40
2:E:330:ASP:OD1	2:E:330:ASP:N	2.54	0.40
2:E:698:GLY:HA2	2:E:703:GLY:HA2	2.03	0.40
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.52	0.40
2:G:4963:ILE:HD13	2:G:5027:CYS:SG	2.61	0.40
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.86	0.40
2:I:2448:GLY:HA2	2:I:2451:LEU:HD12	2.04	0.40
2:I:113:HIS:CE1	2:I:402:ARG:HB3	2.56	0.40
2:I:649:PHE:HB3	2:I:776:LEU:HD13	2.03	0.40
2:B:4657:CYS:HB3	2:B:4792:LEU:HD11	2.03	0.40
2:E:1029:GLU:HB3	2:E:1033:ARG:HH12	1.86	0.40
2:E:113:HIS:CE1	2:E:402:ARG:HB3	2.56	0.40
2:E:894:GLY:HA3	2:E:903:LEU:HD22	2.03	0.40
2:G:1029:GLU:HB3	2:G:1033:ARG:HH12	1.86	0.40
2:I:813:GLU:OE2	2:I:1020:ARG:N	2.54	0.40
2:I:346:CYS:N	2:I:388:LEU:O	2.52	0.40
2:B:4984:ASN:C	2:B:4986:ALA:H	2.24	0.40
2:B:649:PHE:HB3	2:B:776:LEU:HD13	2.03	0.40
2:G:5004:THR:H	2:G:5007:GLU:HB2	1.86	0.40
2:G:813:GLU:OE2	2:G:1020:ARG:N	2.54	0.40
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.86	0.40
2:I:4010:ILE:HD12	2:I:4131:ARG:HD2	2.03	0.40
2:I:894:GLY:HA3	2:I:903:LEU:HD22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	93 (89%)	12 (11%)	0	100	100
1	F	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	H	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	J	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	B	3235/4416 (73%)	2892 (89%)	335 (10%)	8 (0%)	52	86
2	E	3235/4416 (73%)	2893 (89%)	334 (10%)	8 (0%)	52	86
2	G	3235/4416 (73%)	2893 (89%)	334 (10%)	8 (0%)	52	86
2	I	3235/4416 (73%)	2891 (89%)	336 (10%)	8 (0%)	52	86
All	All	13360/18096 (74%)	11941 (89%)	1387 (10%)	32 (0%)	56	86

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5028	PHE
2	I	5028	PHE
2	E	5028	PHE
2	G	5028	PHE
2	B	1708	ARG
2	B	1932	PRO
2	B	4982	GLU
2	I	1708	ARG
2	I	1932	PRO
2	E	1708	ARG
2	E	1932	PRO
2	E	4982	GLU
2	G	1708	ARG
2	G	1932	PRO
2	G	4982	GLU
2	I	4982	GLU
2	B	1840	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	4641	PRO
2	I	1840	PRO
2	I	4641	PRO
2	E	1840	PRO
2	E	4641	PRO
2	G	1840	PRO
2	G	4641	PRO
2	B	2291	GLN
2	B	3762	ARG
2	I	2291	GLN
2	I	3762	ARG
2	E	2291	GLN
2	E	3762	ARG
2	G	2291	GLN
2	G	3762	ARG

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%)	2474 (99%)	19 (1%)	86	93
2	E	2493/3022 (82%)	2474 (99%)	19 (1%)	86	93
2	G	2493/3022 (82%)	2474 (99%)	19 (1%)	86	93
2	I	2493/3022 (82%)	2474 (99%)	19 (1%)	86	93
All	All	10324/12444 (83%)	10248 (99%)	76 (1%)	89	94

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG
2	B	553	ARG
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	3762	ARG
2	B	3787	LYS
2	B	3805	LEU
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4201	ASN
2	B	4959	PHE
2	B	4961	CYS
2	B	5027	CYS
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	3762	ARG
2	I	3787	LYS
2	I	3805	LEU
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4201	ASN
2	I	4959	PHE
2	I	4961	CYS
2	I	5027	CYS
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
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	1964	ARG
2	E	3762	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	4201	ASN
2	E	4959	PHE
2	E	4961	CYS
2	E	5027	CYS
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
2	G	3762	ARG
2	G	3787	LYS
2	G	3805	LEU
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4201	ASN
2	G	4959	PHE
2	G	4961	CYS
2	G	5027	CYS

Some 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	57	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	111	HIS
2	B	113	HIS
2	B	151	HIS
2	B	224	HIS
2	B	273	HIS
2	B	379	HIS
2	B	395	GLN
2	B	479	GLN
2	B	520	ASN
2	B	582	HIS
2	B	1158	ASN
2	B	1691	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	2041	HIS
2	B	2127	GLN
2	B	3766	GLN
2	B	3781	GLN
2	B	3896	ASN
2	B	3950	ASN
2	B	3960	GLN
2	B	4034	ASN
2	B	4102	GLN
2	B	4120	ASN
2	B	4153	HIS
2	B	4201	ASN
2	B	4553	ASN
2	B	4806	ASN
2	I	57	ASN
2	I	111	HIS
2	I	113	HIS
2	I	151	HIS
2	I	224	HIS
2	I	273	HIS
2	I	379	HIS
2	I	395	GLN
2	I	479	GLN
2	I	520	ASN
2	I	582	HIS
2	I	1158	ASN
2	I	1691	GLN
2	I	1719	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	1775	HIS
2	I	2041	HIS
2	I	2127	GLN
2	I	3766	GLN
2	I	3781	GLN
2	I	3896	ASN
2	I	3950	ASN
2	I	3960	GLN
2	I	4034	ASN
2	I	4102	GLN
2	I	4120	ASN
2	I	4153	HIS
2	I	4201	ASN
2	I	4553	ASN
2	I	4806	ASN
2	E	57	ASN
2	E	111	HIS
2	E	113	HIS
2	E	151	HIS
2	E	224	HIS
2	E	273	HIS
2	E	379	HIS
2	E	395	GLN
2	E	479	GLN
2	E	520	ASN
2	E	582	HIS
2	E	1158	ASN
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	2041	HIS
2	E	2127	GLN
2	E	3766	GLN
2	E	3781	GLN
2	E	3896	ASN
2	E	3950	ASN
2	E	3960	GLN
2	E	4034	ASN
2	E	4102	GLN
2	E	4120	ASN
2	E	4153	HIS
2	E	4201	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	4553	ASN
2	E	4806	ASN
2	G	57	ASN
2	G	111	HIS
2	G	113	HIS
2	G	151	HIS
2	G	224	HIS
2	G	273	HIS
2	G	379	HIS
2	G	395	GLN
2	G	479	GLN
2	G	520	ASN
2	G	582	HIS
2	G	1158	ASN
2	G	1691	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	2007	ASN
2	G	2041	HIS
2	G	2127	GLN
2	G	3766	GLN
2	G	3781	GLN
2	G	3896	ASN
2	G	3950	ASN
2	G	3960	GLN
2	G	4034	ASN
2	G	4102	GLN
2	G	4120	ASN
2	G	4153	HIS
2	G	4553	ASN
2	G	4806	ASN

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	73.35
1	I	4345:UNK	C	4540:PHE	N	73.35
1	E	4345:UNK	C	4540:PHE	N	73.35
1	G	4345:UNK	C	4540:PHE	N	73.35
1	B	3613:UNK	C	3639:THR	N	45.90
1	I	3613:UNK	C	3639:THR	N	45.90
1	E	3613:UNK	C	3639:THR	N	45.90
1	G	3613:UNK	C	3639:THR	N	45.90
1	B	4253:GLU	C	4320:UNK	N	27.05

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4253:GLU	C	4320:UNK	N	27.05
1	E	4253:GLU	C	4320:UNK	N	27.05
1	G	4253:GLU	C	4320:UNK	N	27.05
1	B	3163:UNK	C	3170:UNK	N	15.84
1	I	3163:UNK	C	3170:UNK	N	15.84
1	E	3163:UNK	C	3170:UNK	N	15.84
1	G	3163:UNK	C	3170:UNK	N	15.84
1	B	3063:UNK	C	3134:UNK	N	14.98
1	I	3063:UNK	C	3134:UNK	N	14.98
1	E	3063:UNK	C	3134:UNK	N	14.98
1	G	3063:UNK	C	3134:UNK	N	14.98
1	B	3468:UNK	C	3511:UNK	N	14.61
1	I	3468:UNK	C	3511:UNK	N	14.61
1	E	3468:UNK	C	3511:UNK	N	14.61
1	G	3468:UNK	C	3511:UNK	N	14.61
1	B	2703:UNK	C	2734:ASN	N	14.05
1	I	2703:UNK	C	2734:ASN	N	14.05
1	E	2703:UNK	C	2734:ASN	N	14.05
1	G	2703:UNK	C	2734:ASN	N	14.05
1	I	3236:UNK	C	3241:UNK	N	13.51
1	B	3236:UNK	C	3241:UNK	N	13.50
1	E	3236:UNK	C	3241:UNK	N	13.50
1	G	3236:UNK	C	3241:UNK	N	13.50
1	B	2976:UNK	C	2995:UNK	N	12.34
1	I	2976:UNK	C	2995:UNK	N	12.34
1	E	2976:UNK	C	2995:UNK	N	12.34
1	G	2976:UNK	C	2995:UNK	N	12.34
1	B	1564:UNK	C	1573:MET	N	11.71
1	I	1564:UNK	C	1573:MET	N	11.71
1	E	1564:UNK	C	1573:MET	N	11.71
1	G	1564:UNK	C	1573:MET	N	11.71
1	B	3254:UNK	C	3261:UNK	N	8.48
1	I	3254:UNK	C	3261:UNK	N	8.48
1	E	3254:UNK	C	3261:UNK	N	8.48
1	G	3254:UNK	C	3261:UNK	N	8.48
1	B	1297:UNK	C	1430:UNK	N	5.81
1	I	1297:UNK	C	1430:UNK	N	5.81
1	E	1297:UNK	C	1430:UNK	N	5.81
1	G	1297:UNK	C	1430:UNK	N	5.81
1	B	2939:ARG	C	2942:UNK	N	3.79
1	I	2939:ARG	C	2942:UNK	N	3.79
1	E	2939:ARG	C	2942:UNK	N	3.79

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	2939:ARG	C	2942:UNK	N	3.79
1	B	2479:LEU	C	2487:UNK	N	3.33
1	I	2479:LEU	C	2487:UNK	N	3.33
1	E	2479:LEU	C	2487:UNK	N	3.33
1	G	2479:LEU	C	2487:UNK	N	3.33