



Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 11:08 AM JST

PDB ID : 5GO9
EMDB ID : EMD-9528
Title : Cryo-EM structure of RyR2 in closed state
Authors : Peng, W.; Wu, J.P.; Yan, N.
Deposited on : 2016-07-26
Resolution : 4.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

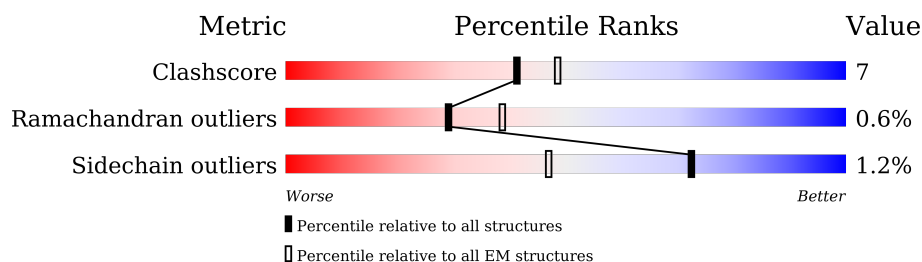
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4968	<div> <div>15%</div> <div>54%</div> <div>14%</div> <div>31%</div> </div>
1	B	4968	<div> <div>15%</div> <div>54%</div> <div>14%</div> <div>31%</div> </div>
1	C	4968	<div> <div>15%</div> <div>54%</div> <div>14%</div> <div>31%</div> </div>
1	D	4968	<div> <div>15%</div> <div>54%</div> <div>14%</div> <div>31%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 105068 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 RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3423	Total 26266	C 16740	N 4498	O 4874	S 154	0	0
1	B	3423	Total 26266	C 16740	N 4498	O 4874	S 154	0	0
1	C	3423	Total 26266	C 16740	N 4498	O 4874	S 154	0	0
1	D	3423	Total 26266	C 16740	N 4498	O 4874	S 154	0	0

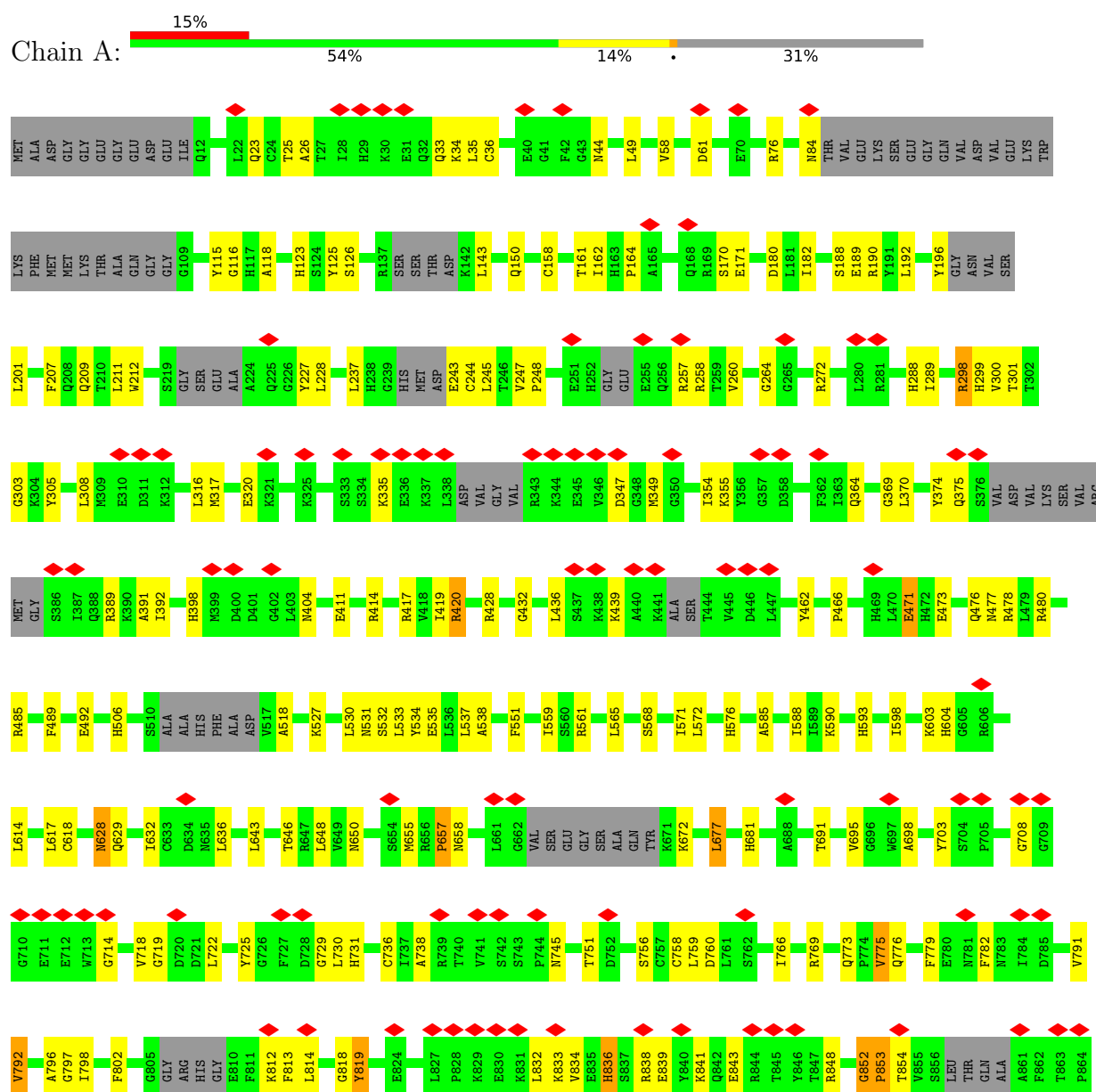
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total 1	Zn 1	0
2	B	1	Total 1	Zn 1	0
2	C	1	Total 1	Zn 1	0
2	D	1	Total 1	Zn 1	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

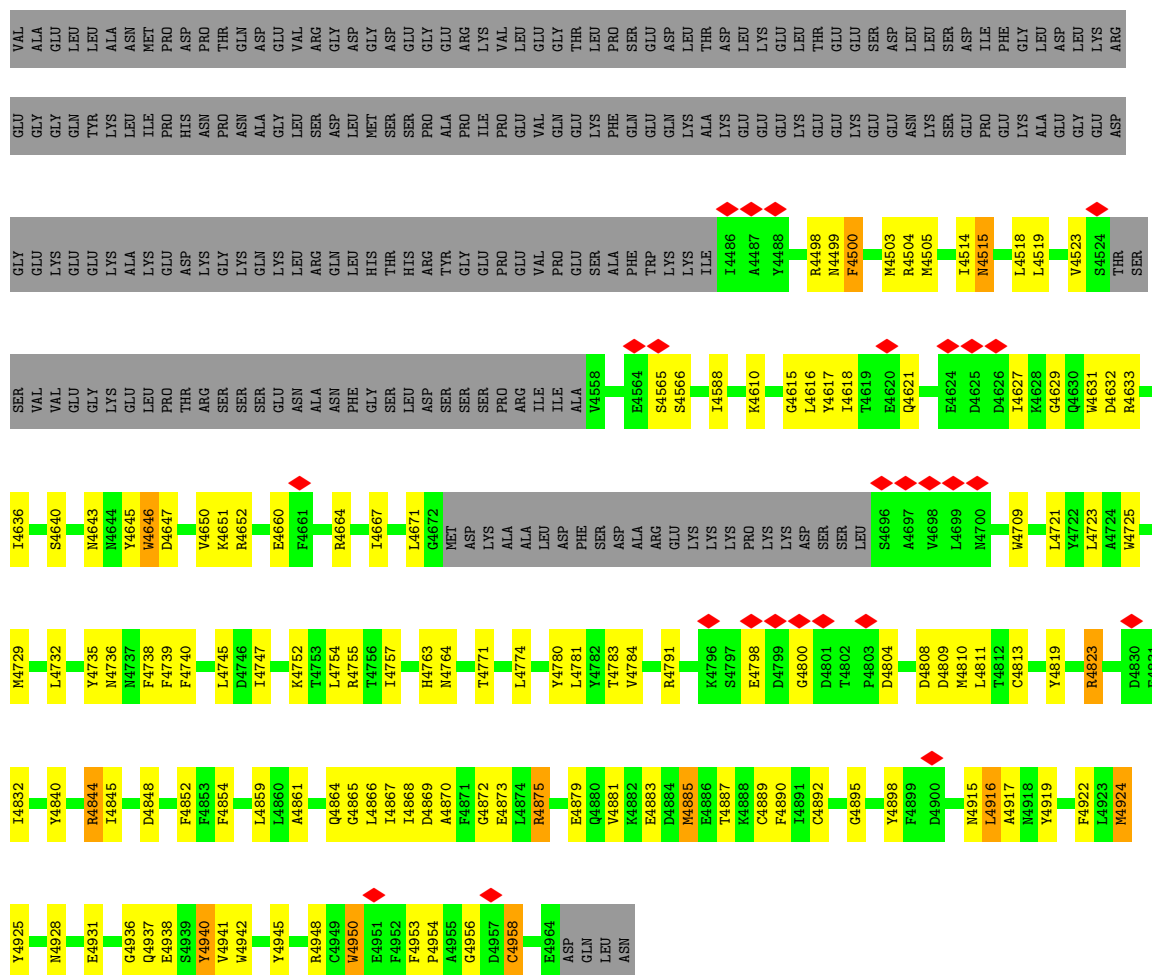
• Molecule 1: RyR2



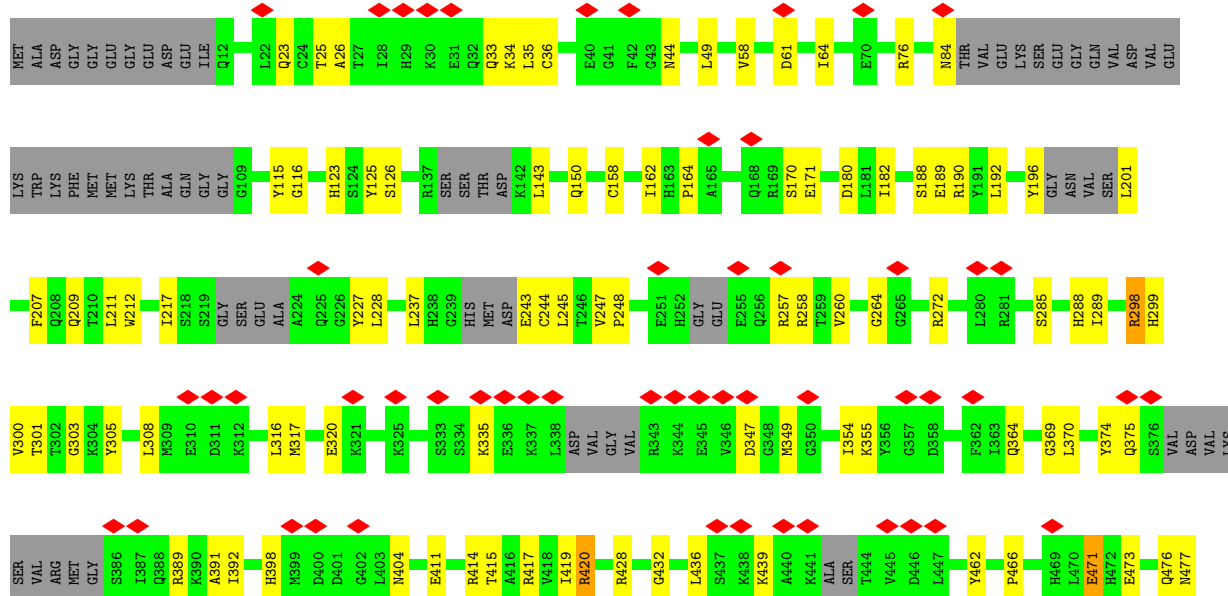


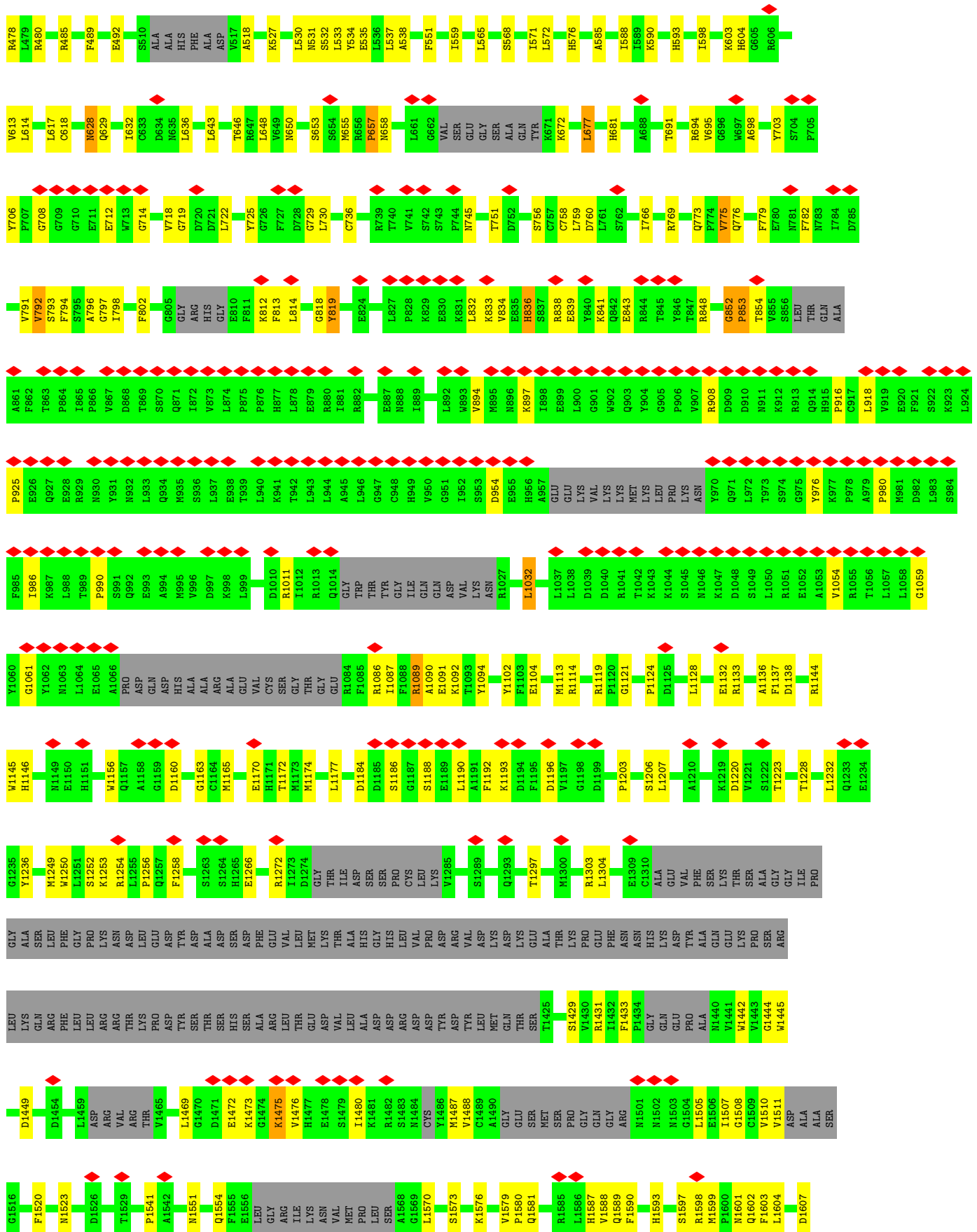






• Molecule 1: RyR2









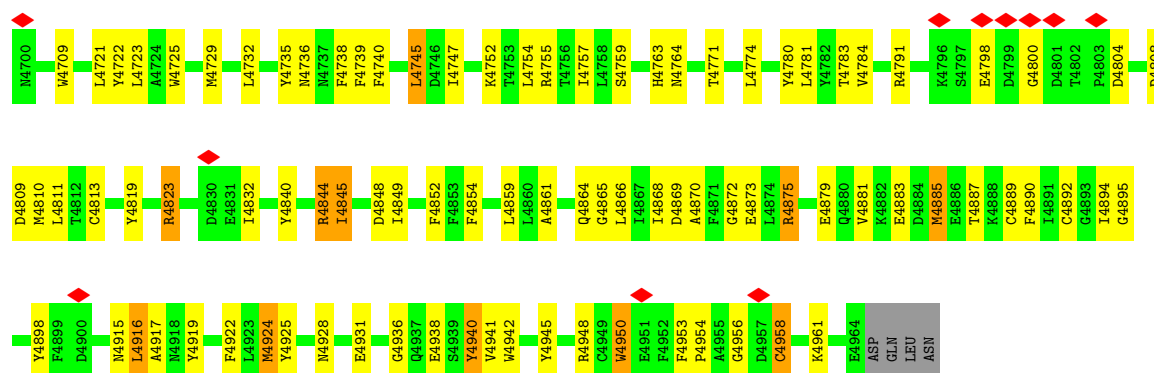




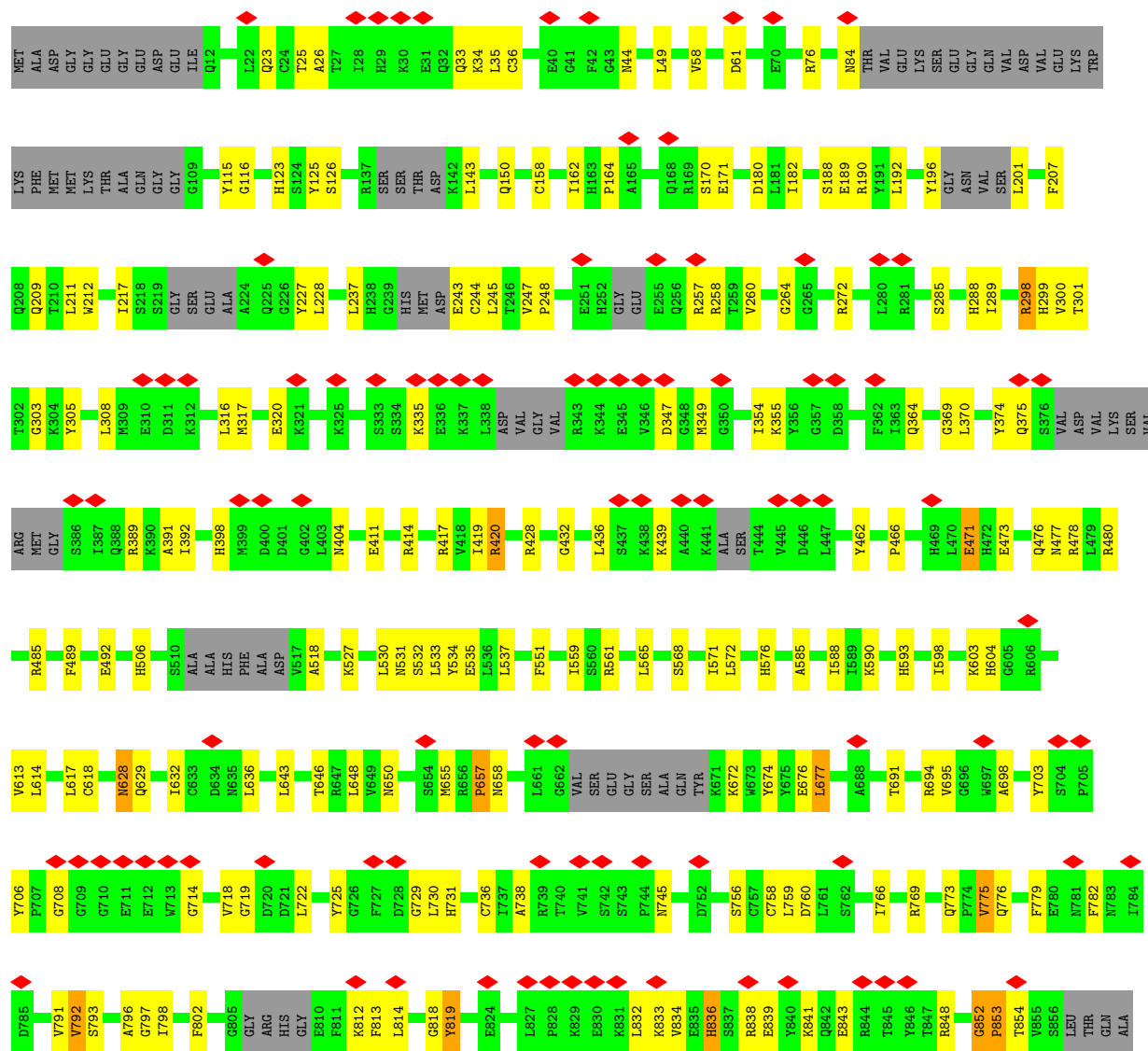








• Molecule 1: RyR2



L1905	P1820	M1720	R1614	SER	W1443	PRO	GLY	L1232	D1138	L1057	F985	P925	A861
L1911	L1824	I1726	W1617	G1516	G1444	SER	ILE	Q1233	R1144	L1058	I986	E926	F862
V1934	F1825	M1729	L1618	F1520	W1445	ARG	GLY	W1234	W1145	G1059	K987	Q927	T863
Q1938	I1830	T1733	L1622	D1526	D1449	LYS	SER	Y1236	H1146	G1061	L988	E928	P864
R1942	I1833	T1738	E1623	L1454	ARG	LEU	LEU	M1249	M1149	Y1062	P990	N930	I865
F1943	F1739	L1738	Q1626	L1459	PHE	PHE	GLY	W1250	H1150	N1063	S991	Y931	V867
R1944	H1835	P1740	S1629	ASP	LEU	ARG	PRO	L1251	H1151	E1064	N932	N932	D868
TYR	E1847	P1741	I1632	VAL	ARG	LYS	ASN	S1252	W1156	E1065	E993	L933	T869
ASN	P1848	GLU	I1637	THR	THR	LYS	LEU	R1254	A1158	A1066	A994	Q934	S870
GLU	S1849	ASN	E1635	V1465	THR	PRO	GLU	L1255	G1159	ASP	M995	M935	Q871
VAL	P1849	LYS	E1636	GLY	GLY	ASP	ASP	P1256	D1160	ASP	V996	S936	I872
MET	P1849	HIS	R1637	L1469	GLY	TYR	TYR	F1257	G1163	HIS	D997	L937	V873
GLN	N1636	LYS	E1556	G1470	THR	ASP	ASP	F1258	C1164	ALA	L999	E938	L874
ALA	R1637	ARG	E1557	D1471	SER	ALA	ALA	S1263	M1165	ALA	D1010	T939	P875
LEU	D1640	GLY	E1558	E1472	SER	ASP	ASP	S1264	E1170	ALA	I1011	L940	P876
ASN	I1641	ILE	E1559	K1473	HIS	SER	SER	E1265	H1171	GLU	I1012	K941	H877
GLY	E1642	LYS	K1473	G1474	ASP	ASP	PHE	H1266	M1172	VAL	R1013	T942	L878
ALA	L1644	ASN	K1475	E1476	ALA	GLU	VAL	R1272	M1173	CYS	R1014	L943	E879
LEU	T1645	VAL	H1476	LEU	THR	LEU	VAL	I1273	G1174	SER	Q1014	L944	R880
THR	K1652	PRO	H1477	THR	GLY	LEU	GLY	I1274	L1177	THR	GLY	A945	I881
ALA	F1653	LEU	E1478	GLY	GLY	MET	THR	GLY	L1177	GLY	TRP	L946	B882
LYS	H1654	SER	S1479	VAL	THR	THR	THR	ILE	L1184	GLU	THR	G947	E887
LEU	T1657	ALA	I1480	LEU	ALA	ALA	ALA	ASP	D1185	R1084	TYR	C948	N888
LYS	K1576	ASP	K1481	ASP	GLY	HIS	HIS	SER	D1186	F1085	ILE	H949	I889
GLU	V1579	ASP	R1482	ASP	GLY	GLY	GLY	ASP	S1186	R1086	GLN	V950	L892
PRO	V1580	ARG	S1483	ARG	LEU	HIS	HIS	PRO	G1187	I1087	ASP	G951	W893
PRO	Q1581	ASP	N1484	ASP	VAL	VAL	VAL	CYS	E1188	F1088	VAL	I952	W894
ASN	V1672	CYS	CYS	TYR	PRO	PRO	PRO	LYS	E1189	A1089	LYS	S953	M895
ASN	I1585	TYR	Y1486	ASP	ASP	ASP	ASP	W1285	L1190	A1090	ASN	D954	M896
GLU	L1586	ASP	M1487	ASP	VAL	ARG	ARG	E1289	A1191	E1091	R1027	E955	N896
GLU	H1587	TYR	C1488	TYR	LEU	VAL	VAL	S1289	F1192	K1092	R1028	H956	K897
TYR	V1588	MET	A1490	GLY	MET	GLY	LYS	Q1293	K1193	Y1094	N1029	P1030	I898
GLN	Q1589	GLY	GLY	THR	THR	LYS	LYS	T1297	F1195	Y1102	P1031	GLU	E999
GLY	L1590	SER	SER	SER	SER	ALA	ALA	T1297	D1196	F1103	L1032	LYS	L900
PRO	H1593	MET	T1426	THR	THR	THR	THR	M1300	V1197	E1104	L1037	VAL	G901
ASN	S1597	SER	S1429	PRO	PRO	LYS	LYS	R1113	G1198	M1113	L1038	LYS	W902
GLY	R1598	PRO	V1430	GLY	GLY	PRO	PRO	R1114	D1199	R1114	D1039	MET	Q903
GLY	M1599	GLN	R1431	GLY	GLY	GLY	GLY	P1119	P1203	R1119	D1040	LYS	Y904
GLY	P1600	GLY	Y1432	GLY	GLY	PHE	PHE	G1121	S1206	G1121	T1042	LYS	G905
ARG	F1433	ARG	F1433	ASN	ASN	ASN	ASN	P1120	L1207	P1120	K1043	PRO	P906
N1501	N1501	N1501	P1434	GLY	GLY	HIS	HIS	P1124	S1207	P1124	K1044	LYS	V907
N1502	N1502	N1502	GLY	GLY	GLY	LYS	LYS	D1125	A1210	D1125	S1045	ASN	R908
N1503	N1503	N1503	GLY	GLY	GLY	ASP	ASP	L1128	K1219	L1128	M1046	VAL	D909
I1507	I1507	I1507	ALA	ALA	ALA	ALA	ALA	PHE	K1219	L1128	M1046	VAL	D910
G1508	G1508	G1508	N1440	GLN	GLN	GLN	GLN	THR	E1132	E1132	K1047	LYS	L972
V1511	V1511	V1511	W1442	THR	THR	THR	THR	ALA	R1133	R1133	D1048	GLY	T973
ASP	ASP	ASP	ASP	ALA	ALA	ALA	ALA	GLY	V1221	V1221	S1049	GLY	G975
ALA	ALA	ALA	ALA	GLY	GLY	GLY	GLY	T1223	T1223	T1223	L1050	GLY	S976
E1613	E1613	E1613	ALA	ALA	ALA	ALA	ALA	T1228	T1228	T1228	E1051	K977	P916
											A1053	P978	C917
											V1054	A979	L918
											R1055	P980	V919
											D981	E981	E920
											F921	D982	F921
											L983	S984	S922
											S984	S984	K923
											L924	L924	L924







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	48454	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.173	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	546.0, 546.0, 546.0	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.98	29/26751 (0.1%)	0.94	78/36149 (0.2%)
1	B	0.98	29/26751 (0.1%)	0.94	78/36149 (0.2%)
1	C	0.98	29/26751 (0.1%)	0.94	78/36149 (0.2%)
1	D	0.98	29/26751 (0.1%)	0.94	78/36149 (0.2%)
All	All	0.98	116/107004 (0.1%)	0.94	312/144596 (0.2%)

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	30
1	B	0	30
1	C	0	30
1	D	0	30
All	All	0	120

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4945	TYR	CG-CD1	-10.60	1.25	1.39
1	B	4945	TYR	CG-CD1	-10.60	1.25	1.39
1	C	4945	TYR	CG-CD1	-10.60	1.25	1.39
1	D	4945	TYR	CG-CD1	-10.60	1.25	1.39
1	A	4950	TRP	CE3-CZ3	-9.89	1.21	1.38
1	B	4950	TRP	CE3-CZ3	-9.89	1.21	1.38
1	C	4950	TRP	CE3-CZ3	-9.89	1.21	1.38
1	D	4950	TRP	CE3-CZ3	-9.89	1.21	1.38
1	A	4190	PHE	CG-CD1	-8.95	1.25	1.38
1	B	4190	PHE	CG-CD1	-8.95	1.25	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4190	PHE	CG-CD1	-8.95	1.25	1.38
1	D	4190	PHE	CG-CD1	-8.95	1.25	1.38
1	A	4919	TYR	CG-CD1	-8.51	1.28	1.39
1	B	4919	TYR	CG-CD1	-8.51	1.28	1.39
1	C	4919	TYR	CG-CD1	-8.51	1.28	1.39
1	D	4919	TYR	CG-CD1	-8.51	1.28	1.39
1	A	4940	TYR	CG-CD1	-8.37	1.28	1.39
1	B	4940	TYR	CG-CD1	-8.37	1.28	1.39
1	C	4940	TYR	CG-CD1	-8.37	1.28	1.39
1	D	4940	TYR	CG-CD1	-8.37	1.28	1.39
1	A	4953	PHE	CG-CD2	-8.12	1.26	1.38
1	B	4953	PHE	CG-CD2	-8.12	1.26	1.38
1	C	4953	PHE	CG-CD2	-8.12	1.26	1.38
1	D	4953	PHE	CG-CD2	-8.12	1.26	1.38
1	A	4945	TYR	CE2-CZ	-7.18	1.29	1.38
1	B	4945	TYR	CE2-CZ	-7.18	1.29	1.38
1	C	4945	TYR	CE2-CZ	-7.18	1.29	1.38
1	D	4945	TYR	CE2-CZ	-7.18	1.29	1.38
1	A	4500	PHE	CG-CD1	-6.99	1.28	1.38
1	B	4500	PHE	CG-CD1	-6.99	1.28	1.38
1	C	4500	PHE	CG-CD1	-6.99	1.28	1.38
1	D	4500	PHE	CG-CD1	-6.99	1.28	1.38
1	A	4953	PHE	CE1-CZ	-6.97	1.24	1.37
1	B	4953	PHE	CE1-CZ	-6.97	1.24	1.37
1	C	4953	PHE	CE1-CZ	-6.97	1.24	1.37
1	D	4953	PHE	CE1-CZ	-6.97	1.24	1.37
1	A	4646	TRP	CG-CD1	-6.90	1.27	1.36
1	B	4646	TRP	CG-CD1	-6.90	1.27	1.36
1	C	4646	TRP	CG-CD1	-6.90	1.27	1.36
1	D	4646	TRP	CG-CD1	-6.90	1.27	1.36
1	A	4898	TYR	CG-CD2	-6.79	1.30	1.39
1	B	4898	TYR	CG-CD2	-6.79	1.30	1.39
1	C	4898	TYR	CG-CD2	-6.79	1.30	1.39
1	D	4898	TYR	CG-CD2	-6.79	1.30	1.39
1	A	4895	GLY	C-O	-6.48	1.13	1.23
1	B	4895	GLY	C-O	-6.48	1.13	1.23
1	C	4895	GLY	C-O	-6.48	1.13	1.23
1	D	4895	GLY	C-O	-6.48	1.13	1.23
1	A	4136	ARG	C-O	-6.46	1.11	1.23
1	B	4136	ARG	C-O	-6.46	1.11	1.23
1	C	4136	ARG	C-O	-6.46	1.11	1.23
1	D	4136	ARG	C-O	-6.46	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4919	TYR	CE1-CZ	-6.08	1.30	1.38
1	B	4919	TYR	CE1-CZ	-6.08	1.30	1.38
1	C	4919	TYR	CE1-CZ	-6.08	1.30	1.38
1	D	4919	TYR	CE1-CZ	-6.08	1.30	1.38
1	A	4138	GLU	CD-OE1	-5.87	1.19	1.25
1	B	4138	GLU	CD-OE1	-5.87	1.19	1.25
1	C	4138	GLU	CD-OE1	-5.87	1.19	1.25
1	D	4138	GLU	CD-OE1	-5.87	1.19	1.25
1	A	4922	PHE	CD2-CE2	-5.83	1.27	1.39
1	B	4922	PHE	CD2-CE2	-5.83	1.27	1.39
1	C	4922	PHE	CD2-CE2	-5.83	1.27	1.39
1	D	4922	PHE	CD2-CE2	-5.83	1.27	1.39
1	A	4950	TRP	CB-CG	-5.79	1.39	1.50
1	B	4950	TRP	CB-CG	-5.79	1.39	1.50
1	C	4950	TRP	CB-CG	-5.79	1.39	1.50
1	D	4950	TRP	CB-CG	-5.79	1.39	1.50
1	A	4854	PHE	CG-CD1	5.72	1.47	1.38
1	B	4854	PHE	CG-CD1	5.72	1.47	1.38
1	C	4854	PHE	CG-CD1	5.72	1.47	1.38
1	D	4854	PHE	CG-CD1	5.72	1.47	1.38
1	A	4954	PRO	CA-C	-5.71	1.41	1.52
1	B	4954	PRO	CA-C	-5.71	1.41	1.52
1	C	4954	PRO	CA-C	-5.71	1.41	1.52
1	D	4954	PRO	CA-C	-5.71	1.41	1.52
1	A	4925	TYR	CG-CD2	-5.62	1.31	1.39
1	B	4925	TYR	CG-CD2	-5.62	1.31	1.39
1	C	4925	TYR	CG-CD2	-5.62	1.31	1.39
1	D	4925	TYR	CG-CD2	-5.62	1.31	1.39
1	A	4735	TYR	CE2-CZ	-5.60	1.31	1.38
1	B	4735	TYR	CE2-CZ	-5.60	1.31	1.38
1	C	4735	TYR	CE2-CZ	-5.60	1.31	1.38
1	D	4735	TYR	CE2-CZ	-5.60	1.31	1.38
1	A	1825	PHE	CG-CD2	-5.56	1.30	1.38
1	B	1825	PHE	CG-CD2	-5.56	1.30	1.38
1	C	1825	PHE	CG-CD2	-5.56	1.30	1.38
1	D	1825	PHE	CG-CD2	-5.56	1.30	1.38
1	A	4890	PHE	CB-CG	-5.45	1.42	1.51
1	B	4890	PHE	CB-CG	-5.45	1.42	1.51
1	C	4890	PHE	CB-CG	-5.45	1.42	1.51
1	D	4890	PHE	CB-CG	-5.45	1.42	1.51
1	A	471	GLU	CG-CD	5.44	1.60	1.51
1	B	471	GLU	CG-CD	5.44	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	471	GLU	CG-CD	5.44	1.60	1.51
1	D	471	GLU	CG-CD	5.44	1.60	1.51
1	A	4958	CYS	CB-SG	-5.40	1.73	1.81
1	B	4958	CYS	CB-SG	-5.40	1.73	1.81
1	C	4958	CYS	CB-SG	-5.40	1.73	1.81
1	D	4958	CYS	CB-SG	-5.40	1.73	1.81
1	A	3781	TYR	CG-CD1	-5.39	1.32	1.39
1	B	3781	TYR	CG-CD1	-5.39	1.32	1.39
1	C	3781	TYR	CG-CD1	-5.39	1.32	1.39
1	D	3781	TYR	CG-CD1	-5.39	1.32	1.39
1	A	3700	CYS	CB-SG	5.37	1.91	1.82
1	B	3700	CYS	CB-SG	5.37	1.91	1.82
1	C	3700	CYS	CB-SG	5.37	1.91	1.82
1	D	3700	CYS	CB-SG	5.37	1.91	1.82
1	A	3890	TYR	CE2-CZ	5.27	1.45	1.38
1	B	3890	TYR	CE2-CZ	5.27	1.45	1.38
1	C	3890	TYR	CE2-CZ	5.27	1.45	1.38
1	D	3890	TYR	CE2-CZ	5.27	1.45	1.38
1	A	4735	TYR	CG-CD1	-5.18	1.32	1.39
1	B	4735	TYR	CG-CD1	-5.18	1.32	1.39
1	C	4735	TYR	CG-CD1	-5.18	1.32	1.39
1	D	4735	TYR	CG-CD1	-5.18	1.32	1.39

All (312) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1089	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	B	1089	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	C	1089	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	D	1089	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	A	4171	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	B	4171	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	C	4171	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	D	4171	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	A	4948	ARG	NE-CZ-NH1	-8.45	116.08	120.30
1	B	4948	ARG	NE-CZ-NH1	-8.45	116.08	120.30
1	C	4948	ARG	NE-CZ-NH1	-8.45	116.08	120.30
1	D	4948	ARG	NE-CZ-NH1	-8.45	116.08	120.30
1	A	2583	PRO	N-CA-CB	8.35	113.31	103.30
1	B	2583	PRO	N-CA-CB	8.35	113.31	103.30
1	C	2583	PRO	N-CA-CB	8.35	113.31	103.30
1	D	2583	PRO	N-CA-CB	8.35	113.31	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3104	PRO	N-CA-CB	8.32	113.29	103.30
1	B	3104	PRO	N-CA-CB	8.32	113.29	103.30
1	C	3104	PRO	N-CA-CB	8.32	113.29	103.30
1	D	3104	PRO	N-CA-CB	8.32	113.29	103.30
1	A	4844	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	B	4844	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	C	4844	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	D	4844	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	A	3778	MET	CG-SD-CE	7.94	112.90	100.20
1	B	3778	MET	CG-SD-CE	7.94	112.90	100.20
1	C	3778	MET	CG-SD-CE	7.94	112.90	100.20
1	D	3778	MET	CG-SD-CE	7.94	112.90	100.20
1	A	2495	PRO	N-CA-CB	7.79	112.64	103.30
1	B	2495	PRO	N-CA-CB	7.79	112.64	103.30
1	C	2495	PRO	N-CA-CB	7.79	112.64	103.30
1	D	2495	PRO	N-CA-CB	7.79	112.64	103.30
1	A	2736	ASP	CB-CG-OD2	7.77	125.30	118.30
1	B	2736	ASP	CB-CG-OD2	7.77	125.30	118.30
1	C	2736	ASP	CB-CG-OD2	7.77	125.30	118.30
1	D	2736	ASP	CB-CG-OD2	7.77	125.30	118.30
1	A	4139	ILE	CG1-CB-CG2	-7.39	95.15	111.40
1	B	4139	ILE	CG1-CB-CG2	-7.39	95.15	111.40
1	C	4139	ILE	CG1-CB-CG2	-7.39	95.15	111.40
1	D	4139	ILE	CG1-CB-CG2	-7.39	95.15	111.40
1	A	347	ASP	CB-CG-OD1	7.38	124.94	118.30
1	B	347	ASP	CB-CG-OD1	7.38	124.94	118.30
1	C	347	ASP	CB-CG-OD1	7.38	124.94	118.30
1	D	347	ASP	CB-CG-OD1	7.38	124.94	118.30
1	A	4885	MET	CG-SD-CE	-7.29	88.53	100.20
1	B	4885	MET	CG-SD-CE	-7.29	88.53	100.20
1	C	4885	MET	CG-SD-CE	-7.29	88.53	100.20
1	D	4885	MET	CG-SD-CE	-7.29	88.53	100.20
1	A	2598	PRO	N-CA-CB	7.25	112.00	103.30
1	B	2598	PRO	N-CA-CB	7.25	112.00	103.30
1	C	2598	PRO	N-CA-CB	7.25	112.00	103.30
1	D	2598	PRO	N-CA-CB	7.25	112.00	103.30
1	A	4505	MET	CB-CG-SD	7.13	133.79	112.40
1	B	4505	MET	CB-CG-SD	7.13	133.79	112.40
1	C	4505	MET	CB-CG-SD	7.13	133.79	112.40
1	D	4505	MET	CB-CG-SD	7.13	133.79	112.40
1	A	4745	LEU	CB-CG-CD2	7.06	123.01	111.00
1	B	4745	LEU	CB-CG-CD2	7.06	123.01	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4745	LEU	CB-CG-CD2	7.06	123.01	111.00
1	D	4745	LEU	CB-CG-CD2	7.06	123.01	111.00
1	A	2534	PRO	N-CA-CB	7.04	111.75	103.30
1	B	2534	PRO	N-CA-CB	7.04	111.75	103.30
1	C	2534	PRO	N-CA-CB	7.04	111.75	103.30
1	D	2534	PRO	N-CA-CB	7.04	111.75	103.30
1	A	3918	PHE	CB-CG-CD2	-7.01	115.89	120.80
1	B	3918	PHE	CB-CG-CD2	-7.01	115.89	120.80
1	C	3918	PHE	CB-CG-CD2	-7.01	115.89	120.80
1	D	3918	PHE	CB-CG-CD2	-7.01	115.89	120.80
1	A	4859	LEU	CB-CG-CD2	6.97	122.84	111.00
1	B	4859	LEU	CB-CG-CD2	6.97	122.84	111.00
1	C	4859	LEU	CB-CG-CD2	6.97	122.84	111.00
1	D	4859	LEU	CB-CG-CD2	6.97	122.84	111.00
1	A	4859	LEU	CB-CG-CD1	-6.85	99.35	111.00
1	B	4859	LEU	CB-CG-CD1	-6.85	99.35	111.00
1	C	4859	LEU	CB-CG-CD1	-6.85	99.35	111.00
1	D	4859	LEU	CB-CG-CD1	-6.85	99.35	111.00
1	A	4136	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	B	4136	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	C	4136	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	D	4136	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	A	2625	PRO	N-CA-CB	6.61	111.23	103.30
1	B	2625	PRO	N-CA-CB	6.61	111.23	103.30
1	C	2625	PRO	N-CA-CB	6.61	111.23	103.30
1	D	2625	PRO	N-CA-CB	6.61	111.23	103.30
1	A	4500	PHE	CB-CG-CD2	6.56	125.39	120.80
1	B	4500	PHE	CB-CG-CD2	6.56	125.39	120.80
1	C	4500	PHE	CB-CG-CD2	6.56	125.39	120.80
1	D	4500	PHE	CB-CG-CD2	6.56	125.39	120.80
1	A	3683	LEU	CB-CG-CD1	-6.41	100.11	111.00
1	B	3683	LEU	CB-CG-CD1	-6.41	100.11	111.00
1	C	3683	LEU	CB-CG-CD1	-6.41	100.11	111.00
1	D	3683	LEU	CB-CG-CD1	-6.41	100.11	111.00
1	A	2678	PRO	N-CA-CB	6.36	110.93	103.30
1	B	2678	PRO	N-CA-CB	6.36	110.93	103.30
1	C	2678	PRO	N-CA-CB	6.36	110.93	103.30
1	D	2678	PRO	N-CA-CB	6.36	110.93	103.30
1	A	4938	GLU	OE1-CD-OE2	6.35	130.92	123.30
1	B	4938	GLU	OE1-CD-OE2	6.35	130.92	123.30
1	C	4938	GLU	OE1-CD-OE2	6.35	130.92	123.30
1	D	4938	GLU	OE1-CD-OE2	6.35	130.92	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4170	LYS	CD-CE-NZ	-6.28	97.25	111.70
1	B	4170	LYS	CD-CE-NZ	-6.28	97.25	111.70
1	C	4170	LYS	CD-CE-NZ	-6.28	97.25	111.70
1	D	4170	LYS	CD-CE-NZ	-6.28	97.25	111.70
1	A	4158	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	B	4158	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	C	4158	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	D	4158	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	A	3803	VAL	N-CA-C	-6.17	94.34	111.00
1	B	3803	VAL	N-CA-C	-6.17	94.34	111.00
1	C	3803	VAL	N-CA-C	-6.17	94.34	111.00
1	D	3803	VAL	N-CA-C	-6.17	94.34	111.00
1	A	2607	PRO	N-CA-CB	6.15	110.68	103.30
1	B	2607	PRO	N-CA-CB	6.15	110.68	103.30
1	C	2607	PRO	N-CA-CB	6.15	110.68	103.30
1	D	2607	PRO	N-CA-CB	6.15	110.68	103.30
1	A	2990	PRO	N-CA-CB	6.12	110.64	103.30
1	B	2990	PRO	N-CA-CB	6.12	110.64	103.30
1	C	2990	PRO	N-CA-CB	6.12	110.64	103.30
1	D	2990	PRO	N-CA-CB	6.12	110.64	103.30
1	A	2679	PRO	N-CA-CB	6.06	110.57	103.30
1	B	2679	PRO	N-CA-CB	6.06	110.57	103.30
1	C	2679	PRO	N-CA-CB	6.06	110.57	103.30
1	D	2679	PRO	N-CA-CB	6.06	110.57	103.30
1	A	4735	TYR	CG-CD2-CE2	6.03	126.12	121.30
1	B	4735	TYR	CG-CD2-CE2	6.03	126.12	121.30
1	C	4735	TYR	CG-CD2-CE2	6.03	126.12	121.30
1	D	4735	TYR	CG-CD2-CE2	6.03	126.12	121.30
1	A	2783	MET	CG-SD-CE	5.97	109.76	100.20
1	B	2783	MET	CG-SD-CE	5.97	109.76	100.20
1	C	2783	MET	CG-SD-CE	5.97	109.76	100.20
1	D	2783	MET	CG-SD-CE	5.97	109.76	100.20
1	A	1303	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	B	1303	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	C	1303	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	D	1303	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	A	3948	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	B	3948	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	C	3948	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	D	3948	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	A	814	LEU	CA-CB-CG	5.81	128.67	115.30
1	B	814	LEU	CA-CB-CG	5.81	128.67	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	814	LEU	CA-CB-CG	5.81	128.67	115.30
1	D	814	LEU	CA-CB-CG	5.81	128.67	115.30
1	A	4134	LEU	CA-CB-CG	5.79	128.62	115.30
1	B	4134	LEU	CA-CB-CG	5.79	128.62	115.30
1	C	4134	LEU	CA-CB-CG	5.79	128.62	115.30
1	D	4134	LEU	CA-CB-CG	5.79	128.62	115.30
1	A	4953	PHE	CB-CG-CD1	5.78	124.84	120.80
1	B	4953	PHE	CB-CG-CD1	5.78	124.84	120.80
1	C	4953	PHE	CB-CG-CD1	5.78	124.84	120.80
1	D	4953	PHE	CB-CG-CD1	5.78	124.84	120.80
1	A	2268	ARG	CB-CG-CD	5.63	126.25	111.60
1	B	2268	ARG	CB-CG-CD	5.63	126.25	111.60
1	C	2268	ARG	CB-CG-CD	5.63	126.25	111.60
1	D	2268	ARG	CB-CG-CD	5.63	126.25	111.60
1	A	2425	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	2425	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	C	2425	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	D	2425	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	2668	PRO	N-CA-CB	5.60	110.02	103.30
1	B	2668	PRO	N-CA-CB	5.60	110.02	103.30
1	C	2668	PRO	N-CA-CB	5.60	110.02	103.30
1	D	2668	PRO	N-CA-CB	5.60	110.02	103.30
1	A	4945	TYR	CB-CG-CD2	5.59	124.35	121.00
1	B	4945	TYR	CB-CG-CD2	5.59	124.35	121.00
1	C	4945	TYR	CB-CG-CD2	5.59	124.35	121.00
1	D	4945	TYR	CB-CG-CD2	5.59	124.35	121.00
1	A	836	HIS	CB-CA-C	-5.58	99.25	110.40
1	B	836	HIS	CB-CA-C	-5.58	99.25	110.40
1	C	836	HIS	CB-CA-C	-5.58	99.25	110.40
1	D	836	HIS	CB-CA-C	-5.58	99.25	110.40
1	A	4504	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	4504	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	C	4504	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	D	4504	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	3803	VAL	CG1-CB-CG2	-5.49	102.11	110.90
1	B	3803	VAL	CG1-CB-CG2	-5.49	102.11	110.90
1	C	3803	VAL	CG1-CB-CG2	-5.49	102.11	110.90
1	D	3803	VAL	CG1-CB-CG2	-5.49	102.11	110.90
1	A	4500	PHE	CB-CG-CD1	-5.49	116.96	120.80
1	B	4500	PHE	CB-CG-CD1	-5.49	116.96	120.80
1	C	4500	PHE	CB-CG-CD1	-5.49	116.96	120.80
1	D	4500	PHE	CB-CG-CD1	-5.49	116.96	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4085	VAL	CG1-CB-CG2	-5.48	102.14	110.90
1	B	4085	VAL	CG1-CB-CG2	-5.48	102.14	110.90
1	C	4085	VAL	CG1-CB-CG2	-5.48	102.14	110.90
1	D	4085	VAL	CG1-CB-CG2	-5.48	102.14	110.90
1	A	2143	MET	CG-SD-CE	-5.45	91.48	100.20
1	B	2143	MET	CG-SD-CE	-5.45	91.48	100.20
1	C	2143	MET	CG-SD-CE	-5.45	91.48	100.20
1	D	2143	MET	CG-SD-CE	-5.45	91.48	100.20
1	A	1599	MET	CG-SD-CE	5.44	108.91	100.20
1	B	1599	MET	CG-SD-CE	5.44	108.91	100.20
1	C	1599	MET	CG-SD-CE	5.44	108.91	100.20
1	D	1599	MET	CG-SD-CE	5.44	108.91	100.20
1	A	4187	MET	CG-SD-CE	5.44	108.90	100.20
1	B	4187	MET	CG-SD-CE	5.44	108.90	100.20
1	C	4187	MET	CG-SD-CE	5.44	108.90	100.20
1	D	4187	MET	CG-SD-CE	5.44	108.90	100.20
1	A	1032	LEU	CB-CG-CD2	-5.43	101.78	111.00
1	B	1032	LEU	CB-CG-CD2	-5.43	101.78	111.00
1	C	1032	LEU	CB-CG-CD2	-5.43	101.78	111.00
1	D	1032	LEU	CB-CG-CD2	-5.43	101.78	111.00
1	A	4916	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	B	4916	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	C	4916	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	D	4916	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	A	4189	LEU	CA-CB-CG	5.36	127.63	115.30
1	B	4189	LEU	CA-CB-CG	5.36	127.63	115.30
1	C	4189	LEU	CA-CB-CG	5.36	127.63	115.30
1	D	4189	LEU	CA-CB-CG	5.36	127.63	115.30
1	A	4197	THR	CA-CB-CG2	-5.35	104.92	112.40
1	B	4197	THR	CA-CB-CG2	-5.35	104.92	112.40
1	C	4197	THR	CA-CB-CG2	-5.35	104.92	112.40
1	D	4197	THR	CA-CB-CG2	-5.35	104.92	112.40
1	A	1738	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	B	1738	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	C	1738	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	D	1738	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	A	4645	TYR	CB-CG-CD1	5.33	124.20	121.00
1	B	4645	TYR	CB-CG-CD1	5.33	124.20	121.00
1	C	4645	TYR	CB-CG-CD1	5.33	124.20	121.00
1	D	4645	TYR	CB-CG-CD1	5.33	124.20	121.00
1	A	2101	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	4940	TYR	CB-CG-CD2	5.29	124.17	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2101	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	4940	TYR	CB-CG-CD2	5.29	124.17	121.00
1	C	2101	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	C	4940	TYR	CB-CG-CD2	5.29	124.17	121.00
1	D	2101	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	D	4940	TYR	CB-CG-CD2	5.29	124.17	121.00
1	A	2166	LEU	CB-CG-CD1	-5.29	102.02	111.00
1	B	2166	LEU	CB-CG-CD1	-5.29	102.02	111.00
1	C	2166	LEU	CB-CG-CD1	-5.29	102.02	111.00
1	D	2166	LEU	CB-CG-CD1	-5.29	102.02	111.00
1	A	2517	LEU	CA-CB-CG	5.28	127.45	115.30
1	B	2517	LEU	CA-CB-CG	5.28	127.45	115.30
1	C	2517	LEU	CA-CB-CG	5.28	127.45	115.30
1	D	2517	LEU	CA-CB-CG	5.28	127.45	115.30
1	A	4823	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	B	4823	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	C	4823	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	D	4823	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	A	4924	MET	CG-SD-CE	-5.25	91.81	100.20
1	B	4924	MET	CG-SD-CE	-5.25	91.81	100.20
1	C	4924	MET	CG-SD-CE	-5.25	91.81	100.20
1	D	4924	MET	CG-SD-CE	-5.25	91.81	100.20
1	A	2736	ASP	CB-CG-OD1	-5.24	113.59	118.30
1	B	2736	ASP	CB-CG-OD1	-5.24	113.59	118.30
1	C	2736	ASP	CB-CG-OD1	-5.24	113.59	118.30
1	D	2736	ASP	CB-CG-OD1	-5.24	113.59	118.30
1	A	677	LEU	CA-CB-CG	5.22	127.30	115.30
1	B	677	LEU	CA-CB-CG	5.22	127.30	115.30
1	C	677	LEU	CA-CB-CG	5.22	127.30	115.30
1	D	677	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	4945	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	B	4945	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	C	4945	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	D	4945	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	A	1824	LEU	CA-CB-CG	5.20	127.26	115.30
1	A	4721	LEU	CA-CB-CG	5.20	127.26	115.30
1	B	1824	LEU	CA-CB-CG	5.20	127.26	115.30
1	B	4721	LEU	CA-CB-CG	5.20	127.26	115.30
1	C	1824	LEU	CA-CB-CG	5.20	127.26	115.30
1	C	4721	LEU	CA-CB-CG	5.20	127.26	115.30
1	D	1824	LEU	CA-CB-CG	5.20	127.26	115.30
1	D	4721	LEU	CA-CB-CG	5.20	127.26	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1942	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	B	1942	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	C	1942	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	D	1942	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	A	1729	MET	CG-SD-CE	5.16	108.45	100.20
1	B	1729	MET	CG-SD-CE	5.16	108.45	100.20
1	C	1729	MET	CG-SD-CE	5.16	108.45	100.20
1	D	1729	MET	CG-SD-CE	5.16	108.45	100.20
1	A	3837	THR	CA-CB-CG2	-5.15	105.19	112.40
1	B	3837	THR	CA-CB-CG2	-5.15	105.19	112.40
1	C	3837	THR	CA-CB-CG2	-5.15	105.19	112.40
1	D	3837	THR	CA-CB-CG2	-5.15	105.19	112.40
1	A	4941	VAL	CG1-CB-CG2	-5.15	102.66	110.90
1	B	4941	VAL	CG1-CB-CG2	-5.15	102.66	110.90
1	C	4941	VAL	CG1-CB-CG2	-5.15	102.66	110.90
1	D	4941	VAL	CG1-CB-CG2	-5.15	102.66	110.90
1	A	4086	LYS	CD-CE-NZ	5.14	123.53	111.70
1	B	4086	LYS	CD-CE-NZ	5.14	123.53	111.70
1	C	4086	LYS	CD-CE-NZ	5.14	123.53	111.70
1	D	4086	LYS	CD-CE-NZ	5.14	123.53	111.70
1	A	3802	SER	C-N-CA	5.13	134.52	121.70
1	B	3802	SER	C-N-CA	5.13	134.52	121.70
1	C	3802	SER	C-N-CA	5.13	134.52	121.70
1	D	3802	SER	C-N-CA	5.13	134.52	121.70
1	A	3945	VAL	CG1-CB-CG2	-5.11	102.72	110.90
1	B	3945	VAL	CG1-CB-CG2	-5.11	102.72	110.90
1	C	3945	VAL	CG1-CB-CG2	-5.11	102.72	110.90
1	D	3945	VAL	CG1-CB-CG2	-5.11	102.72	110.90
1	A	4845	ILE	CG1-CB-CG2	-5.06	100.27	111.40
1	B	4845	ILE	CG1-CB-CG2	-5.06	100.27	111.40
1	C	4845	ILE	CG1-CB-CG2	-5.06	100.27	111.40
1	D	4845	ILE	CG1-CB-CG2	-5.06	100.27	111.40
1	A	2059	LEU	CB-CG-CD1	5.03	119.54	111.00
1	B	2059	LEU	CB-CG-CD1	5.03	119.54	111.00
1	C	2059	LEU	CB-CG-CD1	5.03	119.54	111.00
1	D	2059	LEU	CB-CG-CD1	5.03	119.54	111.00
1	A	3918	PHE	CB-CG-CD1	5.02	124.31	120.80
1	B	3918	PHE	CB-CG-CD1	5.02	124.31	120.80
1	C	3918	PHE	CB-CG-CD1	5.02	124.31	120.80
1	D	3918	PHE	CB-CG-CD1	5.02	124.31	120.80
1	A	2203	TYR	CB-CG-CD2	-5.01	118.00	121.00
1	B	2203	TYR	CB-CG-CD2	-5.01	118.00	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2203	TYR	CB-CG-CD2	-5.01	118.00	121.00
1	D	2203	TYR	CB-CG-CD2	-5.01	118.00	121.00

There are no chirality outliers.

All (120) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1102	TYR	Peptide
1	A	1266	GLU	Peptide
1	A	1297	THR	Peptide
1	A	1475	LYS	Peptide
1	A	1579	VAL	Peptide
1	A	1635	GLU	Peptide
1	A	1739	PHE	Peptide
1	A	1808	ASP	Peptide
1	A	1835	HIS	Peptide
1	A	1847	GLU	Peptide
1	A	2075	VAL	Peptide
1	A	2077	GLU	Peptide
1	A	3767	LEU	Peptide
1	A	3805	ASP	Peptide
1	A	4070	CYS	Peptide
1	A	4144	LYS	Peptide
1	A	4163	LYS	Peptide
1	A	471	GLU	Peptide
1	A	4798	GLU	Peptide
1	A	4956	GLY	Peptide
1	A	4958	CYS	Peptide
1	A	657	PRO	Peptide
1	A	729	GLY	Peptide
1	A	775	VAL	Peptide
1	A	791	VAL	Peptide
1	A	818	GLY	Peptide
1	A	819	TYR	Peptide
1	A	838	ARG	Peptide
1	A	852	GLY	Mainchain,Peptide
1	B	1102	TYR	Peptide
1	B	1266	GLU	Peptide
1	B	1297	THR	Peptide
1	B	1475	LYS	Peptide
1	B	1579	VAL	Peptide
1	B	1635	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	B	1739	PHE	Peptide
1	B	1808	ASP	Peptide
1	B	1835	HIS	Peptide
1	B	1847	GLU	Peptide
1	B	2075	VAL	Peptide
1	B	2077	GLU	Peptide
1	B	3767	LEU	Peptide
1	B	3805	ASP	Peptide
1	B	4070	CYS	Peptide
1	B	4144	LYS	Peptide
1	B	4163	LYS	Peptide
1	B	471	GLU	Peptide
1	B	4798	GLU	Peptide
1	B	4956	GLY	Peptide
1	B	4958	CYS	Peptide
1	B	657	PRO	Peptide
1	B	729	GLY	Peptide
1	B	775	VAL	Peptide
1	B	791	VAL	Peptide
1	B	818	GLY	Peptide
1	B	819	TYR	Peptide
1	B	838	ARG	Peptide
1	B	852	GLY	Mainchain,Peptide
1	C	1102	TYR	Peptide
1	C	1266	GLU	Peptide
1	C	1297	THR	Peptide
1	C	1475	LYS	Peptide
1	C	1579	VAL	Peptide
1	C	1635	GLU	Peptide
1	C	1739	PHE	Peptide
1	C	1808	ASP	Peptide
1	C	1835	HIS	Peptide
1	C	1847	GLU	Peptide
1	C	2075	VAL	Peptide
1	C	2077	GLU	Peptide
1	C	3767	LEU	Peptide
1	C	3805	ASP	Peptide
1	C	4070	CYS	Peptide
1	C	4144	LYS	Peptide
1	C	4163	LYS	Peptide
1	C	471	GLU	Peptide
1	C	4798	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	C	4956	GLY	Peptide
1	C	4958	CYS	Peptide
1	C	657	PRO	Peptide
1	C	729	GLY	Peptide
1	C	775	VAL	Peptide
1	C	791	VAL	Peptide
1	C	818	GLY	Peptide
1	C	819	TYR	Peptide
1	C	838	ARG	Peptide
1	C	852	GLY	Mainchain,Peptide
1	D	1102	TYR	Peptide
1	D	1266	GLU	Peptide
1	D	1297	THR	Peptide
1	D	1475	LYS	Peptide
1	D	1579	VAL	Peptide
1	D	1635	GLU	Peptide
1	D	1739	PHE	Peptide
1	D	1808	ASP	Peptide
1	D	1835	HIS	Peptide
1	D	1847	GLU	Peptide
1	D	2075	VAL	Peptide
1	D	2077	GLU	Peptide
1	D	3767	LEU	Peptide
1	D	3805	ASP	Peptide
1	D	4070	CYS	Peptide
1	D	4144	LYS	Peptide
1	D	4163	LYS	Peptide
1	D	471	GLU	Peptide
1	D	4798	GLU	Peptide
1	D	4956	GLY	Peptide
1	D	4958	CYS	Peptide
1	D	657	PRO	Peptide
1	D	729	GLY	Peptide
1	D	775	VAL	Peptide
1	D	791	VAL	Peptide
1	D	818	GLY	Peptide
1	D	819	TYR	Peptide
1	D	838	ARG	Peptide
1	D	852	GLY	Mainchain,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	26266	0	24898	409	0
1	B	26266	0	24898	421	0
1	C	26266	0	24898	414	0
1	D	26266	0	24898	401	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	105068	0	99592	1515	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 7.

All (1515) 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)
1:A:4873:GLU:HA	1:B:4875:ARG:NH1	1.62	1.15
1:A:4875:ARG:NH1	1:D:4873:GLU:HA	1.62	1.14
1:B:4873:GLU:HA	1:C:4875:ARG:NH1	1.62	1.13
1:C:4873:GLU:OE1	1:D:4875:ARG:HD3	1.49	1.12
1:C:4873:GLU:HA	1:D:4875:ARG:NH1	1.62	1.12
1:B:4873:GLU:OE1	1:C:4875:ARG:HD3	1.49	1.11
1:A:4873:GLU:OE1	1:B:4875:ARG:HD3	1.49	1.11
1:A:4875:ARG:HD3	1:D:4873:GLU:OE1	1.49	1.10
1:A:4823:ARG:HA	1:D:4852:PHE:CZ	1.98	0.98
1:B:4852:PHE:CZ	1:C:4823:ARG:HA	1.98	0.98
1:A:4852:PHE:CZ	1:B:4823:ARG:HA	1.98	0.98
1:C:4852:PHE:CZ	1:D:4823:ARG:HA	1.98	0.98
1:D:4832:ILE:HG21	1:D:4844:ARG:HH21	1.44	0.83
1:B:4832:ILE:HG21	1:B:4844:ARG:HH21	1.44	0.82
1:C:4832:ILE:HG21	1:C:4844:ARG:HH21	1.44	0.82
1:A:4832:ILE:HG21	1:A:4844:ARG:HH21	1.44	0.80
1:A:4872:GLY:C	1:B:4875:ARG:HH22	1.86	0.79
1:A:4875:ARG:HH22	1:D:4872:GLY:C	1.86	0.78
1:A:4810:MET:HG2	1:B:4518:LEU:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4872:GLY:C	1:C:4875:ARG:HH22	1.86	0.78
1:B:4810:MET:HG2	1:C:4518:LEU:O	1.84	0.78
1:C:4872:GLY:C	1:D:4875:ARG:HH22	1.86	0.78
1:A:4518:LEU:O	1:D:4810:MET:HG2	1.84	0.77
1:C:4810:MET:HG2	1:D:4518:LEU:O	1.84	0.77
1:C:76:ARG:HG2	1:D:3891:TRP:HB3	1.68	0.75
1:B:708:GLY:HA2	1:B:714:GLY:HA3	1.69	0.74
1:B:76:ARG:HG2	1:C:3891:TRP:HB3	1.68	0.74
1:D:708:GLY:HA2	1:D:714:GLY:HA3	1.69	0.74
1:A:708:GLY:HA2	1:A:714:GLY:HA3	1.69	0.73
1:A:76:ARG:HG2	1:B:3891:TRP:HB3	1.68	0.73
1:A:3891:TRP:HB3	1:D:76:ARG:HG2	1.68	0.73
1:C:4872:GLY:C	1:D:4875:ARG:NH2	2.42	0.73
1:B:4872:GLY:C	1:C:4875:ARG:NH2	2.42	0.73
1:C:4873:GLU:OE1	1:D:4875:ARG:CD	2.35	0.73
1:C:708:GLY:HA2	1:C:714:GLY:HA3	1.69	0.72
1:B:4873:GLU:OE1	1:C:4875:ARG:CD	2.35	0.72
1:A:4872:GLY:C	1:B:4875:ARG:NH2	2.42	0.72
1:A:4875:ARG:NH2	1:D:4872:GLY:C	2.42	0.71
1:A:4875:ARG:NH1	1:D:4872:GLY:O	2.24	0.71
1:A:4157:SER:OG	1:A:4924:MET:SD	2.50	0.70
1:A:4872:GLY:O	1:B:4875:ARG:NH2	2.25	0.70
1:A:4872:GLY:O	1:B:4875:ARG:NH1	2.24	0.70
1:A:4875:ARG:NH2	1:D:4872:GLY:O	2.25	0.70
1:B:4157:SER:OG	1:B:4924:MET:SD	2.50	0.70
1:C:4872:GLY:O	1:D:4875:ARG:NH1	2.24	0.70
1:D:4157:SER:OG	1:D:4924:MET:SD	2.50	0.70
1:B:4872:GLY:O	1:C:4875:ARG:NH2	2.25	0.70
1:A:2419:ARG:NH1	1:D:189:GLU:OE1	2.25	0.70
1:B:189:GLU:OE1	1:C:2419:ARG:NH1	2.25	0.70
1:C:4873:GLU:CA	1:D:4875:ARG:NH1	2.51	0.69
1:B:4872:GLY:O	1:C:4875:ARG:NH1	2.24	0.69
1:A:189:GLU:OE1	1:B:2419:ARG:NH1	2.25	0.69
1:C:4157:SER:OG	1:C:4924:MET:SD	2.50	0.69
1:C:189:GLU:OE1	1:D:2419:ARG:NH1	2.25	0.69
1:B:4800:GLY:HA2	1:B:4804:ASP:HB3	1.74	0.68
1:A:4873:GLU:CA	1:B:4875:ARG:NH1	2.51	0.68
1:C:4872:GLY:O	1:D:4875:ARG:NH2	2.25	0.68
1:A:3986:MET:HG2	1:A:3996:ILE:HD11	1.75	0.68
1:D:3986:MET:HG2	1:D:3996:ILE:HD11	1.75	0.68
1:A:4875:ARG:NH1	1:D:4873:GLU:CA	2.51	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4011:VAL:HA	1:A:4014:ILE:HG12	1.76	0.68
1:A:1645:THR:HG22	1:A:1695:PRO:HG3	1.76	0.68
1:B:4873:GLU:CA	1:C:4875:ARG:NH1	2.51	0.68
1:C:4011:VAL:HA	1:C:4014:ILE:HG12	1.76	0.68
1:D:4800:GLY:HA2	1:D:4804:ASP:HB3	1.74	0.68
1:C:1645:THR:HG22	1:C:1695:PRO:HG3	1.76	0.67
1:C:4873:GLU:HA	1:D:4875:ARG:HH12	1.59	0.67
1:D:1138:ASP:HB2	1:D:1145:TRP:HE1	1.60	0.67
1:D:4011:VAL:HA	1:D:4014:ILE:HG12	1.76	0.67
1:A:1138:ASP:HB2	1:A:1145:TRP:HE1	1.60	0.67
1:C:1138:ASP:HB2	1:C:1145:TRP:HE1	1.60	0.67
1:C:4800:GLY:HA2	1:C:4804:ASP:HB3	1.74	0.67
1:A:4800:GLY:HA2	1:A:4804:ASP:HB3	1.74	0.67
1:B:1645:THR:HG22	1:B:1695:PRO:HG3	1.76	0.67
1:B:4873:GLU:HA	1:C:4875:ARG:HH12	1.59	0.67
1:C:3986:MET:HG2	1:C:3996:ILE:HD11	1.75	0.67
1:B:3986:MET:HG2	1:B:3996:ILE:HD11	1.75	0.67
1:B:4011:VAL:HA	1:B:4014:ILE:HG12	1.76	0.67
1:B:1138:ASP:HB2	1:B:1145:TRP:HE1	1.60	0.67
1:D:1645:THR:HG22	1:D:1695:PRO:HG3	1.76	0.67
1:D:35:LEU:HD13	1:D:49:LEU:HD22	1.77	0.66
1:A:299:HIS:HE2	1:A:301:THR:HG1	1.43	0.66
1:B:35:LEU:HD13	1:B:49:LEU:HD22	1.77	0.66
1:A:4875:ARG:CD	1:D:4873:GLU:OE1	2.35	0.65
1:A:4873:GLU:HA	1:B:4875:ARG:HH12	1.59	0.65
1:C:3875:THR:HG21	1:C:3924:TYR:HE2	1.62	0.65
1:A:35:LEU:HD13	1:A:49:LEU:HD22	1.77	0.65
1:B:248:PRO:HG2	1:B:257:ARG:HA	1.79	0.65
1:A:3875:THR:HG21	1:A:3924:TYR:HE2	1.62	0.65
1:A:248:PRO:HG2	1:A:257:ARG:HA	1.79	0.65
1:A:4873:GLU:OE1	1:B:4875:ARG:CD	2.35	0.65
1:C:35:LEU:HD13	1:C:49:LEU:HD22	1.77	0.65
1:D:248:PRO:HG2	1:D:257:ARG:HA	1.79	0.65
1:B:243:GLU:HA	1:B:264:GLY:HA2	1.79	0.65
1:B:1602:GLN:HE22	1:B:1642:LEU:HB3	1.62	0.65
1:A:1602:GLN:HE22	1:A:1642:LEU:HB3	1.62	0.65
1:B:299:HIS:HE2	1:B:301:THR:HG1	1.45	0.65
1:C:243:GLU:HA	1:C:264:GLY:HA2	1.79	0.65
1:C:248:PRO:HG2	1:C:257:ARG:HA	1.79	0.64
1:D:1602:GLN:HE22	1:D:1642:LEU:HB3	1.62	0.64
1:A:243:GLU:HA	1:A:264:GLY:HA2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1602:GLN:HE22	1:C:1642:LEU:HB3	1.62	0.64
1:D:3875:THR:HG21	1:D:3924:TYR:HE2	1.62	0.64
1:D:243:GLU:HA	1:D:264:GLY:HA2	1.79	0.64
1:B:1304:LEU:HB3	1:B:1541:PRO:HG2	1.80	0.64
1:B:3875:THR:HG21	1:B:3924:TYR:HE2	1.62	0.63
1:A:227:TYR:HE1	1:A:355:LYS:HG2	1.64	0.63
1:A:4868:ILE:HG12	1:D:4865:GLY:HA3	1.81	0.63
1:B:3845:GLN:HB2	1:B:3920:THR:HG22	1.81	0.63
1:D:188:SER:HB2	1:D:190:ARG:HH21	1.64	0.63
1:D:227:TYR:HE1	1:D:355:LYS:HG2	1.64	0.63
1:C:227:TYR:HE1	1:C:355:LYS:HG2	1.64	0.63
1:D:1304:LEU:HB3	1:D:1541:PRO:HG2	1.80	0.63
1:B:188:SER:HB2	1:B:190:ARG:HH21	1.64	0.62
1:A:188:SER:HB2	1:A:190:ARG:HH21	1.64	0.62
1:A:3922:THR:O	1:A:3926:GLN:N	2.32	0.62
1:A:4865:GLY:HA3	1:B:4868:ILE:HG12	1.81	0.62
1:C:188:SER:HB2	1:C:190:ARG:HH21	1.64	0.62
1:C:3922:THR:O	1:C:3926:GLN:N	2.32	0.62
1:A:1304:LEU:HB3	1:A:1541:PRO:HG2	1.80	0.62
1:A:3845:GLN:HB2	1:A:3920:THR:HG22	1.81	0.62
1:C:1304:LEU:HB3	1:C:1541:PRO:HG2	1.80	0.62
1:B:3922:THR:O	1:B:3926:GLN:N	2.32	0.62
1:B:227:TYR:HE1	1:B:355:LYS:HG2	1.64	0.62
1:D:3922:THR:O	1:D:3926:GLN:N	2.32	0.62
1:B:4865:GLY:HA3	1:C:4868:ILE:HG12	1.81	0.62
1:D:3845:GLN:HB2	1:D:3920:THR:HG22	1.81	0.62
1:C:4865:GLY:HA3	1:D:4868:ILE:HG12	1.81	0.62
1:B:1272:ARG:NH1	1:B:1587:HIS:O	2.34	0.61
1:D:1272:ARG:NH1	1:D:1587:HIS:O	2.34	0.61
1:D:299:HIS:HE2	1:D:301:THR:HG1	1.46	0.61
1:C:4072:GLU:HB3	1:C:4074:ASP:HB2	1.83	0.61
1:C:1272:ARG:NH1	1:C:1587:HIS:O	2.34	0.61
1:A:4875:ARG:HH12	1:D:4873:GLU:HA	1.59	0.61
1:B:3841:PHE:HB3	1:B:3920:THR:HG21	1.82	0.61
1:D:779:PHE:HB3	1:D:782:PHE:HE2	1.66	0.61
1:A:3841:PHE:HB3	1:A:3920:THR:HG21	1.82	0.60
1:B:4072:GLU:HB3	1:B:4074:ASP:HB2	1.83	0.60
1:D:3841:PHE:HB3	1:D:3920:THR:HG21	1.82	0.60
1:A:4140:MET:HG2	1:A:4146:ILE:HG12	1.82	0.60
1:B:1258:PHE:HB2	1:B:1593:HIS:HB3	1.83	0.60
1:D:4140:MET:HG2	1:D:4146:ILE:HG12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:THR:HG22	1:A:34:LYS:HG2	1.83	0.60
1:A:779:PHE:HB3	1:A:782:PHE:HE2	1.66	0.60
1:C:3802:SER:OG	1:C:3833:ASP:O	2.18	0.60
1:C:779:PHE:HB3	1:C:782:PHE:HE2	1.66	0.60
1:A:954:ASP:HB3	1:A:1061:GLY:HA3	1.84	0.60
1:B:779:PHE:HB3	1:B:782:PHE:HE2	1.66	0.60
1:D:954:ASP:HB3	1:D:1061:GLY:HA3	1.84	0.60
1:A:1469:LEU:HG	1:A:1480:ILE:HD11	1.84	0.60
1:A:3802:SER:OG	1:A:3833:ASP:O	2.18	0.60
1:B:143:LEU:HD23	1:C:2426:SER:HB3	1.84	0.60
1:C:123:HIS:HD2	1:C:126:SER:H	1.50	0.60
1:C:3845:GLN:HB2	1:C:3920:THR:HG22	1.81	0.60
1:D:802:PHE:HB2	1:D:1617:TRP:HB2	1.84	0.60
1:D:1469:LEU:HG	1:D:1480:ILE:HD11	1.84	0.60
1:B:954:ASP:HB3	1:B:1061:GLY:HA3	1.84	0.60
1:C:802:PHE:HB2	1:C:1617:TRP:HB2	1.84	0.60
1:C:4140:MET:HG2	1:C:4146:ILE:HG12	1.82	0.60
1:D:25:THR:HG22	1:D:34:LYS:HG2	1.83	0.60
1:A:802:PHE:HB2	1:A:1617:TRP:HB2	1.84	0.60
1:A:1258:PHE:HB2	1:A:1593:HIS:HB3	1.83	0.60
1:C:1137:PHE:HA	1:C:1144:ARG:HA	1.82	0.60
1:A:1272:ARG:NH1	1:A:1587:HIS:O	2.34	0.60
1:B:25:THR:HG22	1:B:34:LYS:HG2	1.83	0.60
1:B:123:HIS:HD2	1:B:126:SER:H	1.50	0.60
1:B:4140:MET:HG2	1:B:4146:ILE:HG12	1.82	0.60
1:C:1258:PHE:HB2	1:C:1593:HIS:HB3	1.83	0.60
1:A:756:SER:HB3	1:A:769:ARG:HB2	1.84	0.60
1:A:4072:GLU:HB3	1:A:4074:ASP:HB2	1.83	0.60
1:B:672:LYS:HA	1:B:760:ASP:HA	1.84	0.60
1:B:4617:TYR:OH	1:B:4629:GLY:O	2.20	0.60
1:D:1113:MET:HG3	1:D:1156:TRP:HZ2	1.67	0.60
1:B:756:SER:HB3	1:B:769:ARG:HB2	1.84	0.59
1:D:123:HIS:HD2	1:D:126:SER:H	1.50	0.59
1:A:1137:PHE:HA	1:A:1144:ARG:HA	1.82	0.59
1:D:4072:GLU:HB3	1:D:4074:ASP:HB2	1.83	0.59
1:A:672:LYS:HA	1:A:760:ASP:HA	1.84	0.59
1:A:4617:TYR:OH	1:A:4629:GLY:O	2.20	0.59
1:B:802:PHE:HB2	1:B:1617:TRP:HB2	1.84	0.59
1:B:1469:LEU:HG	1:B:1480:ILE:HD11	1.84	0.59
1:C:954:ASP:HB3	1:C:1061:GLY:HA3	1.84	0.59
1:D:1137:PHE:HA	1:D:1144:ARG:HA	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3802:SER:OG	1:D:3833:ASP:O	2.18	0.59
1:A:559:ILE:HD13	1:A:593:HIS:HB3	1.85	0.59
1:B:1137:PHE:HA	1:B:1144:ARG:HA	1.82	0.59
1:D:1445:TRP:HE1	1:D:1508:GLY:HA3	1.67	0.59
1:A:2426:SER:HB3	1:D:143:LEU:HD23	1.84	0.59
1:C:3914:ALA:HA	1:C:3917:VAL:HG12	1.85	0.59
1:D:559:ILE:HD13	1:D:593:HIS:HB3	1.85	0.59
1:A:123:HIS:HD2	1:A:126:SER:H	1.50	0.59
1:A:143:LEU:HD23	1:B:2426:SER:HB3	1.84	0.59
1:A:3914:ALA:HA	1:A:3917:VAL:HG12	1.85	0.59
1:D:3914:ALA:HA	1:D:3917:VAL:HG12	1.85	0.59
1:C:143:LEU:HD23	1:D:2426:SER:HB3	1.84	0.59
1:D:3924:TYR:O	1:D:3932:ASN:ND2	2.36	0.59
1:B:3914:ALA:HA	1:B:3917:VAL:HG12	1.85	0.59
1:C:25:THR:HG22	1:C:34:LYS:HG2	1.83	0.59
1:C:3841:PHE:HB3	1:C:3920:THR:HG21	1.82	0.59
1:D:1258:PHE:HB2	1:D:1593:HIS:HB3	1.83	0.59
1:A:1113:MET:HG3	1:A:1156:TRP:HZ2	1.67	0.59
1:C:756:SER:HB3	1:C:769:ARG:HB2	1.84	0.59
1:C:1469:LEU:HG	1:C:1480:ILE:HD11	1.84	0.59
1:B:1113:MET:HG3	1:B:1156:TRP:HZ2	1.67	0.58
1:C:672:LYS:HA	1:C:760:ASP:HA	1.84	0.58
1:C:1113:MET:HG3	1:C:1156:TRP:HZ2	1.67	0.58
1:A:3924:TYR:O	1:A:3932:ASN:ND2	2.36	0.58
1:C:4883:GLU:O	1:C:4887:THR:HG23	2.04	0.58
1:B:1445:TRP:HE1	1:B:1508:GLY:HA3	1.67	0.58
1:C:1706:LEU:HD21	1:C:1787:LEU:HD21	1.85	0.58
1:B:3802:SER:OG	1:B:3833:ASP:O	2.18	0.58
1:C:4617:TYR:OH	1:C:4629:GLY:O	2.20	0.58
1:D:756:SER:HB3	1:D:769:ARG:HB2	1.84	0.58
1:A:1104:GLU:HA	1:A:1163:GLY:HA2	1.85	0.58
1:B:3924:TYR:O	1:B:3932:ASN:ND2	2.36	0.58
1:C:897:LYS:HD3	1:C:918:LEU:HD21	1.86	0.58
1:B:559:ILE:HD13	1:B:593:HIS:HB3	1.85	0.58
1:D:672:LYS:HA	1:D:760:ASP:HA	1.84	0.58
1:B:897:LYS:HD3	1:B:918:LEU:HD21	1.86	0.58
1:B:1706:LEU:HD21	1:B:1787:LEU:HD21	1.85	0.58
1:D:4617:TYR:OH	1:D:4629:GLY:O	2.20	0.58
1:A:247:VAL:O	1:A:272:ARG:NH1	2.36	0.58
1:C:559:ILE:HD13	1:C:593:HIS:HB3	1.85	0.58
1:A:897:LYS:HD3	1:A:918:LEU:HD21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4883:GLU:O	1:A:4887:THR:HG23	2.04	0.58
1:C:1104:GLU:HA	1:C:1163:GLY:HA2	1.85	0.58
1:D:897:LYS:HD3	1:D:918:LEU:HD21	1.86	0.58
1:D:4883:GLU:O	1:D:4887:THR:HG23	2.04	0.58
1:A:1445:TRP:HE1	1:A:1508:GLY:HA3	1.67	0.57
1:C:3924:TYR:O	1:C:3932:ASN:ND2	2.36	0.57
1:C:4915:ASN:O	1:C:4917:ALA:N	2.38	0.57
1:D:1104:GLU:HA	1:D:1163:GLY:HA2	1.85	0.57
1:A:1124:PRO:HB2	1:A:1252:SER:HB3	1.86	0.57
1:A:4915:ASN:O	1:A:4917:ALA:N	2.38	0.57
1:C:1445:TRP:HE1	1:C:1508:GLY:HA3	1.67	0.57
1:D:247:VAL:O	1:D:272:ARG:NH1	2.36	0.57
1:B:4915:ASN:O	1:B:4917:ALA:N	2.38	0.57
1:C:1114:ARG:HB2	1:C:1206:SER:HB3	1.86	0.57
1:D:1706:LEU:HD21	1:D:1787:LEU:HD21	1.85	0.57
1:B:1114:ARG:HB2	1:B:1206:SER:HB3	1.86	0.57
1:D:1124:PRO:HB2	1:D:1252:SER:HB3	1.86	0.57
1:D:4915:ASN:O	1:D:4917:ALA:N	2.38	0.57
1:B:4883:GLU:O	1:B:4887:THR:HG23	2.04	0.57
1:C:299:HIS:HE2	1:C:301:THR:HG1	1.51	0.57
1:C:530:LEU:HD23	1:C:533:LEU:HD12	1.87	0.57
1:C:1429:SER:HA	1:C:1507:ILE:HG12	1.87	0.57
1:D:1429:SER:HA	1:D:1507:ILE:HG12	1.87	0.57
1:A:530:LEU:HD23	1:A:533:LEU:HD12	1.87	0.57
1:C:1433:PHE:HD2	1:C:1551:ASN:HB3	1.70	0.57
1:D:530:LEU:HD23	1:D:533:LEU:HD12	1.87	0.57
1:A:1429:SER:HA	1:A:1507:ILE:HG12	1.87	0.57
1:B:1104:GLU:HA	1:B:1163:GLY:HA2	1.85	0.57
1:A:1706:LEU:HD21	1:A:1787:LEU:HD21	1.85	0.56
1:A:1433:PHE:HD2	1:A:1551:ASN:HB3	1.70	0.56
1:D:1442:TRP:HD1	1:D:1488:VAL:HG13	1.71	0.56
1:B:4791:ARG:NE	1:C:4523:VAL:HG11	2.20	0.56
1:C:473:GLU:OE2	1:C:477:ASN:ND2	2.39	0.56
1:C:1124:PRO:HB2	1:C:1252:SER:HB3	1.86	0.56
1:C:1442:TRP:HD1	1:C:1488:VAL:HG13	1.71	0.56
1:C:1699:ARG:NH1	1:C:1816:PHE:O	2.39	0.56
1:D:1433:PHE:HD2	1:D:1551:ASN:HB3	1.70	0.56
1:B:1429:SER:HA	1:B:1507:ILE:HG12	1.87	0.56
1:C:58:VAL:HG22	1:C:320:GLU:HA	1.87	0.56
1:C:4015:LEU:HD22	1:C:4126:VAL:HG21	1.87	0.56
1:D:473:GLU:OE2	1:D:477:ASN:ND2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1442:TRP:HD1	1:A:1488:VAL:HG13	1.71	0.56
1:A:1114:ARG:HB2	1:A:1206:SER:HB3	1.86	0.56
1:B:530:LEU:HD23	1:B:533:LEU:HD12	1.87	0.56
1:B:4161:TRP:HD1	1:B:4201:MET:HE1	1.71	0.56
1:D:4015:LEU:HD22	1:D:4126:VAL:HG21	1.87	0.56
1:A:1121:GLY:O	1:A:1133:ARG:NH1	2.38	0.56
1:C:2060:GLN:NE2	1:C:2092:GLN:O	2.39	0.56
1:D:1114:ARG:HB2	1:D:1206:SER:HB3	1.86	0.56
1:A:4015:LEU:HD22	1:A:4126:VAL:HG21	1.87	0.56
1:B:58:VAL:HG22	1:B:320:GLU:HA	1.87	0.56
1:D:1121:GLY:O	1:D:1133:ARG:NH1	2.38	0.56
1:A:58:VAL:HG22	1:A:320:GLU:HA	1.87	0.56
1:A:4791:ARG:NE	1:B:4523:VAL:HG11	2.20	0.56
1:B:1699:ARG:NH1	1:B:1816:PHE:O	2.39	0.56
1:B:4015:LEU:HD22	1:B:4126:VAL:HG21	1.87	0.56
1:A:2060:GLN:NE2	1:A:2092:GLN:O	2.39	0.56
1:A:4618:ILE:HD12	1:A:4667:ILE:HD12	1.88	0.56
1:B:986:ILE:HD12	1:B:1059:GLY:HA2	1.88	0.56
1:C:4161:TRP:HD1	1:C:4201:MET:HE1	1.71	0.56
1:C:4618:ILE:HD12	1:C:4667:ILE:HD12	1.88	0.56
1:C:4791:ARG:NE	1:D:4523:VAL:HG11	2.20	0.56
1:B:1124:PRO:HB2	1:B:1252:SER:HB3	1.86	0.55
1:D:2060:GLN:NE2	1:D:2092:GLN:O	2.39	0.55
1:B:1433:PHE:HD2	1:B:1551:ASN:HB3	1.70	0.55
1:B:2060:GLN:NE2	1:B:2092:GLN:O	2.39	0.55
1:D:1272:ARG:NH2	1:D:1590:PHE:O	2.39	0.55
1:A:1272:ARG:NH2	1:A:1590:PHE:O	2.39	0.55
1:A:4523:VAL:HG11	1:D:4791:ARG:NE	2.20	0.55
1:B:375:GLN:HE21	1:B:392:ILE:HD13	1.72	0.55
1:B:473:GLU:OE2	1:B:477:ASN:ND2	2.39	0.55
1:C:1726:ILE:HD11	1:C:2121:LEU:HD11	1.89	0.55
1:D:1726:ILE:HD11	1:D:2121:LEU:HD11	1.89	0.55
1:A:618:CYS:SG	1:A:629:GLN:NE2	2.80	0.55
1:A:986:ILE:HD12	1:A:1059:GLY:HA2	1.88	0.55
1:A:2463:PRO:HB3	1:A:2516:ALA:HA	1.88	0.55
1:B:4618:ILE:HD12	1:B:4667:ILE:HD12	1.88	0.55
1:B:4819:TYR:O	1:B:4823:ARG:NH2	2.33	0.55
1:C:1272:ARG:NH2	1:C:1590:PHE:O	2.39	0.55
1:D:58:VAL:HG22	1:D:320:GLU:HA	1.87	0.55
1:A:375:GLN:HE21	1:A:392:ILE:HD13	1.72	0.55
1:A:1699:ARG:NH1	1:A:1816:PHE:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4618:ILE:HD12	1:D:4667:ILE:HD12	1.88	0.55
1:B:2843:GLU:OE1	1:B:2887:ARG:NH2	2.40	0.55
1:C:2843:GLU:OE1	1:C:2887:ARG:NH2	2.40	0.55
1:C:4840:TYR:O	1:C:4844:ARG:N	2.40	0.55
1:B:1272:ARG:NH2	1:B:1590:PHE:O	2.39	0.55
1:C:247:VAL:O	1:C:272:ARG:NH1	2.36	0.55
1:C:2463:PRO:HB3	1:C:2516:ALA:HA	1.88	0.55
1:B:618:CYS:SG	1:B:629:GLN:NE2	2.80	0.55
1:B:1442:TRP:HD1	1:B:1488:VAL:HG13	1.71	0.55
1:C:797:GLY:HA2	1:C:1622:LEU:HA	1.89	0.55
1:D:375:GLN:HE21	1:D:392:ILE:HD13	1.72	0.55
1:D:1699:ARG:NH1	1:D:1816:PHE:O	2.39	0.55
1:C:618:CYS:SG	1:C:629:GLN:NE2	2.80	0.55
1:D:797:GLY:HA2	1:D:1622:LEU:HA	1.89	0.55
1:D:2463:PRO:HB3	1:D:2516:ALA:HA	1.88	0.55
1:A:4514:ILE:HG21	1:A:4740:PHE:HE2	1.72	0.55
1:B:1726:ILE:HD11	1:B:2121:LEU:HD11	1.89	0.55
1:B:4514:ILE:HG21	1:B:4740:PHE:HE2	1.72	0.55
1:C:986:ILE:HD12	1:C:1059:GLY:HA2	1.88	0.55
1:C:4514:ILE:HG21	1:C:4740:PHE:HE2	1.72	0.55
1:A:473:GLU:OE2	1:A:477:ASN:ND2	2.39	0.54
1:A:1510:VAL:HG12	1:A:1511:VAL:HG23	1.89	0.54
1:B:3960:SER:HG	1:B:4070:CYS:HG	1.53	0.54
1:D:2158:GLN:O	1:D:3616:ARG:NH1	2.40	0.54
1:A:1156:TRP:HB3	1:A:1177:LEU:HD11	1.90	0.54
1:B:4840:TYR:O	1:B:4844:ARG:N	2.40	0.54
1:C:258:ARG:NH1	1:C:317:MET:SD	2.80	0.54
1:A:258:ARG:NH1	1:A:317:MET:SD	2.80	0.54
1:A:1726:ILE:HD11	1:A:2121:LEU:HD11	1.89	0.54
1:B:258:ARG:NH1	1:B:317:MET:SD	2.80	0.54
1:B:2158:GLN:O	1:B:3616:ARG:NH1	2.40	0.54
1:D:258:ARG:NH1	1:D:317:MET:SD	2.80	0.54
1:D:986:ILE:HD12	1:D:1059:GLY:HA2	1.88	0.54
1:D:2843:GLU:OE1	1:D:2887:ARG:NH2	2.40	0.54
1:A:2158:GLN:O	1:A:3616:ARG:NH1	2.40	0.54
1:C:375:GLN:HE21	1:C:392:ILE:HD13	1.72	0.54
1:C:2158:GLN:O	1:C:3616:ARG:NH1	2.40	0.54
1:D:618:CYS:SG	1:D:629:GLN:NE2	2.80	0.54
1:D:4514:ILE:HG21	1:D:4740:PHE:HE2	1.72	0.54
1:A:797:GLY:HA2	1:A:1622:LEU:HA	1.89	0.54
1:B:4046:LYS:HG3	1:B:4068:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1601:ASN:ND2	1:C:1643:GLU:OE2	2.41	0.54
1:A:2843:GLU:OE1	1:A:2887:ARG:NH2	2.40	0.54
1:B:247:VAL:O	1:B:272:ARG:NH1	2.36	0.54
1:B:1156:TRP:HB3	1:B:1177:LEU:HD11	1.90	0.54
1:B:1601:ASN:ND2	1:B:1643:GLU:OE2	2.41	0.54
1:C:1156:TRP:HB3	1:C:1177:LEU:HD11	1.90	0.54
1:C:4046:LYS:HG3	1:C:4068:LEU:HD22	1.90	0.54
1:D:1510:VAL:HG12	1:D:1511:VAL:HG23	1.89	0.54
1:A:1607:ASP:HB3	1:A:1608:VAL:HG23	1.90	0.54
1:B:228:LEU:HB3	1:B:289:ILE:HB	1.90	0.54
1:B:1510:VAL:HG12	1:B:1511:VAL:HG23	1.89	0.54
1:C:1607:ASP:HB3	1:C:1608:VAL:HG23	1.90	0.54
1:D:1156:TRP:HB3	1:D:1177:LEU:HD11	1.90	0.54
1:A:1601:ASN:ND2	1:A:1643:GLU:OE2	2.41	0.54
1:A:4161:TRP:HD1	1:A:4201:MET:HE1	1.71	0.54
1:C:228:LEU:HB3	1:C:289:ILE:HB	1.90	0.54
1:D:598:ILE:HG23	1:D:636:LEU:HD12	1.90	0.54
1:B:797:GLY:HA2	1:B:1622:LEU:HA	1.89	0.54
1:B:2463:PRO:HB3	1:B:2516:ALA:HA	1.88	0.54
1:B:1121:GLY:O	1:B:1133:ARG:NH1	2.38	0.54
1:B:1607:ASP:HB3	1:B:1608:VAL:HG23	1.90	0.54
1:D:1601:ASN:ND2	1:D:1643:GLU:OE2	2.41	0.54
1:A:4840:TYR:O	1:A:4844:ARG:N	2.40	0.53
1:C:26:ALA:HB3	1:C:33:GLN:HB3	1.90	0.53
1:C:1911:LEU:HD11	1:C:2063:ILE:HG12	1.90	0.53
1:D:4819:TYR:O	1:D:4823:ARG:NH2	2.33	0.53
1:C:3926:GLN:HE21	1:C:4936:GLY:H	1.56	0.53
1:C:4660:GLU:HG3	1:C:4664:ARG:HH21	1.73	0.53
1:B:598:ILE:HG23	1:B:636:LEU:HD12	1.90	0.53
1:D:4161:TRP:HD1	1:D:4201:MET:HE1	1.71	0.53
1:A:3926:GLN:HE21	1:A:4936:GLY:H	1.56	0.53
1:C:1121:GLY:O	1:C:1133:ARG:NH1	2.38	0.53
1:D:636:LEU:HD21	1:D:643:LEU:HD21	1.90	0.53
1:D:1607:ASP:HB3	1:D:1608:VAL:HG23	1.90	0.53
1:D:1726:ILE:HB	1:D:2109:ILE:HD11	1.91	0.53
1:D:4840:TYR:O	1:D:4844:ARG:N	2.40	0.53
1:C:3730:ALA:HA	1:C:3733:HIS:CE1	2.44	0.53
1:D:1911:LEU:HD11	1:D:2063:ILE:HG12	1.90	0.53
1:D:2488:LEU:O	1:D:2492:GLY:N	2.42	0.53
1:B:3730:ALA:HA	1:B:3733:HIS:CE1	2.44	0.53
1:C:61:ASP:OD2	1:C:417:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:598:ILE:HG23	1:C:636:LEU:HD12	1.90	0.53
1:D:26:ALA:HB3	1:D:33:GLN:HB3	1.90	0.53
1:D:4046:LYS:HG3	1:D:4068:LEU:HD22	1.90	0.53
1:A:1726:ILE:HB	1:A:2109:ILE:HD11	1.91	0.53
1:A:3730:ALA:HA	1:A:3733:HIS:CE1	2.44	0.53
1:A:3798:MET:HE1	1:A:3875:THR:HB	1.91	0.53
1:A:598:ILE:HG23	1:A:636:LEU:HD12	1.90	0.53
1:B:61:ASP:OD2	1:B:417:ARG:NH2	2.42	0.53
1:B:1726:ILE:HB	1:B:2109:ILE:HD11	1.91	0.53
1:C:1510:VAL:HG12	1:C:1511:VAL:HG23	1.89	0.53
1:D:4660:GLU:HG3	1:D:4664:ARG:HH21	1.73	0.53
1:B:677:LEU:HD11	1:B:792:VAL:HG21	1.91	0.53
1:B:4660:GLU:HG3	1:B:4664:ARG:HH21	1.73	0.53
1:C:4889:CYS:HB3	1:C:4892:CYS:SG	2.49	0.53
1:D:3798:MET:HE1	1:D:3875:THR:HB	1.91	0.53
1:D:4889:CYS:HB3	1:D:4892:CYS:SG	2.49	0.53
1:A:228:LEU:HB3	1:A:289:ILE:HB	1.90	0.52
1:A:2488:LEU:O	1:A:2492:GLY:N	2.42	0.52
1:A:2793:THR:OG1	1:A:2901:GLY:O	2.25	0.52
1:B:4889:CYS:HB3	1:B:4892:CYS:SG	2.49	0.52
1:D:61:ASP:OD2	1:D:417:ARG:NH2	2.42	0.52
1:D:228:LEU:HB3	1:D:289:ILE:HB	1.90	0.52
1:D:3729:GLN:O	1:D:3733:HIS:ND1	2.41	0.52
1:D:4108:GLU:HG3	1:D:4136:ARG:HH22	1.74	0.52
1:B:636:LEU:HD21	1:B:643:LEU:HD21	1.90	0.52
1:B:1094:TYR:OH	1:B:1808:ASP:OD1	2.28	0.52
1:B:4050:HIS:HB2	1:B:4068:LEU:HD11	1.91	0.52
1:C:677:LEU:HD11	1:C:792:VAL:HG21	1.91	0.52
1:B:1911:LEU:HD11	1:B:2063:ILE:HG12	1.90	0.52
1:B:3798:MET:HE1	1:B:3875:THR:HB	1.91	0.52
1:C:1094:TYR:OH	1:C:1808:ASP:OD1	2.28	0.52
1:C:3798:MET:HE1	1:C:3875:THR:HB	1.92	0.52
1:A:1911:LEU:HD11	1:A:2063:ILE:HG12	1.90	0.52
1:B:2488:LEU:O	1:B:2492:GLY:N	2.42	0.52
1:B:4791:ARG:CZ	1:C:4523:VAL:HG11	2.39	0.52
1:A:26:ALA:HB3	1:A:33:GLN:HB3	1.90	0.52
1:A:364:GLN:HE21	1:A:369:GLY:HA2	1.75	0.52
1:A:4889:CYS:HB3	1:A:4892:CYS:SG	2.49	0.52
1:C:2488:LEU:O	1:C:2492:GLY:N	2.42	0.52
1:A:4660:GLU:HG3	1:A:4664:ARG:HH21	1.73	0.52
1:A:4819:TYR:O	1:A:4823:ARG:NH2	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ALA:HB3	1:B:33:GLN:HB3	1.90	0.52
1:B:1487:MET:HB3	1:B:1520:PHE:HZ	1.75	0.52
1:B:3926:GLN:HE21	1:B:4936:GLY:H	1.56	0.52
1:C:4108:GLU:HG3	1:C:4136:ARG:HH22	1.74	0.52
1:A:192:LEU:O	1:A:212:TRP:NE1	2.42	0.52
1:A:1487:MET:HB3	1:A:1520:PHE:HZ	1.75	0.52
1:A:4046:LYS:HG3	1:A:4068:LEU:HD22	1.90	0.52
1:A:4791:ARG:CZ	1:B:4523:VAL:HG11	2.39	0.52
1:C:636:LEU:HD21	1:C:643:LEU:HD21	1.90	0.52
1:C:1726:ILE:HB	1:C:2109:ILE:HD11	1.91	0.52
1:D:3730:ALA:HA	1:D:3733:HIS:CE1	2.44	0.52
1:A:61:ASP:OD2	1:A:417:ARG:NH2	2.42	0.52
1:C:1938:GLN:HE22	1:C:3614:ARG:HA	1.75	0.52
1:A:1252:SER:HB2	1:A:1598:ARG:HB2	1.92	0.52
1:A:4108:GLU:HG3	1:A:4136:ARG:HH22	1.74	0.52
1:A:4523:VAL:HG11	1:D:4791:ARG:CZ	2.39	0.52
1:C:4791:ARG:CZ	1:D:4523:VAL:HG11	2.39	0.52
1:D:1094:TYR:OH	1:D:1808:ASP:OD1	2.28	0.52
1:D:1632:ILE:HD11	1:D:1637:ARG:HG2	1.92	0.52
1:A:476:GLN:NE2	1:A:3679:GLU:OE1	2.43	0.52
1:A:636:LEU:HD21	1:A:643:LEU:HD21	1.90	0.52
1:A:677:LEU:HD11	1:A:792:VAL:HG21	1.91	0.52
1:A:1703:TYR:HD2	1:A:1820:PRO:HB2	1.75	0.52
1:B:2192:LYS:O	1:B:2196:ASN:ND2	2.43	0.52
1:B:4108:GLU:HG3	1:B:4136:ARG:HH22	1.74	0.52
1:C:1632:ILE:HD11	1:C:1637:ARG:HG2	1.92	0.52
1:C:4050:HIS:HB2	1:C:4068:LEU:HD11	1.91	0.52
1:C:4873:GLU:HA	1:D:4875:ARG:HH11	1.68	0.52
1:D:3926:GLN:HE21	1:D:4936:GLY:H	1.56	0.52
1:A:4873:GLU:HA	1:B:4875:ARG:HH11	1.68	0.51
1:B:1252:SER:HB2	1:B:1598:ARG:HB2	1.92	0.51
1:D:1487:MET:HB3	1:D:1520:PHE:HZ	1.75	0.51
1:A:1938:GLN:HE22	1:A:3614:ARG:HA	1.75	0.51
1:B:1629:SER:HA	1:B:1640:ASP:HA	1.93	0.51
1:B:2103:LEU:HA	1:B:2106:THR:HG22	1.93	0.51
1:C:1487:MET:HB3	1:C:1520:PHE:HZ	1.75	0.51
1:C:2103:LEU:HA	1:C:2106:THR:HG22	1.93	0.51
1:C:2192:LYS:O	1:C:2196:ASN:ND2	2.43	0.51
1:D:4809:ASP:O	1:D:4813:CYS:N	2.39	0.51
1:A:1613:GLU:HB2	1:A:1618:LEU:H	1.76	0.51
1:B:476:GLN:NE2	1:B:3679:GLU:OE1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1613:GLU:HB2	1:B:1618:LEU:H	1.76	0.51
1:D:677:LEU:HD11	1:D:792:VAL:HG21	1.91	0.51
1:D:1613:GLU:HB2	1:D:1618:LEU:H	1.76	0.51
1:D:1629:SER:HA	1:D:1640:ASP:HA	1.93	0.51
1:C:1629:SER:HA	1:C:1640:ASP:HA	1.93	0.51
1:C:1703:TYR:HD2	1:C:1820:PRO:HB2	1.75	0.51
1:C:4809:ASP:O	1:C:4813:CYS:N	2.39	0.51
1:D:476:GLN:NE2	1:D:3679:GLU:OE1	2.43	0.51
1:B:364:GLN:HE21	1:B:369:GLY:HA2	1.75	0.51
1:C:476:GLN:NE2	1:C:3679:GLU:OE1	2.43	0.51
1:C:1613:GLU:HB2	1:C:1618:LEU:H	1.76	0.51
1:C:3980:VAL:HA	1:C:3983:LEU:HD23	1.92	0.51
1:D:364:GLN:HE21	1:D:369:GLY:HA2	1.75	0.51
1:D:1703:TYR:HD2	1:D:1820:PRO:HB2	1.75	0.51
1:A:4050:HIS:HB2	1:A:4068:LEU:HD11	1.91	0.51
1:B:23:GLN:HA	1:B:36:CYS:HA	1.92	0.51
1:B:1654:HIS:O	1:B:1657:THR:OG1	2.26	0.51
1:B:4163:LYS:HB2	1:B:4164:PRO:HD3	1.92	0.51
1:C:4636:ILE:O	1:C:4651:LYS:NZ	2.44	0.51
1:D:192:LEU:O	1:D:212:TRP:NE1	2.42	0.51
1:D:1252:SER:HB2	1:D:1598:ARG:HB2	1.92	0.51
1:D:1938:GLN:HE22	1:D:3614:ARG:HA	1.75	0.51
1:D:2192:LYS:O	1:D:2196:ASN:ND2	2.43	0.51
1:D:4636:ILE:O	1:D:4651:LYS:NZ	2.44	0.51
1:A:1094:TYR:OH	1:A:1808:ASP:OD1	2.28	0.51
1:A:4163:LYS:HB2	1:A:4164:PRO:HD3	1.92	0.51
1:B:1576:LYS:NZ	1:B:1589:GLN:OE1	2.44	0.51
1:B:4636:ILE:O	1:B:4651:LYS:NZ	2.44	0.51
1:C:364:GLN:HE21	1:C:369:GLY:HA2	1.75	0.51
1:C:1252:SER:HB2	1:C:1598:ARG:HB2	1.92	0.51
1:A:4875:ARG:CZ	1:D:4872:GLY:O	2.59	0.51
1:B:1703:TYR:HD2	1:B:1820:PRO:HB2	1.75	0.51
1:A:1576:LYS:NZ	1:A:1589:GLN:OE1	2.44	0.51
1:A:2103:LEU:HA	1:A:2106:THR:HG22	1.93	0.51
1:A:4636:ILE:O	1:A:4651:LYS:NZ	2.44	0.51
1:C:4872:GLY:O	1:D:4875:ARG:CZ	2.59	0.51
1:A:2192:LYS:O	1:A:2196:ASN:ND2	2.43	0.51
1:B:4872:GLY:O	1:C:4875:ARG:CZ	2.59	0.51
1:C:4819:TYR:O	1:C:4823:ARG:NH2	2.33	0.51
1:D:2103:LEU:HA	1:D:2106:THR:HG22	1.93	0.51
1:D:4050:HIS:HB2	1:D:4068:LEU:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1632:ILE:HD11	1:B:1637:ARG:HG2	1.92	0.50
1:B:4052:ALA:O	1:B:4056:HIS:ND1	2.44	0.50
1:C:150:GLN:NE2	1:C:158:CYS:SG	2.80	0.50
1:C:4052:ALA:O	1:C:4056:HIS:ND1	2.44	0.50
1:D:1726:ILE:HG13	1:D:1757:LEU:HD23	1.93	0.50
1:D:4174:ILE:HG21	1:D:4885:MET:HE2	1.93	0.50
1:A:1629:SER:HA	1:A:1640:ASP:HA	1.93	0.50
1:A:2857:LYS:HE3	1:A:2861:LEU:HD11	1.93	0.50
1:B:260:VAL:HG12	1:B:391:ALA:HB3	1.92	0.50
1:B:3980:VAL:HA	1:B:3983:LEU:HD23	1.92	0.50
1:C:419:ILE:HD13	1:C:492:GLU:HG3	1.93	0.50
1:A:3980:VAL:HA	1:A:3983:LEU:HD23	1.92	0.50
1:A:260:VAL:HG12	1:A:391:ALA:HB3	1.92	0.50
1:A:1911:LEU:HD22	1:A:2088:LEU:HD13	1.94	0.50
1:C:23:GLN:HA	1:C:36:CYS:HA	1.92	0.50
1:C:1128:LEU:HD13	1:C:1206:SER:HB2	1.94	0.50
1:C:1654:HIS:O	1:C:1657:THR:OG1	2.26	0.50
1:C:4647:ASP:O	1:C:4650:VAL:HG23	2.12	0.50
1:A:812:LYS:HD3	1:A:813:PHE:HB2	1.93	0.50
1:A:1632:ILE:HD11	1:A:1637:ARG:HG2	1.92	0.50
1:A:3729:GLN:O	1:A:3733:HIS:ND1	2.41	0.50
1:B:150:GLN:NE2	1:B:158:CYS:SG	2.80	0.50
1:B:1431:ARG:HB3	1:B:1554:GLN:HB2	1.94	0.50
1:B:1726:ILE:HG13	1:B:1757:LEU:HD23	1.93	0.50
1:B:1938:GLN:HE22	1:B:3614:ARG:HA	1.75	0.50
1:B:2857:LYS:HE3	1:B:2861:LEU:HD11	1.93	0.50
1:D:1128:LEU:HD13	1:D:1206:SER:HB2	1.94	0.50
1:D:1911:LEU:HD22	1:D:2088:LEU:HD13	1.94	0.50
1:C:260:VAL:HG12	1:C:391:ALA:HB3	1.92	0.50
1:C:812:LYS:HD3	1:C:813:PHE:HB2	1.93	0.50
1:C:1576:LYS:NZ	1:C:1589:GLN:OE1	2.44	0.50
1:D:1228:THR:HA	1:D:1232:LEU:HD12	1.94	0.50
1:A:1726:ILE:HG13	1:A:1757:LEU:HD23	1.93	0.50
1:A:2783:MET:HG2	1:A:2788:TRP:HE3	1.77	0.50
1:D:23:GLN:HA	1:D:36:CYS:HA	1.92	0.50
1:A:2439:ILE:HD13	1:A:2465:HIS:HB3	1.94	0.50
1:B:1444:GLY:HA2	1:B:1487:MET:HB2	1.94	0.50
1:C:565:LEU:HG	1:C:604:HIS:CE1	2.47	0.50
1:C:1228:THR:HA	1:C:1232:LEU:HD12	1.94	0.50
1:C:1726:ILE:HG13	1:C:1757:LEU:HD23	1.93	0.50
1:A:23:GLN:HA	1:A:36:CYS:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4780:TYR:HA	1:A:4783:THR:HG22	1.94	0.50
1:B:419:ILE:HD13	1:B:492:GLU:HG3	1.93	0.50
1:C:4861:ALA:HA	1:C:4864:GLN:HB2	1.94	0.50
1:D:260:VAL:HG12	1:D:391:ALA:HB3	1.92	0.50
1:D:4163:LYS:HB2	1:D:4164:PRO:HD3	1.92	0.50
1:A:3961:GLN:NE2	1:A:4069:SER:OG	2.45	0.49
1:A:4052:ALA:O	1:A:4056:HIS:ND1	2.44	0.49
1:B:565:LEU:HG	1:B:604:HIS:CE1	2.47	0.49
1:B:2439:ILE:HD13	1:B:2465:HIS:HB3	1.94	0.49
1:B:4647:ASP:O	1:B:4650:VAL:HG23	2.12	0.49
1:C:1444:GLY:HA2	1:C:1487:MET:HB2	1.94	0.49
1:D:1576:LYS:NZ	1:D:1589:GLN:OE1	2.44	0.49
1:A:4811:LEU:HD23	1:B:4519:LEU:HG	1.94	0.49
1:A:4872:GLY:O	1:B:4875:ARG:CZ	2.59	0.49
1:B:4784:VAL:HG13	1:C:4738:PHE:CE2	2.47	0.49
1:B:4861:ALA:HA	1:B:4864:GLN:HB2	1.94	0.49
1:C:1911:LEU:HD22	1:C:2088:LEU:HD13	1.94	0.49
1:D:719:GLY:H	1:D:722:LEU:HD12	1.77	0.49
1:D:1654:HIS:O	1:D:1657:THR:OG1	2.26	0.49
1:D:2857:LYS:HE3	1:D:2861:LEU:HD11	1.93	0.49
1:A:4632:ASP:OD1	1:A:4709:TRP:NE1	2.42	0.49
1:A:4784:VAL:HG13	1:B:4738:PHE:CE2	2.47	0.49
1:B:2783:MET:HG2	1:B:2788:TRP:HE3	1.77	0.49
1:B:4811:LEU:HD23	1:C:4519:LEU:HG	1.94	0.49
1:C:4784:VAL:HG13	1:D:4738:PHE:CE2	2.47	0.49
1:D:3961:GLN:NE2	1:D:4069:SER:OG	2.45	0.49
1:D:4610:LYS:HB3	1:D:4616:LEU:HD22	1.94	0.49
1:A:477:ASN:OD1	1:A:480:ARG:NH1	2.46	0.49
1:A:1444:GLY:HA2	1:A:1487:MET:HB2	1.94	0.49
1:A:2521:LEU:HD22	1:A:2565:ALA:HB2	1.94	0.49
1:A:4519:LEU:HG	1:D:4811:LEU:HD23	1.94	0.49
1:B:3961:GLN:NE2	1:B:4069:SER:OG	2.45	0.49
1:B:4780:TYR:HA	1:B:4783:THR:HG22	1.94	0.49
1:D:812:LYS:HD3	1:D:813:PHE:HB2	1.93	0.49
1:D:3980:VAL:HA	1:D:3983:LEU:HD23	1.92	0.49
1:A:1228:THR:HA	1:A:1232:LEU:HD12	1.94	0.49
1:A:1431:ARG:HB3	1:A:1554:GLN:HB2	1.94	0.49
1:D:1444:GLY:HA2	1:D:1487:MET:HB2	1.94	0.49
1:D:2521:LEU:HD22	1:D:2565:ALA:HB2	1.94	0.49
1:A:288:HIS:ND1	1:A:349:MET:O	2.43	0.49
1:B:1911:LEU:HD22	1:B:2088:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2783:MET:HG2	1:C:2788:TRP:HE3	1.77	0.49
1:C:4163:LYS:HB2	1:C:4164:PRO:HD3	1.92	0.49
1:D:4003:MET:HG3	1:D:4004:LEU:HG	1.95	0.49
1:A:419:ILE:HD13	1:A:492:GLU:HG3	1.93	0.49
1:A:4647:ASP:O	1:A:4650:VAL:HG23	2.12	0.49
1:B:1184:ASP:HB3	1:B:1186:SER:H	1.78	0.49
1:B:1228:THR:HA	1:B:1232:LEU:HD12	1.94	0.49
1:C:2857:LYS:HE3	1:C:2861:LEU:HD11	1.93	0.49
1:D:227:TYR:CE1	1:D:355:LYS:HG2	2.47	0.49
1:D:477:ASN:OD1	1:D:480:ARG:NH1	2.46	0.49
1:D:4052:ALA:O	1:D:4056:HIS:ND1	2.44	0.49
1:A:1128:LEU:HD13	1:A:1206:SER:HB2	1.94	0.49
1:A:4610:LYS:HB3	1:A:4616:LEU:HD22	1.94	0.49
1:B:335:LYS:NZ	1:B:398:HIS:O	2.44	0.49
1:B:812:LYS:HD3	1:B:813:PHE:HB2	1.93	0.49
1:B:2521:LEU:HD22	1:B:2565:ALA:HB2	1.94	0.49
1:B:3729:GLN:O	1:B:3733:HIS:ND1	2.41	0.49
1:C:227:TYR:CE1	1:C:355:LYS:HG2	2.47	0.49
1:C:335:LYS:NZ	1:C:398:HIS:O	2.44	0.49
1:D:4647:ASP:O	1:D:4650:VAL:HG23	2.12	0.49
1:B:1473:LYS:HE2	1:B:1475:LYS:HE3	1.95	0.49
1:C:2439:ILE:HD13	1:C:2465:HIS:HB3	1.94	0.49
1:C:4610:LYS:HB3	1:C:4616:LEU:HD22	1.94	0.49
1:D:419:ILE:HD13	1:D:492:GLU:HG3	1.93	0.49
1:D:565:LEU:HG	1:D:604:HIS:CE1	2.47	0.49
1:D:1086:ARG:HH22	1:D:1254:ARG:HB2	1.78	0.49
1:D:4780:TYR:HA	1:D:4783:THR:HG22	1.94	0.49
1:A:565:LEU:HG	1:A:604:HIS:CE1	2.47	0.49
1:A:1184:ASP:HB3	1:A:1186:SER:H	1.78	0.49
1:B:719:GLY:H	1:B:722:LEU:HD12	1.77	0.49
1:B:2421:ARG:HH21	1:B:2425:ARG:HH21	1.61	0.49
1:C:1431:ARG:HB3	1:C:1554:GLN:HB2	1.94	0.49
1:C:2521:LEU:HD22	1:C:2565:ALA:HB2	1.94	0.49
1:C:4003:MET:HG3	1:C:4004:LEU:HG	1.95	0.49
1:D:1184:ASP:HB3	1:D:1186:SER:H	1.78	0.49
1:D:1431:ARG:HB3	1:D:1554:GLN:HB2	1.94	0.49
1:A:3663:ASP:OD2	1:A:3735:ARG:NH2	2.46	0.48
1:A:150:GLN:NE2	1:A:158:CYS:SG	2.80	0.48
1:A:4774:LEU:HD13	1:B:4754:LEU:HD21	1.95	0.48
1:B:1086:ARG:HB2	1:B:1207:LEU:HB2	1.95	0.48
1:B:1220:ASP:O	1:B:1223:THR:N	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:ASN:OD1	1:C:480:ARG:NH1	2.46	0.48
1:C:4174:ILE:HD13	1:C:4885:MET:HE1	1.96	0.48
1:D:2783:MET:HG2	1:D:2788:TRP:HE3	1.77	0.48
1:A:4191:VAL:HA	1:A:4194:CYS:HB2	1.96	0.48
1:A:4732:LEU:O	1:A:4736:ASN:N	2.44	0.48
1:A:4861:ALA:HA	1:A:4864:GLN:HB2	1.94	0.48
1:B:1128:LEU:HD13	1:B:1206:SER:HB2	1.94	0.48
1:B:2345:LEU:HD21	1:B:2434:VAL:HB	1.96	0.48
1:C:3663:ASP:OD2	1:C:3735:ARG:NH2	2.46	0.48
1:C:4764:ASN:ND2	1:C:4866:LEU:O	2.47	0.48
1:C:4780:TYR:HA	1:C:4783:THR:HG22	1.94	0.48
1:D:3663:ASP:OD2	1:D:3735:ARG:NH2	2.46	0.48
1:D:4861:ALA:HA	1:D:4864:GLN:HB2	1.94	0.48
1:A:719:GLY:H	1:A:722:LEU:HD12	1.77	0.48
1:A:1934:VAL:O	1:A:1938:GLN:N	2.43	0.48
1:A:2345:LEU:HD21	1:A:2434:VAL:HB	1.96	0.48
1:B:477:ASN:OD1	1:B:480:ARG:NH1	2.46	0.48
1:B:653:SER:OG	1:B:794:PHE:O	2.31	0.48
1:B:1184:ASP:OD2	1:B:1188:SER:OG	2.31	0.48
1:B:3663:ASP:OD2	1:B:3735:ARG:NH2	2.46	0.48
1:C:192:LEU:O	1:C:212:TRP:NE1	2.42	0.48
1:C:2723:ASN:OD1	1:C:2773:ARG:NH2	2.47	0.48
1:C:4774:LEU:HD13	1:D:4754:LEU:HD21	1.95	0.48
1:D:150:GLN:NE2	1:D:158:CYS:SG	2.80	0.48
1:D:2209:ARG:HG3	1:D:2251:ASN:HD21	1.79	0.48
1:D:2345:LEU:HD21	1:D:2434:VAL:HB	1.96	0.48
1:A:4003:MET:HG3	1:A:4004:LEU:HG	1.95	0.48
1:B:1086:ARG:HH22	1:B:1254:ARG:HB2	1.78	0.48
1:C:2421:ARG:HH21	1:C:2425:ARG:HH21	1.61	0.48
1:C:4811:LEU:HD23	1:D:4519:LEU:HG	1.94	0.48
1:D:1184:ASP:OD2	1:D:1188:SER:OG	2.31	0.48
1:A:4013:MET:O	1:A:4017:PHE:N	2.46	0.48
1:C:2345:LEU:HD21	1:C:2434:VAL:HB	1.96	0.48
1:C:4780:TYR:OH	1:D:4515:ASN:ND2	2.46	0.48
1:D:1473:LYS:HE2	1:D:1475:LYS:HE3	1.95	0.48
1:A:1220:ASP:O	1:A:1223:THR:N	2.35	0.48
1:A:1473:LYS:HE2	1:A:1475:LYS:HE3	1.95	0.48
1:A:2421:ARG:HH21	1:A:2425:ARG:HH21	1.61	0.48
1:C:374:TYR:HA	1:C:391:ALA:HA	1.96	0.48
1:C:719:GLY:H	1:C:722:LEU:HD12	1.77	0.48
1:C:852:GLY:HA2	1:C:853:PRO:HA	1.69	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3961:GLN:NE2	1:C:4069:SER:OG	2.45	0.48
1:D:2723:ASN:OD1	1:D:2773:ARG:NH2	2.47	0.48
1:A:428:ARG:O	1:A:432:GLY:N	2.46	0.48
1:A:1833:ILE:HG22	1:A:1834:PHE:H	1.79	0.48
1:A:4515:ASN:ND2	1:D:4780:TYR:OH	2.46	0.48
1:A:4738:PHE:CE2	1:D:4784:VAL:HG13	2.47	0.48
1:A:4780:TYR:OH	1:B:4515:ASN:ND2	2.46	0.48
1:C:2717:LYS:HB2	1:C:2792:ARG:HH22	1.79	0.48
1:D:4764:ASN:ND2	1:D:4866:LEU:O	2.47	0.48
1:A:4130:PHE:O	1:A:4134:LEU:N	2.45	0.48
1:B:2723:ASN:OD1	1:B:2773:ARG:NH2	2.47	0.48
1:B:4771:THR:OG1	1:C:4757:ILE:HD13	2.14	0.48
1:B:4780:TYR:OH	1:C:4515:ASN:ND2	2.46	0.48
1:D:2439:ILE:HD13	1:D:2465:HIS:HB3	1.94	0.48
1:B:192:LEU:O	1:B:212:TRP:NE1	2.42	0.48
1:B:1833:ILE:HG22	1:B:1834:PHE:H	1.79	0.48
1:B:3911:ILE:HG21	1:B:3971:GLU:HB3	1.96	0.48
1:B:4610:LYS:HB3	1:B:4616:LEU:HD22	1.94	0.48
1:C:1184:ASP:HB3	1:C:1186:SER:H	1.78	0.48
1:D:1086:ARG:HB2	1:D:1207:LEU:HB2	1.95	0.48
1:D:1626:GLN:O	1:D:1687:TYR:OH	2.32	0.48
1:B:4191:VAL:HA	1:B:4194:CYS:HB2	1.96	0.47
1:C:1473:LYS:HE2	1:C:1475:LYS:HE3	1.95	0.47
1:D:2717:LYS:HB2	1:D:2792:ARG:HH22	1.79	0.47
1:D:4013:MET:O	1:D:4017:PHE:N	2.46	0.47
1:D:4191:VAL:HA	1:D:4194:CYS:HB2	1.96	0.47
1:B:115:TYR:HB3	1:B:164:PRO:HD3	1.97	0.47
1:C:3729:GLN:O	1:C:3733:HIS:ND1	2.41	0.47
1:C:3911:ILE:HG21	1:C:3971:GLU:HB3	1.96	0.47
1:D:374:TYR:HA	1:D:391:ALA:HA	1.96	0.47
1:D:2421:ARG:HH21	1:D:2425:ARG:HH21	1.61	0.47
1:D:3911:ILE:HG21	1:D:3971:GLU:HB3	1.96	0.47
1:A:1086:ARG:HH22	1:A:1254:ARG:HB2	1.78	0.47
1:A:2723:ASN:OD1	1:A:2773:ARG:NH2	2.47	0.47
1:A:4764:ASN:ND2	1:A:4866:LEU:O	2.47	0.47
1:A:4771:THR:OG1	1:B:4757:ILE:HD13	2.14	0.47
1:D:2076:ILE:HG21	1:D:2081:LEU:HD22	1.97	0.47
1:D:3804:LEU:HD13	1:D:3910:ALA:HB2	1.96	0.47
1:A:115:TYR:HB3	1:A:164:PRO:HD3	1.97	0.47
1:A:3911:ILE:HG21	1:A:3971:GLU:HB3	1.96	0.47
1:B:4764:ASN:ND2	1:B:4866:LEU:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4774:LEU:HD13	1:C:4754:LEU:HD21	1.95	0.47
1:C:1086:ARG:HH22	1:C:1254:ARG:HB2	1.78	0.47
1:D:115:TYR:HB3	1:D:164:PRO:HD3	1.97	0.47
1:D:2793:THR:OG1	1:D:2901:GLY:O	2.25	0.47
1:A:374:TYR:HA	1:A:391:ALA:HA	1.96	0.47
1:A:1184:ASP:OD2	1:A:1188:SER:OG	2.31	0.47
1:A:2076:ILE:HG21	1:A:2081:LEU:HD22	1.97	0.47
1:B:4003:MET:HG3	1:B:4004:LEU:HG	1.95	0.47
1:C:590:LYS:HB2	1:C:593:HIS:HD2	1.80	0.47
1:C:718:VAL:HA	1:C:736:CYS:HB2	1.96	0.47
1:A:572:LEU:O	1:A:576:HIS:N	2.47	0.47
1:A:2717:LYS:HB2	1:A:2792:ARG:HH22	1.79	0.47
1:A:3804:LEU:HD13	1:A:3910:ALA:HB2	1.96	0.47
1:A:4757:ILE:HD13	1:D:4771:THR:OG1	2.14	0.47
1:B:300:VAL:O	1:B:420:ARG:NH2	2.48	0.47
1:B:572:LEU:O	1:B:576:HIS:N	2.47	0.47
1:B:3800:SER:OG	1:B:3801:CYS:N	2.47	0.47
1:B:4191:VAL:HB	1:B:4950:TRP:HH2	1.79	0.47
1:C:115:TYR:HB3	1:C:164:PRO:HD3	1.97	0.47
1:C:1086:ARG:HB2	1:C:1207:LEU:HB2	1.95	0.47
1:C:1184:ASP:OD2	1:C:1188:SER:OG	2.31	0.47
1:C:2737:LYS:HB3	1:C:2742:TRP:HB2	1.96	0.47
1:D:4191:VAL:HB	1:D:4950:TRP:HH2	1.79	0.47
1:A:1086:ARG:HB2	1:A:1207:LEU:HB2	1.95	0.47
1:A:1707:ILE:HA	1:A:1711:LEU:HB2	1.97	0.47
1:A:2209:ARG:HG3	1:A:2251:ASN:HD21	1.79	0.47
1:B:374:TYR:HA	1:B:391:ALA:HA	1.96	0.47
1:B:2076:ILE:HG21	1:B:2081:LEU:HD22	1.97	0.47
1:B:2717:LYS:HB2	1:B:2792:ARG:HH22	1.79	0.47
1:C:2076:ILE:HG21	1:C:2081:LEU:HD22	1.97	0.47
1:C:2121:LEU:O	1:C:2125:GLY:N	2.47	0.47
1:C:2793:THR:OG1	1:C:2901:GLY:O	2.25	0.47
1:C:4752:LYS:HA	1:C:4755:ARG:HE	1.80	0.47
1:C:4771:THR:OG1	1:D:4757:ILE:HD13	2.14	0.47
1:D:125:TYR:CZ	1:D:417:ARG:HB3	2.50	0.47
1:D:335:LYS:NZ	1:D:398:HIS:O	2.44	0.47
1:D:718:VAL:HA	1:D:736:CYS:HB2	1.96	0.47
1:B:2209:ARG:HG3	1:B:2251:ASN:HD21	1.79	0.47
1:B:2424:LEU:HD23	1:B:2476:VAL:HG22	1.97	0.47
1:B:2737:LYS:HB3	1:B:2742:TRP:HB2	1.96	0.47
1:B:4174:ILE:HG21	1:B:4885:MET:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4207:ILE:HG22	1:B:4498:ARG:HE	1.80	0.47
1:C:4191:VAL:HA	1:C:4194:CYS:HB2	1.96	0.47
1:D:300:VAL:O	1:D:420:ARG:NH2	2.48	0.47
1:D:590:LYS:HB2	1:D:593:HIS:HD2	1.80	0.47
1:D:4732:LEU:O	1:D:4736:ASN:N	2.44	0.47
1:A:4207:ILE:HG22	1:A:4498:ARG:HE	1.80	0.47
1:C:125:TYR:CZ	1:C:417:ARG:HB3	2.50	0.47
1:B:2301:ASP:OD1	1:B:2304:ARG:NH2	2.48	0.47
1:B:3696:MET:O	1:B:3699:SER:OG	2.26	0.47
1:B:4130:PHE:O	1:B:4134:LEU:N	2.45	0.47
1:B:4752:LYS:HA	1:B:4755:ARG:HE	1.80	0.47
1:A:125:TYR:CZ	1:A:417:ARG:HB3	2.50	0.46
1:A:298:ARG:HE	1:A:303:GLY:HA2	1.81	0.46
1:A:300:VAL:O	1:A:420:ARG:NH2	2.48	0.46
1:A:1172:THR:HG21	1:A:1190:LEU:HD13	1.97	0.46
1:A:2301:ASP:OD1	1:A:2304:ARG:NH2	2.48	0.46
1:A:2737:LYS:HB3	1:A:2742:TRP:HB2	1.96	0.46
1:B:125:TYR:CZ	1:B:417:ARG:HB3	2.50	0.46
1:C:1833:ILE:HG22	1:C:1834:PHE:H	1.79	0.46
1:C:2424:LEU:HD23	1:C:2476:VAL:HG22	1.97	0.46
1:D:1172:THR:HG21	1:D:1190:LEU:HD13	1.97	0.46
1:A:1174:MET:SD	1:A:1236:TYR:OH	2.73	0.46
1:B:590:LYS:HB2	1:B:593:HIS:HD2	1.80	0.46
1:B:1445:TRP:H	1:B:1487:MET:HB2	1.81	0.46
1:C:300:VAL:O	1:C:420:ARG:NH2	2.48	0.46
1:C:1172:THR:HG21	1:C:1190:LEU:HD13	1.97	0.46
1:C:2209:ARG:HG3	1:C:2251:ASN:HD21	1.79	0.46
1:D:1833:ILE:HG22	1:D:1834:PHE:H	1.79	0.46
1:D:2301:ASP:OD1	1:D:2304:ARG:NH2	2.48	0.46
1:D:2737:LYS:HB3	1:D:2742:TRP:HB2	1.96	0.46
1:D:4565:SER:OG	1:D:4566:SER:N	2.49	0.46
1:A:590:LYS:HB2	1:A:593:HIS:HD2	1.80	0.46
1:A:2858:LYS:HG2	1:A:2872:LEU:HD13	1.96	0.46
1:A:4565:SER:OG	1:A:4566:SER:N	2.49	0.46
1:A:4754:LEU:HD21	1:D:4774:LEU:HD13	1.95	0.46
1:B:657:PRO:HA	1:B:834:VAL:HA	1.97	0.46
1:B:1172:THR:HG21	1:B:1190:LEU:HD13	1.97	0.46
1:B:1763:PHE:HB3	1:B:1781:GLU:HB3	1.98	0.46
1:B:3804:LEU:HD13	1:B:3910:ALA:HB2	1.96	0.46
1:B:4627:ILE:O	1:B:4631:TRP:N	2.48	0.46
1:C:1626:GLN:O	1:C:1687:TYR:OH	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4191:VAL:HB	1:C:4950:TRP:HH2	1.79	0.46
1:D:4752:LYS:HA	1:D:4755:ARG:HE	1.80	0.46
1:A:718:VAL:HA	1:A:736:CYS:HB2	1.96	0.46
1:A:1445:TRP:H	1:A:1487:MET:HB2	1.81	0.46
1:A:4752:LYS:HA	1:A:4755:ARG:HE	1.80	0.46
1:B:428:ARG:O	1:B:432:GLY:N	2.46	0.46
1:B:1707:ILE:HA	1:B:1711:LEU:HB2	1.97	0.46
1:B:2121:LEU:O	1:B:2125:GLY:N	2.47	0.46
1:C:648:LEU:HD23	1:C:1684:GLN:HA	1.98	0.46
1:A:648:LEU:HD23	1:A:1684:GLN:HA	1.98	0.46
1:B:648:LEU:HD23	1:B:1684:GLN:HA	1.98	0.46
1:B:718:VAL:HA	1:B:736:CYS:HB2	1.96	0.46
1:B:4201:MET:O	1:B:4205:ALA:N	2.49	0.46
1:C:180:ASP:HB3	1:C:211:LEU:HD22	1.97	0.46
1:C:3804:LEU:HD13	1:C:3910:ALA:HB2	1.96	0.46
1:D:2858:LYS:HG2	1:D:2872:LEU:HD13	1.96	0.46
1:A:1763:PHE:HB3	1:A:1781:GLU:HB3	1.98	0.46
1:A:2326:ILE:HD13	1:A:2326:ILE:HA	1.83	0.46
1:A:2424:LEU:HD23	1:A:2476:VAL:HG22	1.97	0.46
1:A:4191:VAL:HB	1:A:4950:TRP:HH2	1.79	0.46
1:B:852:GLY:HA2	1:B:853:PRO:HA	1.69	0.46
1:D:2424:LEU:HD23	1:D:2476:VAL:HG22	1.97	0.46
1:A:657:PRO:HA	1:A:834:VAL:HA	1.97	0.46
1:A:4174:ILE:HG21	1:A:4885:MET:HE2	1.97	0.46
1:B:436:LEU:HD13	1:B:518:ALA:HA	1.98	0.46
1:B:2858:LYS:HG2	1:B:2872:LEU:HD13	1.96	0.46
1:C:298:ARG:HA	1:C:305:TYR:HA	1.97	0.46
1:C:698:ALA:HB2	1:C:722:LEU:HD23	1.98	0.46
1:C:1174:MET:SD	1:C:1236:TYR:OH	2.73	0.46
1:C:2301:ASP:OD1	1:C:2304:ARG:NH2	2.48	0.46
1:C:4632:ASP:OD1	1:C:4709:TRP:NE1	2.42	0.46
1:D:298:ARG:HA	1:D:305:TYR:HA	1.97	0.46
1:D:698:ALA:HB2	1:D:722:LEU:HD23	1.98	0.46
1:A:298:ARG:HA	1:A:305:TYR:HA	1.97	0.46
1:A:436:LEU:HD13	1:A:518:ALA:HA	1.98	0.46
1:A:4875:ARG:HH11	1:D:4873:GLU:HA	1.68	0.46
1:B:180:ASP:HB3	1:B:211:LEU:HD22	1.97	0.46
1:C:170:SER:OG	1:C:171:GLU:N	2.49	0.46
1:C:572:LEU:O	1:C:576:HIS:N	2.47	0.46
1:C:1707:ILE:HA	1:C:1711:LEU:HB2	1.97	0.46
1:C:4627:ILE:O	1:C:4631:TRP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:ARG:HE	1:D:303:GLY:HA2	1.81	0.46
1:D:657:PRO:HA	1:D:834:VAL:HA	1.97	0.46
1:D:4201:MET:O	1:D:4205:ALA:N	2.49	0.46
1:A:189:GLU:CG	1:B:2419:ARG:NH2	2.79	0.46
1:B:189:GLU:CG	1:C:2419:ARG:NH2	2.79	0.46
1:B:298:ARG:HA	1:B:305:TYR:HA	1.97	0.46
1:B:1174:MET:SD	1:B:1236:TYR:OH	2.73	0.46
1:B:4565:SER:OG	1:B:4566:SER:N	2.49	0.46
1:C:189:GLU:OE1	1:D:2419:ARG:CZ	2.64	0.46
1:C:2858:LYS:HG2	1:C:2872:LEU:HD13	1.96	0.46
1:D:537:LEU:HD11	1:D:551:PHE:HZ	1.81	0.46
1:D:1174:MET:SD	1:D:1236:TYR:OH	2.73	0.46
1:A:695:VAL:O	1:A:725:TYR:N	2.49	0.46
1:B:537:LEU:HD11	1:B:551:PHE:HZ	1.81	0.46
1:C:189:GLU:CG	1:D:2419:ARG:NH2	2.79	0.46
1:C:288:HIS:ND1	1:C:349:MET:O	2.43	0.46
1:C:478:ARG:HE	1:C:485:ARG:HH22	1.64	0.46
1:D:478:ARG:HE	1:D:485:ARG:HH22	1.64	0.46
1:D:648:LEU:HD23	1:D:1684:GLN:HA	1.98	0.46
1:D:1707:ILE:HA	1:D:1711:LEU:HB2	1.97	0.46
1:A:537:LEU:HD11	1:A:551:PHE:HZ	1.81	0.45
1:C:298:ARG:HE	1:C:303:GLY:HA2	1.81	0.45
1:C:4565:SER:OG	1:C:4566:SER:N	2.49	0.45
1:D:428:ARG:O	1:D:432:GLY:N	2.46	0.45
1:D:4207:ILE:HG22	1:D:4498:ARG:HE	1.80	0.45
1:D:4627:ILE:O	1:D:4631:TRP:N	2.48	0.45
1:A:170:SER:OG	1:A:171:GLU:N	2.49	0.45
1:A:2419:ARG:CZ	1:D:189:GLU:OE1	2.64	0.45
1:B:237:LEU:N	1:B:404:ASN:O	2.49	0.45
1:B:4869:ASP:O	1:B:4873:GLU:N	2.49	0.45
1:C:237:LEU:N	1:C:404:ASN:O	2.49	0.45
1:C:646:THR:OG1	1:C:1684:GLN:NE2	2.49	0.45
1:C:657:PRO:HA	1:C:834:VAL:HA	1.97	0.45
1:D:1763:PHE:HB3	1:D:1781:GLU:HB3	1.98	0.45
1:A:180:ASP:HB3	1:A:211:LEU:HD22	1.97	0.45
1:A:848:ARG:HB2	1:A:1603:PHE:HZ	1.81	0.45
1:C:1445:TRP:H	1:C:1487:MET:HB2	1.81	0.45
1:C:1763:PHE:HB3	1:C:1781:GLU:HB3	1.98	0.45
1:D:848:ARG:HB2	1:D:1603:PHE:HZ	1.81	0.45
1:A:646:THR:OG1	1:A:1684:GLN:NE2	2.49	0.45
1:A:698:ALA:HB2	1:A:722:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2419:ARG:NH2	1:D:189:GLU:CG	2.79	0.45
1:B:189:GLU:OE1	1:C:2419:ARG:CZ	2.64	0.45
1:B:698:ALA:HB2	1:B:722:LEU:HD23	1.98	0.45
1:C:4207:ILE:HG22	1:C:4498:ARG:HE	1.80	0.45
1:D:180:ASP:HB3	1:D:211:LEU:HD22	1.97	0.45
1:D:4869:ASP:O	1:D:4873:GLU:N	2.49	0.45
1:A:189:GLU:OE1	1:B:2419:ARG:CZ	2.64	0.45
1:A:4201:MET:O	1:A:4205:ALA:N	2.49	0.45
1:B:298:ARG:HE	1:B:303:GLY:HA2	1.81	0.45
1:C:4013:MET:O	1:C:4017:PHE:N	2.46	0.45
1:D:843:GLU:HA	1:D:848:ARG:HG2	1.98	0.45
1:D:3859:LEU:HD22	1:D:3871:ILE:HG21	1.98	0.45
1:A:227:TYR:CE1	1:A:355:LYS:HG2	2.47	0.45
1:A:4588:ILE:HG22	1:A:4723:LEU:HD23	1.99	0.45
1:B:1602:GLN:HB3	1:B:1604:LEU:HD12	1.99	0.45
1:B:4142:SER:HB3	1:B:4940:TYR:CE1	2.52	0.45
1:D:436:LEU:HD13	1:D:518:ALA:HA	1.98	0.45
1:D:766:ILE:HB	1:D:779:PHE:HB2	1.99	0.45
1:D:4588:ILE:HG22	1:D:4723:LEU:HD23	1.99	0.45
1:A:478:ARG:HE	1:A:485:ARG:HH22	1.64	0.45
1:A:4142:SER:HB3	1:A:4940:TYR:CE1	2.52	0.45
1:B:478:ARG:HE	1:B:485:ARG:HH22	1.64	0.45
1:C:537:LEU:HD11	1:C:551:PHE:HZ	1.81	0.45
1:C:766:ILE:HB	1:C:779:PHE:HB2	1.99	0.45
1:C:1220:ASP:O	1:C:1223:THR:N	2.35	0.45
1:C:4142:SER:HB3	1:C:4940:TYR:CE1	2.52	0.45
1:C:4201:MET:O	1:C:4205:ALA:N	2.49	0.45
1:D:1445:TRP:H	1:D:1487:MET:HB2	1.81	0.45
1:D:3800:SER:OG	1:D:3801:CYS:N	2.47	0.45
1:A:843:GLU:HA	1:A:848:ARG:HG2	1.98	0.45
1:B:1934:VAL:O	1:B:1938:GLN:N	2.43	0.45
1:C:419:ILE:HG12	1:C:489:PHE:CE1	2.52	0.45
1:C:4588:ILE:HG22	1:C:4723:LEU:HD23	1.99	0.45
1:D:289:ILE:HG22	1:D:354:ILE:HD12	1.99	0.45
1:A:2525:VAL:HG13	1:A:2528:LEU:HD12	1.99	0.45
1:B:695:VAL:O	1:B:725:TYR:N	2.49	0.45
1:C:3743:GLN:NE2	1:C:3781:TYR:OH	2.43	0.45
1:C:3952:PHE:HB3	1:C:3976:GLN:HE22	1.82	0.45
1:D:3737:ALA:O	1:D:3740:MET:HG2	2.17	0.45
1:A:3952:PHE:HB3	1:A:3976:GLN:HE22	1.82	0.45
1:B:308:LEU:HD22	1:B:370:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3737:ALA:O	1:B:3740:MET:HG2	2.17	0.45
1:C:428:ARG:O	1:C:432:GLY:N	2.46	0.45
1:C:436:LEU:HD13	1:C:518:ALA:HA	1.98	0.45
1:C:4203:LEU:O	1:C:4207:ILE:HG12	2.17	0.45
1:A:766:ILE:HB	1:A:779:PHE:HB2	1.99	0.44
1:B:419:ILE:HG12	1:B:489:PHE:CE1	2.52	0.44
1:B:4036:TYR:HE2	1:B:4048:ASP:HB3	1.82	0.44
1:C:143:LEU:CD2	1:D:2426:SER:HB3	2.47	0.44
1:C:843:GLU:HA	1:C:848:ARG:HG2	1.98	0.44
1:C:1602:GLN:HB3	1:C:1604:LEU:HD12	1.99	0.44
1:C:4747:ILE:HG13	1:C:4754:LEU:HD22	1.99	0.44
1:D:419:ILE:HG12	1:D:489:PHE:CE1	2.52	0.44
1:D:745:ASN:ND2	1:D:773:GLN:OE1	2.48	0.44
1:D:4844:ARG:HH12	1:D:4848:ASP:HB2	1.83	0.44
1:A:419:ILE:HG12	1:A:489:PHE:CE1	2.52	0.44
1:A:1626:GLN:O	1:A:1687:TYR:OH	2.32	0.44
1:A:4627:ILE:O	1:A:4631:TRP:N	2.48	0.44
1:A:4844:ARG:HH12	1:A:4848:ASP:HB2	1.83	0.44
1:A:4869:ASP:O	1:A:4873:GLU:N	2.49	0.44
1:B:848:ARG:HB2	1:B:1603:PHE:HZ	1.81	0.44
1:B:4747:ILE:HG13	1:B:4754:LEU:HD22	1.99	0.44
1:B:4844:ARG:HH12	1:B:4848:ASP:HB2	1.83	0.44
1:B:4845:ILE:O	1:B:4849:ILE:N	2.44	0.44
1:C:3737:ALA:O	1:C:3740:MET:HG2	2.17	0.44
1:D:1170:GLU:O	1:D:1172:THR:N	2.50	0.44
1:D:2121:LEU:O	1:D:2125:GLY:N	2.47	0.44
1:D:4203:LEU:O	1:D:4207:ILE:HG12	2.17	0.44
1:D:4632:ASP:OD1	1:D:4709:TRP:NE1	2.42	0.44
1:A:308:LEU:HD22	1:A:370:LEU:HD12	1.98	0.44
1:A:3859:LEU:HD22	1:A:3871:ILE:HG21	1.98	0.44
1:B:766:ILE:HB	1:B:779:PHE:HB2	1.99	0.44
1:B:1799:VAL:O	1:B:1803:SER:N	2.46	0.44
1:B:2525:VAL:HG13	1:B:2528:LEU:HD12	1.99	0.44
1:B:3859:LEU:HD22	1:B:3871:ILE:HG21	1.98	0.44
1:B:3925:ILE:HG21	1:B:3925:ILE:HD13	1.70	0.44
1:B:4013:MET:O	1:B:4017:PHE:N	2.46	0.44
1:B:4588:ILE:HG22	1:B:4723:LEU:HD23	1.99	0.44
1:C:289:ILE:HG22	1:C:354:ILE:HD12	1.99	0.44
1:C:695:VAL:O	1:C:725:TYR:N	2.49	0.44
1:C:1087:ILE:HG23	1:C:1128:LEU:HD12	2.00	0.44
1:D:466:PRO:HB3	1:D:478:ARG:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:ASN:ND2	1:A:773:GLN:OE1	2.48	0.44
1:A:4747:ILE:HG13	1:A:4754:LEU:HD22	1.99	0.44
1:B:466:PRO:HB3	1:B:478:ARG:HG2	1.99	0.44
1:B:4203:LEU:O	1:B:4207:ILE:HG12	2.17	0.44
1:D:308:LEU:HD22	1:D:370:LEU:HD12	1.98	0.44
1:D:695:VAL:O	1:D:725:TYR:N	2.49	0.44
1:A:2390:MET:HG3	1:A:2465:HIS:CE1	2.53	0.44
1:A:3767:LEU:O	1:A:3770:GLY:N	2.51	0.44
1:A:4203:LEU:O	1:A:4207:ILE:HG12	2.17	0.44
1:B:646:THR:OG1	1:B:1684:GLN:NE2	2.49	0.44
1:C:848:ARG:HB2	1:C:1603:PHE:HZ	1.81	0.44
1:C:2390:MET:HG3	1:C:2465:HIS:CE1	2.53	0.44
1:C:4130:PHE:O	1:C:4134:LEU:N	2.45	0.44
1:D:1011:ARG:HB3	1:D:1032:LEU:HD21	2.00	0.44
1:D:1934:VAL:O	1:D:1938:GLN:N	2.43	0.44
1:D:4747:ILE:HG13	1:D:4754:LEU:HD22	1.99	0.44
1:A:466:PRO:HB3	1:A:478:ARG:HG2	1.99	0.44
1:A:1136:ALA:HB3	1:A:1145:TRP:HB2	2.00	0.44
1:A:1602:GLN:HB3	1:A:1604:LEU:HD12	1.99	0.44
1:A:2121:LEU:O	1:A:2125:GLY:N	2.47	0.44
1:A:2832:VAL:O	1:A:2895:LYS:NZ	2.45	0.44
1:B:843:GLU:HA	1:B:848:ARG:HG2	1.98	0.44
1:C:299:HIS:NE2	1:C:301:THR:OG1	2.46	0.44
1:C:308:LEU:HD22	1:C:370:LEU:HD12	1.98	0.44
1:C:2525:VAL:HG13	1:C:2528:LEU:HD12	1.99	0.44
1:D:237:LEU:N	1:D:404:ASN:O	2.49	0.44
1:D:1087:ILE:HG23	1:D:1128:LEU:HD12	2.00	0.44
1:D:2390:MET:HG3	1:D:2465:HIS:CE1	2.53	0.44
1:D:3952:PHE:HB3	1:D:3976:GLN:HE22	1.82	0.44
1:D:4142:SER:HB3	1:D:4940:TYR:CE1	2.52	0.44
1:A:1664:VAL:HG12	1:A:1672:VAL:HG11	2.00	0.44
1:A:1799:VAL:O	1:A:1803:SER:N	2.46	0.44
1:A:4867:ILE:HD12	1:A:4867:ILE:HG23	1.80	0.44
1:B:123:HIS:CD2	1:B:126:SER:H	2.34	0.44
1:B:655:MET:HG2	1:B:836:HIS:HA	2.00	0.44
1:B:1092:LYS:H	1:B:1250:TRP:HZ3	1.66	0.44
1:B:4632:ASP:OD1	1:B:4709:TRP:NE1	2.42	0.44
1:C:123:HIS:CD2	1:C:126:SER:H	2.34	0.44
1:C:655:MET:HG2	1:C:836:HIS:HA	2.00	0.44
1:C:4732:LEU:O	1:C:4736:ASN:N	2.44	0.44
1:B:196:TYR:O	1:B:201:LEU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1626:GLN:O	1:B:1687:TYR:OH	2.32	0.44
1:B:2390:MET:HG3	1:B:2465:HIS:CE1	2.53	0.44
1:B:2732:LYS:HD2	1:B:2732:LYS:HA	1.82	0.44
1:B:4500:PHE:HA	1:B:4503:MET:HB2	2.00	0.44
1:B:4732:LEU:O	1:B:4736:ASN:N	2.44	0.44
1:C:4500:PHE:HA	1:C:4503:MET:HB2	2.00	0.44
1:D:1664:VAL:HG12	1:D:1672:VAL:HG11	2.00	0.44
1:D:1720:MET:HE2	1:D:2128:ARG:HD2	2.00	0.44
1:D:4036:TYR:HE2	1:D:4048:ASP:HB3	1.82	0.44
1:A:289:ILE:HG22	1:A:354:ILE:HD12	1.99	0.44
1:A:655:MET:HG2	1:A:836:HIS:HA	2.00	0.44
1:B:4610:LYS:O	1:B:4615:GLY:N	2.51	0.44
1:D:196:TYR:O	1:D:201:LEU:N	2.51	0.44
1:D:3767:LEU:O	1:D:3770:GLY:N	2.51	0.44
1:A:196:TYR:O	1:A:201:LEU:N	2.51	0.43
1:A:1449:ASP:OD1	1:A:1449:ASP:N	2.51	0.43
1:A:4178:VAL:HG11	1:A:4881:VAL:HA	1.99	0.43
1:A:4610:LYS:O	1:A:4615:GLY:N	2.51	0.43
1:B:3743:GLN:NE2	1:B:3781:TYR:OH	2.43	0.43
1:B:4739:PHE:HD1	1:B:4739:PHE:HA	1.76	0.43
1:C:1011:ARG:HB3	1:C:1032:LEU:HD21	2.00	0.43
1:D:646:THR:OG1	1:D:1684:GLN:NE2	2.49	0.43
1:D:655:MET:HG2	1:D:836:HIS:HA	2.00	0.43
1:D:4610:LYS:O	1:D:4615:GLY:N	2.51	0.43
1:A:908:ARG:HA	1:A:916:PRO:HD3	2.00	0.43
1:A:2426:SER:HB3	1:D:143:LEU:CD2	2.47	0.43
1:B:227:TYR:CE1	1:B:355:LYS:HG2	2.47	0.43
1:B:288:HIS:ND1	1:B:349:MET:O	2.43	0.43
1:B:289:ILE:HG22	1:B:354:ILE:HD12	1.99	0.43
1:C:758:CYS:SG	1:C:759:LEU:N	2.91	0.43
1:C:3859:LEU:HD22	1:C:3871:ILE:HG21	1.98	0.43
1:C:4759:SER:O	1:C:4763:HIS:ND1	2.30	0.43
1:C:4763:HIS:CE1	1:C:4870:ALA:HB1	2.53	0.43
1:C:4869:ASP:O	1:C:4873:GLU:N	2.49	0.43
1:D:170:SER:OG	1:D:171:GLU:N	2.49	0.43
1:D:758:CYS:SG	1:D:759:LEU:N	2.91	0.43
1:D:908:ARG:HA	1:D:916:PRO:HD3	2.00	0.43
1:D:1602:GLN:HB3	1:D:1604:LEU:HD12	1.99	0.43
1:D:2525:VAL:HG13	1:D:2528:LEU:HD12	1.99	0.43
1:D:4763:HIS:CE1	1:D:4870:ALA:HB1	2.53	0.43
1:A:143:LEU:CD2	1:B:2426:SER:HB3	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:HB2	1:B:2419:ARG:HH22	1.84	0.43
1:A:1720:MET:HE2	1:A:2128:ARG:HD2	2.00	0.43
1:A:2419:ARG:HH22	1:D:189:GLU:HB2	1.84	0.43
1:A:4763:HIS:CE1	1:A:4870:ALA:HB1	2.53	0.43
1:B:908:ARG:HA	1:B:916:PRO:HD3	2.00	0.43
1:B:1664:VAL:HG12	1:B:1672:VAL:HG11	2.00	0.43
1:C:466:PRO:HB3	1:C:478:ARG:HG2	1.99	0.43
1:C:4178:VAL:HG11	1:C:4881:VAL:HA	1.99	0.43
1:A:462:TYR:O	1:A:485:ARG:NH1	2.51	0.43
1:A:758:CYS:SG	1:A:759:LEU:N	2.91	0.43
1:A:1092:LYS:H	1:A:1250:TRP:HZ3	1.66	0.43
1:A:1654:HIS:O	1:A:1657:THR:OG1	2.26	0.43
1:A:4036:TYR:HE2	1:A:4048:ASP:HB3	1.82	0.43
1:A:4514:ILE:HG21	1:A:4740:PHE:CE2	2.52	0.43
1:A:4523:VAL:HG22	1:D:4808:ASP:OD2	2.19	0.43
1:B:170:SER:OG	1:B:171:GLU:N	2.49	0.43
1:B:189:GLU:HB2	1:C:2419:ARG:HH22	1.84	0.43
1:C:462:TYR:O	1:C:485:ARG:NH1	2.51	0.43
1:C:1090:ALA:HB3	1:C:1203:PRO:HD2	2.00	0.43
1:D:1136:ALA:HB3	1:D:1145:TRP:HB2	2.00	0.43
1:A:237:LEU:N	1:A:404:ASN:O	2.49	0.43
1:A:3737:ALA:O	1:A:3740:MET:HG2	2.17	0.43
1:A:4791:ARG:HD2	1:A:4808:ASP:HB2	2.00	0.43
1:A:4924:MET:O	1:A:4928:ASN:HB2	2.18	0.43
1:B:745:ASN:ND2	1:B:773:GLN:OE1	2.48	0.43
1:B:758:CYS:SG	1:B:759:LEU:N	2.91	0.43
1:B:1449:ASP:OD1	1:B:1449:ASP:N	2.51	0.43
1:B:4763:HIS:CE1	1:B:4870:ALA:HB1	2.53	0.43
1:B:4809:ASP:O	1:B:4813:CYS:N	2.39	0.43
1:C:189:GLU:HB2	1:D:2419:ARG:HH22	1.84	0.43
1:C:4036:TYR:HE2	1:C:4048:ASP:HB3	1.82	0.43
1:D:1220:ASP:O	1:D:1223:THR:N	2.35	0.43
1:A:335:LYS:NZ	1:A:398:HIS:O	2.44	0.43
1:A:1165:MET:HB2	1:A:1174:MET:HB2	2.01	0.43
1:A:2440:ALA:HB2	1:A:2466:LYS:HD2	2.01	0.43
1:A:4500:PHE:HA	1:A:4503:MET:HB2	2.00	0.43
1:A:4808:ASP:OD2	1:B:4523:VAL:HG22	2.19	0.43
1:B:1011:ARG:HB3	1:B:1032:LEU:HD21	2.00	0.43
1:B:1087:ILE:HG23	1:B:1128:LEU:HD12	2.00	0.43
1:C:604:HIS:HA	1:C:1588:VAL:HB	2.01	0.43
1:C:691:THR:HB	1:C:796:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:832:LEU:O	1:C:1614:ARG:NH1	2.51	0.43
1:C:1092:LYS:H	1:C:1250:TRP:HZ3	1.66	0.43
1:C:4739:PHE:HD1	1:C:4739:PHE:HA	1.76	0.43
1:C:4844:ARG:HH12	1:C:4848:ASP:HB2	1.83	0.43
1:D:691:THR:HB	1:D:796:ALA:HB2	2.01	0.43
1:D:1719:LEU:HD21	1:D:1830:ILE:HD13	2.01	0.43
1:A:532:SER:HA	1:A:535:GLU:HB3	2.01	0.43
1:A:1011:ARG:HB3	1:A:1032:LEU:HD21	2.00	0.43
1:B:1136:ALA:HB3	1:B:1145:TRP:HB2	2.00	0.43
1:B:1790:LYS:O	1:B:1794:MET:N	2.44	0.43
1:B:3952:PHE:HB3	1:B:3976:GLN:HE22	1.82	0.43
1:B:4178:VAL:HG11	1:B:4881:VAL:HA	1.99	0.43
1:C:196:TYR:O	1:C:201:LEU:N	2.51	0.43
1:C:1719:LEU:HD21	1:C:1830:ILE:HD13	2.01	0.43
1:C:2832:VAL:O	1:C:2895:LYS:NZ	2.45	0.43
1:C:4610:LYS:O	1:C:4615:GLY:N	2.51	0.43
1:C:4791:ARG:HD2	1:C:4808:ASP:HB2	2.00	0.43
1:C:4845:ILE:O	1:C:4849:ILE:N	2.44	0.43
1:D:4725:TRP:O	1:D:4729:MET:HG2	2.19	0.43
1:A:1090:ALA:HB3	1:A:1203:PRO:HD2	2.00	0.43
1:A:1719:LEU:HD21	1:A:1830:ILE:HD13	2.01	0.43
1:B:1090:ALA:HB3	1:B:1203:PRO:HD2	2.00	0.43
1:C:745:ASN:ND2	1:C:773:GLN:OE1	2.48	0.43
1:C:1091:GLU:HB3	1:C:1094:TYR:HD2	1.84	0.43
1:C:1449:ASP:OD1	1:C:1449:ASP:N	2.51	0.43
1:C:1664:VAL:HG12	1:C:1672:VAL:HG11	2.00	0.43
1:C:1733:THR:HG22	1:C:1755:THR:HB	2.00	0.43
1:C:2102:ALA:O	1:C:2106:THR:N	2.47	0.43
1:C:4514:ILE:HG21	1:C:4740:PHE:CE2	2.52	0.43
1:C:4571:PRO:O	1:C:4575:ILE:N	2.49	0.43
1:D:462:TYR:O	1:D:485:ARG:NH1	2.51	0.43
1:D:1165:MET:HB2	1:D:1174:MET:HB2	2.01	0.43
1:D:4178:VAL:HG11	1:D:4881:VAL:HA	1.99	0.43
1:D:4791:ARG:HD2	1:D:4808:ASP:HB2	2.00	0.43
1:A:629:GLN:OE1	1:A:1669:ASN:ND2	2.52	0.43
1:A:1170:GLU:O	1:A:1172:THR:N	2.50	0.43
1:A:1733:THR:HG22	1:A:1755:THR:HB	2.00	0.43
1:A:4725:TRP:O	1:A:4729:MET:HG2	2.19	0.43
1:B:4808:ASP:OD2	1:C:4523:VAL:HG22	2.19	0.43
1:C:1119:ARG:NH2	1:C:1196:ASP:O	2.48	0.43
1:C:1799:VAL:O	1:C:1803:SER:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3800:SER:OG	1:C:3801:CYS:N	2.47	0.43
1:A:832:LEU:O	1:A:1614:ARG:NH1	2.51	0.43
1:A:1087:ILE:HG23	1:A:1128:LEU:HD12	2.00	0.43
1:A:4809:ASP:O	1:A:4813:CYS:N	2.39	0.43
1:B:629:GLN:OE1	1:B:1669:ASN:ND2	2.52	0.43
1:B:1172:THR:HG22	1:B:1193:LYS:HG3	2.01	0.43
1:B:1719:LEU:HD21	1:B:1830:ILE:HD13	2.01	0.43
1:B:3767:LEU:O	1:B:3770:GLY:N	2.51	0.43
1:B:4791:ARG:HD2	1:B:4808:ASP:HB2	2.00	0.43
1:C:411:GLU:HA	1:C:414:ARG:HB2	2.01	0.43
1:C:1032:LEU:HD23	1:C:1032:LEU:HA	1.82	0.43
1:C:1790:LYS:O	1:C:1794:MET:N	2.44	0.43
1:C:2196:ASN:OD1	1:C:2199:ARG:NH1	2.52	0.43
1:C:4924:MET:O	1:C:4928:ASN:HB2	2.18	0.43
1:D:1090:ALA:HB3	1:D:1203:PRO:HD2	2.00	0.43
1:D:1733:THR:HG22	1:D:1755:THR:HB	2.00	0.43
1:D:2196:ASN:OD1	1:D:2199:ARG:NH1	2.52	0.43
1:D:4130:PHE:O	1:D:4134:LEU:N	2.45	0.43
1:D:4500:PHE:HA	1:D:4503:MET:HB2	2.00	0.43
1:D:4514:ILE:HG21	1:D:4740:PHE:CE2	2.52	0.43
1:D:4867:ILE:HD12	1:D:4867:ILE:HG23	1.80	0.43
1:D:4924:MET:O	1:D:4928:ASN:HB2	2.18	0.43
1:A:691:THR:HB	1:A:796:ALA:HB2	2.01	0.42
1:B:258:ARG:HA	1:B:316:LEU:HB2	2.01	0.42
1:B:565:LEU:HD11	1:B:603:LYS:HG2	2.01	0.42
1:B:832:LEU:O	1:B:1614:ARG:NH1	2.51	0.42
1:B:2102:ALA:O	1:B:2106:THR:N	2.47	0.42
1:B:3919:ASN:O	1:B:3922:THR:OG1	2.35	0.42
1:C:258:ARG:HA	1:C:316:LEU:HB2	2.01	0.42
1:C:565:LEU:HD11	1:C:603:LYS:HG2	2.01	0.42
1:D:2834:LEU:HG	1:D:2895:LYS:HZ3	1.84	0.42
1:A:1156:TRP:HB2	1:A:1160:ASP:HB2	2.01	0.42
1:B:462:TYR:O	1:B:485:ARG:NH1	2.51	0.42
1:B:604:HIS:HA	1:B:1588:VAL:HB	2.01	0.42
1:B:703:TYR:CZ	1:B:722:LEU:HD21	2.54	0.42
1:B:1091:GLU:HB3	1:B:1094:TYR:HD2	1.84	0.42
1:B:4514:ILE:HG21	1:B:4740:PHE:CE2	2.52	0.42
1:C:908:ARG:HA	1:C:916:PRO:HD3	2.00	0.42
1:C:1136:ALA:HB3	1:C:1145:TRP:HB2	2.00	0.42
1:C:4808:ASP:OD2	1:D:4523:VAL:HG22	2.19	0.42
1:D:604:HIS:HA	1:D:1588:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:629:GLN:OE1	1:D:1669:ASN:ND2	2.52	0.42
1:A:1172:THR:HG22	1:A:1193:LYS:HG3	2.01	0.42
1:A:4161:TRP:CD1	1:A:4201:MET:HE1	2.53	0.42
1:B:694:ARG:N	1:B:793:SER:O	2.45	0.42
1:B:1119:ARG:NH2	1:B:1196:ASP:O	2.48	0.42
1:B:1165:MET:HB2	1:B:1174:MET:HB2	2.01	0.42
1:C:703:TYR:CZ	1:C:722:LEU:HD21	2.54	0.42
1:D:532:SER:HA	1:D:535:GLU:HB3	2.01	0.42
1:D:1449:ASP:N	1:D:1449:ASP:OD1	2.51	0.42
1:D:3696:MET:O	1:D:3699:SER:OG	2.26	0.42
1:D:4161:TRP:CD1	1:D:4201:MET:HE1	2.53	0.42
1:A:355:LYS:HE3	1:A:355:LYS:HB3	1.94	0.42
1:A:585:ALA:HA	1:A:588:ILE:HD12	2.02	0.42
1:B:613:VAL:O	1:B:617:LEU:N	2.46	0.42
1:B:1733:THR:HG22	1:B:1755:THR:HB	2.00	0.42
1:B:4166:VAL:O	1:B:4170:LYS:N	2.52	0.42
1:C:189:GLU:HG3	1:D:2419:ARG:NH2	2.35	0.42
1:C:629:GLN:OE1	1:C:1669:ASN:ND2	2.52	0.42
1:C:3759:THR:O	1:C:3763:GLY:N	2.51	0.42
1:C:4725:TRP:O	1:C:4729:MET:HG2	2.19	0.42
1:D:585:ALA:HA	1:D:588:ILE:HD12	2.02	0.42
1:D:1092:LYS:H	1:D:1250:TRP:HZ3	1.66	0.42
1:A:2419:ARG:NH2	1:D:189:GLU:HG3	2.35	0.42
1:B:1570:LEU:O	1:B:1573:SER:OG	2.36	0.42
1:B:4924:MET:O	1:B:4928:ASN:HB2	2.18	0.42
1:C:243:GLU:OE2	1:C:389:ARG:NH1	2.53	0.42
1:C:565:LEU:HA	1:C:568:SER:HB2	2.02	0.42
1:C:4636:ILE:HG22	1:C:4671:LEU:HD22	2.02	0.42
1:D:116:GLY:N	1:D:162:ILE:O	2.45	0.42
1:D:123:HIS:CD2	1:D:126:SER:H	2.34	0.42
1:D:243:GLU:OE2	1:D:389:ARG:NH1	2.53	0.42
1:D:572:LEU:O	1:D:576:HIS:N	2.47	0.42
1:D:832:LEU:O	1:D:1614:ARG:NH1	2.51	0.42
1:D:1029:ASN:HA	1:D:1030:PRO:HD3	1.82	0.42
1:D:1091:GLU:HB3	1:D:1094:TYR:HD2	1.84	0.42
1:D:1682:GLU:HA	1:D:1685:LEU:HD13	2.02	0.42
1:A:190:ARG:HG2	1:A:207:PHE:CE1	2.55	0.42
1:A:2196:ASN:OD1	1:A:2199:ARG:NH1	2.52	0.42
1:B:1170:GLU:O	1:B:1172:THR:N	2.50	0.42
1:B:4725:TRP:O	1:B:4729:MET:HG2	2.19	0.42
1:C:1692:LYS:HA	1:C:1810:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3921:LEU:HD23	1:C:3921:LEU:HA	1.84	0.42
1:D:852:GLY:HA3	1:D:1086:ARG:HG3	2.01	0.42
1:D:1799:VAL:O	1:D:1803:SER:N	2.46	0.42
1:D:2326:ILE:HD13	1:D:2326:ILE:HA	1.83	0.42
1:A:123:HIS:CD2	1:A:126:SER:H	2.34	0.42
1:A:565:LEU:HA	1:A:568:SER:HB2	2.02	0.42
1:A:1730:THR:O	1:A:1733:THR:OG1	2.31	0.42
1:B:532:SER:HA	1:B:535:GLU:HB3	2.01	0.42
1:B:691:THR:HB	1:B:796:ALA:HB2	2.01	0.42
1:B:2440:ALA:HB2	1:B:2466:LYS:HD2	2.01	0.42
1:B:2834:LEU:HG	1:B:2895:LYS:HZ3	1.84	0.42
1:C:585:ALA:HA	1:C:588:ILE:HD12	2.02	0.42
1:C:2440:ALA:HB2	1:C:2466:LYS:HD2	2.01	0.42
1:C:3767:LEU:O	1:C:3770:GLY:N	2.51	0.42
1:C:3925:ILE:HG21	1:C:3925:ILE:HD13	1.70	0.42
1:D:565:LEU:HA	1:D:568:SER:HB2	2.02	0.42
1:D:1172:THR:HG22	1:D:1193:LYS:HG3	2.01	0.42
1:D:2440:ALA:HB2	1:D:2466:LYS:HD2	2.01	0.42
1:D:3759:THR:O	1:D:3763:GLY:N	2.51	0.42
1:D:3797:LEU:HD13	1:D:3840:LEU:HD11	2.02	0.42
1:D:3914:ALA:HB3	1:D:3975:LEU:HD11	2.02	0.42
1:A:189:GLU:HG3	1:B:2419:ARG:NH2	2.35	0.42
1:A:258:ARG:HA	1:A:316:LEU:HB2	2.01	0.42
1:A:4636:ILE:HG22	1:A:4671:LEU:HD22	2.02	0.42
1:B:1091:GLU:HA	1:B:1250:TRP:CZ3	2.55	0.42
1:B:1692:LYS:HA	1:B:1810:VAL:HG13	2.02	0.42
1:B:2326:ILE:HD13	1:B:2326:ILE:HA	1.83	0.42
1:C:776:GLN:HG2	1:C:1472:GLU:HA	2.01	0.42
1:D:190:ARG:HG2	1:D:207:PHE:CE1	2.55	0.42
1:D:258:ARG:HA	1:D:316:LEU:HB2	2.01	0.42
1:D:4636:ILE:HG22	1:D:4671:LEU:HD22	2.02	0.42
1:A:604:HIS:HA	1:A:1588:VAL:HB	2.01	0.42
1:A:1682:GLU:HA	1:A:1685:LEU:HD13	2.02	0.42
1:A:2102:ALA:O	1:A:2106:THR:N	2.47	0.42
1:A:4931:GLU:OE2	1:A:4942:TRP:NE1	2.53	0.42
1:B:243:GLU:OE2	1:B:389:ARG:NH1	2.53	0.42
1:B:565:LEU:HA	1:B:568:SER:HB2	2.02	0.42
1:B:4621:GLN:HE22	1:B:4633:ARG:HH12	1.68	0.42
1:C:1090:ALA:HA	1:C:1249:MET:HG2	2.02	0.42
1:C:1172:THR:HG22	1:C:1193:LYS:HG3	2.01	0.42
1:C:3797:LEU:HD13	1:C:3840:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:GLU:HA	1:D:414:ARG:HB2	2.01	0.42
1:D:674:TYR:OH	1:D:676:GLU:OE2	2.27	0.42
1:D:852:GLY:HA2	1:D:853:PRO:HA	1.69	0.42
1:D:4515:ASN:HD22	1:D:4518:LEU:HB2	1.85	0.42
1:A:565:LEU:HD11	1:A:603:LYS:HG2	2.01	0.42
1:A:852:GLY:HA3	1:A:1086:ARG:HG3	2.01	0.42
1:A:1091:GLU:HA	1:A:1250:TRP:CZ3	2.55	0.42
1:A:4621:GLN:HE22	1:A:4633:ARG:HH12	1.68	0.42
1:A:4739:PHE:HD1	1:A:4739:PHE:HA	1.76	0.42
1:B:614:LEU:HD23	1:B:617:LEU:HD12	2.01	0.42
1:B:1682:GLU:HA	1:B:1685:LEU:HD13	2.02	0.42
1:B:2196:ASN:OD1	1:B:2199:ARG:NH1	2.52	0.42
1:B:2858:LYS:HG3	1:B:2872:LEU:HD22	2.02	0.42
1:B:4636:ILE:HG22	1:B:4671:LEU:HD22	2.02	0.42
1:C:534:TYR:O	1:C:538:ALA:N	2.51	0.42
1:C:796:ALA:HB3	1:C:798:ILE:HG13	2.02	0.42
1:C:1156:TRP:HB2	1:C:1160:ASP:HB2	2.01	0.42
1:C:1165:MET:HB2	1:C:1174:MET:HB2	2.01	0.42
1:C:3914:ALA:HB3	1:C:3975:LEU:HD11	2.02	0.42
1:C:3919:ASN:O	1:C:3922:THR:OG1	2.35	0.42
1:D:796:ALA:HB3	1:D:798:ILE:HG13	2.02	0.42
1:D:2421:ARG:HA	1:D:2424:LEU:HB2	2.01	0.42
1:A:1029:ASN:HA	1:A:1030:PRO:HD3	1.82	0.41
1:A:3743:GLN:NE2	1:A:3781:TYR:OH	2.43	0.41
1:B:189:GLU:HG3	1:C:2419:ARG:NH2	2.35	0.41
1:B:190:ARG:HG2	1:B:207:PHE:CE1	2.55	0.41
1:B:712:GLU:OE2	1:B:1636:ASN:ND2	2.46	0.41
1:B:4852:PHE:CG	1:C:4823:ARG:HG2	2.55	0.41
1:C:4931:GLU:OE2	1:C:4942:TRP:NE1	2.53	0.41
1:D:565:LEU:HD11	1:D:603:LYS:HG2	2.01	0.41
1:D:614:LEU:HD23	1:D:617:LEU:HD12	2.01	0.41
1:D:1156:TRP:HB2	1:D:1160:ASP:HB2	2.01	0.41
1:A:703:TYR:CZ	1:A:722:LEU:HD21	2.54	0.41
1:A:4515:ASN:HD22	1:A:4518:LEU:HB2	1.85	0.41
1:B:585:ALA:HA	1:B:588:ILE:HD12	2.02	0.41
1:B:776:GLN:HG2	1:B:1472:GLU:HA	2.01	0.41
1:B:2421:ARG:HA	1:B:2424:LEU:HB2	2.01	0.41
1:B:3911:ILE:HD13	1:B:3911:ILE:HA	1.91	0.41
1:C:1682:GLU:HA	1:C:1685:LEU:HD13	2.02	0.41
1:C:4852:PHE:CG	1:D:4823:ARG:HG2	2.55	0.41
1:D:182:ILE:HD12	1:D:209:GLN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:703:TYR:CZ	1:D:722:LEU:HD21	2.54	0.41
1:D:1090:ALA:HA	1:D:1249:MET:HG2	2.02	0.41
1:D:1119:ARG:NH2	1:D:1196:ASP:O	2.48	0.41
1:D:1146:HIS:HB2	1:D:1192:PHE:HE1	1.85	0.41
1:D:4739:PHE:HD1	1:D:4739:PHE:HA	1.76	0.41
1:A:243:GLU:OE2	1:A:389:ARG:NH1	2.53	0.41
1:A:411:GLU:HA	1:A:414:ARG:HB2	2.01	0.41
1:A:725:TYR:OH	1:A:775:VAL:HG11	2.21	0.41
1:A:1091:GLU:HB3	1:A:1094:TYR:HD2	1.84	0.41
1:B:143:LEU:CD2	1:C:2426:SER:HB3	2.47	0.41
1:B:833:LYS:HA	1:B:1614:ARG:HH12	1.86	0.41
1:C:836:HIS:HB2	1:C:839:GLU:HG2	2.03	0.41
1:C:852:GLY:HA3	1:C:1086:ARG:HG3	2.01	0.41
1:C:1905:LEU:HD23	1:C:2081:LEU:HA	2.03	0.41
1:C:2858:LYS:HG3	1:C:2872:LEU:HD22	2.02	0.41
1:D:1692:LYS:HA	1:D:1810:VAL:HG13	2.02	0.41
1:A:796:ALA:HB3	1:A:798:ILE:HG13	2.02	0.41
1:A:1146:HIS:HB2	1:A:1192:PHE:HE1	1.85	0.41
1:A:1256:PRO:HB3	1:A:1597:SER:HA	2.02	0.41
1:A:3914:ALA:HB3	1:A:3975:LEU:HD11	2.02	0.41
1:A:4823:ARG:HG2	1:D:4852:PHE:CG	2.55	0.41
1:B:796:ALA:HB3	1:B:798:ILE:HG13	2.02	0.41
1:B:836:HIS:HB2	1:B:839:GLU:HG2	2.03	0.41
1:B:2160:PRO:HB3	1:B:2207:ILE:HD12	2.02	0.41
1:C:532:SER:HA	1:C:535:GLU:HB3	2.01	0.41
1:C:1256:PRO:HB3	1:C:1597:SER:HA	2.02	0.41
1:C:1934:VAL:O	1:C:1938:GLN:N	2.43	0.41
1:C:2884:ALA:HA	1:C:2887:ARG:HB3	2.03	0.41
1:C:3779:LEU:HD11	1:C:3783:LYS:HE2	2.03	0.41
1:D:244:CYS:SG	1:D:245:LEU:N	2.93	0.41
1:A:614:LEU:HD23	1:A:617:LEU:HD12	2.01	0.41
1:A:833:LYS:HA	1:A:1614:ARG:HH12	1.86	0.41
1:A:1090:ALA:HA	1:A:1249:MET:HG2	2.02	0.41
1:A:2421:ARG:HA	1:A:2424:LEU:HB2	2.01	0.41
1:A:2858:LYS:HG3	1:A:2872:LEU:HD22	2.02	0.41
1:A:3800:SER:OG	1:A:3801:CYS:N	2.47	0.41
1:B:852:GLY:HA3	1:B:1086:ARG:HG3	2.01	0.41
1:B:1090:ALA:HA	1:B:1249:MET:HG2	2.02	0.41
1:B:1137:PHE:HD1	1:B:1144:ARG:HB3	1.86	0.41
1:B:1905:LEU:HD23	1:B:2081:LEU:HA	2.03	0.41
1:B:2127:ILE:HD12	1:B:2127:ILE:HA	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2541:HIS:O	1:B:2545:LEU:N	2.49	0.41
1:C:244:CYS:SG	1:C:245:LEU:N	2.93	0.41
1:C:653:SER:OG	1:C:794:PHE:O	2.31	0.41
1:C:4161:TRP:CD1	1:C:4201:MET:HE1	2.53	0.41
1:D:725:TYR:OH	1:D:775:VAL:HG11	2.21	0.41
1:D:833:LYS:HA	1:D:1614:ARG:HH12	1.86	0.41
1:D:3743:GLN:NE2	1:D:3781:TYR:OH	2.43	0.41
1:A:1905:LEU:HD23	1:A:2081:LEU:HA	2.03	0.41
1:A:2732:LYS:HD2	1:A:2732:LYS:HA	1.82	0.41
1:A:3925:ILE:HG21	1:A:3925:ILE:HD13	1.70	0.41
1:A:4045:SER:HA	1:A:4078:THR:HG22	2.03	0.41
1:B:1156:TRP:HB2	1:B:1160:ASP:HB2	2.01	0.41
1:B:2884:ALA:HA	1:B:2887:ARG:HB3	2.03	0.41
1:C:182:ILE:HD12	1:C:209:GLN:HB3	2.02	0.41
1:C:3743:GLN:O	1:C:3746:SER:OG	2.32	0.41
1:D:288:HIS:ND1	1:D:349:MET:O	2.43	0.41
1:D:1091:GLU:HA	1:D:1250:TRP:CZ3	2.55	0.41
1:D:4621:GLN:HE22	1:D:4633:ARG:HH12	1.68	0.41
1:A:244:CYS:SG	1:A:245:LEU:N	2.93	0.41
1:A:1137:PHE:HD1	1:A:1144:ARG:HB3	1.86	0.41
1:A:1692:LYS:HA	1:A:1810:VAL:HG13	2.02	0.41
1:A:2154:LYS:HD3	1:A:2154:LYS:HA	1.90	0.41
1:A:3797:LEU:HD13	1:A:3840:LEU:HD11	2.02	0.41
1:B:3921:LEU:HA	1:B:3921:LEU:HD23	1.84	0.41
1:C:614:LEU:HD23	1:C:617:LEU:HD12	2.01	0.41
1:C:1132:GLU:HG2	1:C:1133:ARG:HG3	2.03	0.41
1:C:1170:GLU:O	1:C:1172:THR:N	2.50	0.41
1:C:2463:PRO:HD3	1:C:2516:ALA:HB2	2.02	0.41
1:D:534:TYR:CZ	1:D:571:ILE:HG13	2.56	0.41
1:D:613:VAL:O	1:D:617:LEU:N	2.46	0.41
1:D:3779:LEU:HD11	1:D:3783:LYS:HE2	2.03	0.41
1:D:3996:ILE:H	1:D:3996:ILE:HG22	1.64	0.41
1:A:182:ILE:HD12	1:A:209:GLN:HB3	2.02	0.41
1:A:534:TYR:CZ	1:A:571:ILE:HG13	2.56	0.41
1:A:650:ASN:HA	1:A:1626:GLN:HA	2.03	0.41
1:A:836:HIS:HB2	1:A:839:GLU:HG2	2.03	0.41
1:A:935:MET:O	1:A:939:THR:OG1	2.36	0.41
1:A:4852:PHE:CG	1:B:4823:ARG:HG2	2.55	0.41
1:B:534:TYR:CZ	1:B:571:ILE:HG13	2.56	0.41
1:B:3914:ALA:HB3	1:B:3975:LEU:HD11	2.02	0.41
1:C:299:HIS:N	1:C:304:LYS:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1029:ASN:HA	1:C:1030:PRO:HD3	1.82	0.41
1:C:1137:PHE:HD1	1:C:1144:ARG:HB3	1.86	0.41
1:C:2421:ARG:HA	1:C:2424:LEU:HB2	2.01	0.41
1:C:4872:GLY:C	1:D:4875:ARG:CZ	2.89	0.41
1:C:4894:ILE:HD12	1:C:4961:LYS:HE3	2.03	0.41
1:D:776:GLN:HG2	1:D:1472:GLU:HA	2.01	0.41
1:D:836:HIS:HB2	1:D:839:GLU:HG2	2.03	0.41
1:D:1256:PRO:HB3	1:D:1597:SER:HA	2.02	0.41
1:D:4045:SER:HA	1:D:4078:THR:HG22	2.03	0.41
1:A:551:PHE:HD1	1:A:551:PHE:HA	1.74	0.41
1:A:776:GLN:HG2	1:A:1472:GLU:HA	2.01	0.41
1:A:881:ILE:HG21	1:A:1062:TYR:CZ	2.56	0.41
1:A:2160:PRO:HB3	1:A:2207:ILE:HD12	2.02	0.41
1:B:182:ILE:HD12	1:B:209:GLN:HB3	2.02	0.41
1:B:244:CYS:SG	1:B:245:LEU:N	2.93	0.41
1:B:411:GLU:HA	1:B:414:ARG:HB2	2.01	0.41
1:B:725:TYR:OH	1:B:775:VAL:HG11	2.21	0.41
1:B:1132:GLU:HG2	1:B:1133:ARG:HG3	2.03	0.41
1:B:1146:HIS:HB2	1:B:1192:PHE:HE1	1.85	0.41
1:B:1699:ARG:HH22	1:B:1821:LEU:HD11	1.86	0.41
1:B:2829:MET:HE1	1:B:2896:PHE:HB2	2.03	0.41
1:B:3779:LEU:HD11	1:B:3783:LYS:HE2	2.03	0.41
1:B:4022:LEU:HA	1:B:4022:LEU:HD23	1.85	0.41
1:B:4161:TRP:CD1	1:B:4201:MET:HE1	2.53	0.41
1:B:4872:GLY:C	1:C:4875:ARG:CZ	2.89	0.41
1:C:190:ARG:HG2	1:C:207:PHE:CE1	2.55	0.41
1:C:534:TYR:CZ	1:C:571:ILE:HG13	2.56	0.41
1:C:650:ASN:HA	1:C:1626:GLN:HA	2.03	0.41
1:C:706:TYR:CD1	1:C:1253:LYS:HD2	2.56	0.41
1:C:1091:GLU:HA	1:C:1250:TRP:CZ3	2.55	0.41
1:C:3911:ILE:HD13	1:C:3911:ILE:HA	1.91	0.41
1:C:4515:ASN:HD22	1:C:4518:LEU:HB2	1.85	0.41
1:C:4621:GLN:HE22	1:C:4633:ARG:HH12	1.68	0.41
1:D:650:ASN:HA	1:D:1626:GLN:HA	2.03	0.41
1:D:881:ILE:HG21	1:D:1062:TYR:CZ	2.56	0.41
1:D:1132:GLU:HG2	1:D:1133:ARG:HG3	2.03	0.41
1:D:1652:LYS:HE2	1:D:1652:LYS:HB3	1.90	0.41
1:D:1716:THR:HA	1:D:1719:LEU:HD12	2.03	0.41
1:D:1905:LEU:HD23	1:D:2081:LEU:HA	2.03	0.41
1:D:2160:PRO:HB3	1:D:2207:ILE:HD12	2.02	0.41
1:D:4853:PHE:HA	1:D:4857:VAL:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ALA:HA	1:A:161:THR:HA	2.03	0.41
1:A:681:HIS:HA	1:A:751:THR:HG22	2.03	0.41
1:A:852:GLY:HA2	1:A:853:PRO:HA	1.69	0.41
1:A:1255:LEU:HA	1:A:1256:PRO:HD3	1.92	0.41
1:A:1716:THR:HA	1:A:1719:LEU:HD12	2.03	0.41
1:A:2463:PRO:HD3	1:A:2516:ALA:HB2	2.02	0.41
1:A:4823:ARG:HA	1:D:4852:PHE:CE1	2.53	0.41
1:B:1505:LEU:H	1:B:1523:ASN:HA	1.86	0.41
1:B:2463:PRO:HD3	1:B:2516:ALA:HB2	2.02	0.41
1:C:64:ILE:HG12	1:C:417:ARG:HH21	1.86	0.41
1:C:217:ILE:HG23	1:C:285:SER:HB3	2.03	0.41
1:C:506:HIS:HB2	1:C:561:ARG:NH1	2.36	0.41
1:C:833:LYS:HA	1:C:1614:ARG:HH12	1.86	0.41
1:C:1177:LEU:HD12	1:C:1177:LEU:HA	1.92	0.41
1:C:3808:ALA:HA	1:C:3811:ARG:HD2	2.03	0.41
1:C:4045:SER:HA	1:C:4078:THR:HG22	2.03	0.41
1:D:2884:ALA:HA	1:D:2887:ARG:HB3	2.03	0.41
1:A:1132:GLU:HG2	1:A:1133:ARG:HG3	2.03	0.40
1:A:1783:PRO:HB3	1:A:1786:ILE:HD12	2.02	0.40
1:A:4875:ARG:CZ	1:D:4872:GLY:C	2.89	0.40
1:B:534:TYR:O	1:B:538:ALA:N	2.51	0.40
1:B:681:HIS:HA	1:B:751:THR:HG22	2.03	0.40
1:B:3797:LEU:HD13	1:B:3840:LEU:HD11	2.02	0.40
1:B:4045:SER:HA	1:B:4078:THR:HG22	2.03	0.40
1:B:4515:ASN:HD22	1:B:4518:LEU:HB2	1.85	0.40
1:C:3642:ILE:HD12	1:C:3642:ILE:HG23	1.91	0.40
1:D:217:ILE:HG23	1:D:285:SER:HB3	2.03	0.40
1:D:1137:PHE:HD1	1:D:1144:ARG:HB3	1.86	0.40
1:D:2858:LYS:HG3	1:D:2872:LEU:HD22	2.02	0.40
1:D:4640:SER:HB3	1:D:4643:ASN:ND2	2.37	0.40
1:D:4931:GLU:OE2	1:D:4942:TRP:NE1	2.53	0.40
1:A:731:HIS:HE1	1:A:738:ALA:HB1	1.87	0.40
1:A:1699:ARG:HH22	1:A:1821:LEU:HD11	1.86	0.40
1:A:2270:LEU:HD21	1:A:2299:TYR:HB2	2.04	0.40
1:A:4166:VAL:O	1:A:4170:LYS:N	2.52	0.40
1:B:64:ILE:H	1:B:64:ILE:HG13	1.79	0.40
1:B:706:TYR:CD1	1:B:1253:LYS:HD2	2.56	0.40
1:B:1032:LEU:HD23	1:B:1032:LEU:HA	1.82	0.40
1:B:3808:ALA:HA	1:B:3811:ARG:HD2	2.03	0.40
1:B:4591:TYR:CE1	1:B:4595:LYS:HB2	2.57	0.40
1:B:4722:TYR:OH	1:B:4745:LEU:O	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4770:LEU:HD23	1:B:4770:LEU:HA	1.98	0.40
1:B:4853:PHE:HA	1:B:4857:VAL:HB	2.03	0.40
1:A:116:GLY:N	1:A:162:ILE:O	2.45	0.40
1:A:534:TYR:O	1:A:538:ALA:N	2.51	0.40
1:A:2069:ARG:HA	1:A:2069:ARG:HD3	1.92	0.40
1:A:3779:LEU:HD11	1:A:3783:LYS:HE2	2.03	0.40
1:B:217:ILE:HG23	1:B:285:SER:HB3	2.03	0.40
1:B:415:THR:O	1:B:419:ILE:HG13	2.22	0.40
1:B:2270:LEU:HD21	1:B:2299:TYR:HB2	2.04	0.40
1:B:4873:GLU:HA	1:C:4875:ARG:HH11	1.68	0.40
1:C:681:HIS:HA	1:C:751:THR:HG22	2.03	0.40
1:C:725:TYR:OH	1:C:775:VAL:HG11	2.21	0.40
1:C:3777:LYS:HE3	1:C:3777:LYS:HB2	1.94	0.40
1:C:4640:SER:HB3	1:C:4643:ASN:ND2	2.37	0.40
1:D:506:HIS:HB2	1:D:561:ARG:NH1	2.36	0.40
1:D:2775:PRO:HB2	1:D:2889:LYS:NZ	2.36	0.40
1:A:628:ASN:O	1:A:632:ILE:HG12	2.22	0.40
1:A:2834:LEU:HG	1:A:2895:LYS:HZ3	1.87	0.40
1:A:4852:PHE:CE1	1:B:4823:ARG:HA	2.53	0.40
1:B:551:PHE:HD1	1:B:551:PHE:HA	1.74	0.40
1:B:650:ASN:HA	1:B:1626:GLN:HA	2.03	0.40
1:B:1256:PRO:HB3	1:B:1597:SER:HA	2.02	0.40
1:B:1716:THR:HA	1:B:1719:LEU:HD12	2.03	0.40
1:B:1729:MET:HG2	1:B:2110:ASN:HA	2.03	0.40
1:B:2775:PRO:HB2	1:B:2889:LYS:NZ	2.36	0.40
1:B:3747:ALA:O	1:B:3749:LYS:HD2	2.22	0.40
1:C:881:ILE:HG21	1:C:1062:TYR:CZ	2.56	0.40
1:C:1146:HIS:HB2	1:C:1192:PHE:HE1	1.85	0.40
1:C:1783:PRO:HB3	1:C:1786:ILE:HD12	2.02	0.40
1:C:2270:LEU:HD21	1:C:2299:TYR:HB2	2.04	0.40
1:C:3886:ILE:HD12	1:C:3886:ILE:HG23	1.92	0.40
1:D:628:ASN:O	1:D:632:ILE:HG12	2.22	0.40
1:D:694:ARG:N	1:D:793:SER:O	2.45	0.40
1:D:706:TYR:CD1	1:D:1253:LYS:HD2	2.56	0.40
1:D:731:HIS:HE1	1:D:738:ALA:HB1	1.87	0.40
1:D:3756:VAL:O	1:D:3759:THR:OG1	2.31	0.40
1:A:506:HIS:HB2	1:A:561:ARG:NH1	2.36	0.40
1:A:3747:ALA:O	1:A:3749:LYS:HD2	2.22	0.40
1:A:3808:ALA:HA	1:A:3811:ARG:HD2	2.03	0.40
1:A:3919:ASN:O	1:A:3922:THR:OG1	2.35	0.40
1:A:3921:LEU:HA	1:A:3921:LEU:HD23	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3988:GLU:HB2	1:A:4937:GLN:NE2	2.37	0.40
1:A:4640:SER:HB3	1:A:4643:ASN:ND2	2.37	0.40
1:A:4804:ASP:OD1	1:A:4804:ASP:N	2.54	0.40
1:B:64:ILE:HG12	1:B:417:ARG:HH21	1.86	0.40
1:B:116:GLY:N	1:B:162:ILE:O	2.45	0.40
1:B:189:GLU:CD	1:C:2419:ARG:CZ	2.90	0.40
1:B:628:ASN:O	1:B:632:ILE:HG12	2.22	0.40
1:B:894:VAL:HG11	1:B:976:TYR:HD2	1.87	0.40
1:B:2788:TRP:HH2	1:B:2844:MET:HB2	1.87	0.40
1:B:3993:ASN:HD22	1:B:4110:MET:HG3	1.87	0.40
1:C:49:LEU:HD21	1:C:203:VAL:HG23	2.04	0.40
1:C:118:ALA:HA	1:C:161:THR:HA	2.03	0.40
1:C:894:VAL:HG11	1:C:976:TYR:HD2	1.87	0.40
1:C:1255:LEU:HA	1:C:1256:PRO:HD3	1.92	0.40
1:C:2160:PRO:HB3	1:C:2207:ILE:HD12	2.02	0.40
1:C:3993:ASN:HD22	1:C:4110:MET:HG3	1.87	0.40
1:C:4722:TYR:OH	1:C:4745:LEU:O	2.40	0.40
1:D:1783:PRO:HB3	1:D:1786:ILE:HD12	2.02	0.40
1:D:3808:ALA:HA	1:D:3811:ARG:HD2	2.03	0.40
1:D:4894:ILE:HD12	1:D:4961:LYS:HE3	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	3289/4968 (66%)	2983 (91%)	285 (9%)	21 (1%)	25	65
1	B	3289/4968 (66%)	2983 (91%)	285 (9%)	21 (1%)	25	65
1	C	3289/4968 (66%)	2983 (91%)	285 (9%)	21 (1%)	25	65
1	D	3289/4968 (66%)	2983 (91%)	285 (9%)	21 (1%)	25	65
All	All	13156/19872 (66%)	11932 (91%)	1140 (9%)	84 (1%)	29	65

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4071	ALA
1	B	4071	ALA
1	C	4071	ALA
1	D	4071	ALA
1	A	730	LEU
1	A	1580	PRO
1	A	3802	SER
1	A	4164	PRO
1	A	4916	LEU
1	B	730	LEU
1	B	1580	PRO
1	B	3802	SER
1	B	4164	PRO
1	B	4916	LEU
1	C	730	LEU
1	C	1580	PRO
1	C	3802	SER
1	C	4164	PRO
1	C	4916	LEU
1	D	730	LEU
1	D	1580	PRO
1	D	3802	SER
1	D	4164	PRO
1	D	4916	LEU
1	A	1581	GLN
1	A	1809	PRO
1	A	2075	VAL
1	A	3805	ASP
1	A	4030	SER
1	A	4646	TRP
1	B	1581	GLN
1	B	1809	PRO
1	B	2075	VAL
1	B	3805	ASP
1	B	4030	SER
1	B	4646	TRP
1	C	1581	GLN
1	C	1809	PRO
1	C	2075	VAL
1	C	3805	ASP
1	C	4030	SER
1	C	4646	TRP

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Mol	Chain	Res	Type
1	D	1581	GLN
1	D	1809	PRO
1	D	2075	VAL
1	D	3805	ASP
1	D	4030	SER
1	D	4646	TRP
1	A	819	TYR
1	A	980	PRO
1	A	3804	LEU
1	B	819	TYR
1	B	980	PRO
1	B	3804	LEU
1	C	819	TYR
1	C	980	PRO
1	C	3804	LEU
1	D	819	TYR
1	D	980	PRO
1	D	3804	LEU
1	A	792	VAL
1	B	792	VAL
1	C	792	VAL
1	D	792	VAL
1	A	853	PRO
1	A	1848	PRO
1	B	853	PRO
1	B	1848	PRO
1	C	853	PRO
1	C	1848	PRO
1	D	853	PRO
1	D	1848	PRO
1	A	1476	VAL
1	A	2329	PRO
1	A	4163	LYS
1	B	1476	VAL
1	B	2329	PRO
1	B	4163	LYS
1	C	1476	VAL
1	C	2329	PRO
1	C	4163	LYS
1	D	1476	VAL
1	D	2329	PRO
1	D	4163	LYS

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	2659/4355 (61%)	2628 (99%)	31 (1%)	71	84
1	B	2658/4355 (61%)	2627 (99%)	31 (1%)	71	84
1	C	2659/4355 (61%)	2627 (99%)	32 (1%)	71	84
1	D	2660/4355 (61%)	2628 (99%)	32 (1%)	71	84
All	All	10636/17420 (61%)	10510 (99%)	126 (1%)	72	84

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	84	ASN
1	A	298	ARG
1	A	420	ARG
1	A	439	LYS
1	A	527	LYS
1	A	531	ASN
1	A	628	ASN
1	A	658	ASN
1	A	841	LYS
1	A	854	THR
1	A	925	PRO
1	A	990	PRO
1	A	1054	VAL
1	A	1089	ARG
1	A	1761	MET
1	A	2211	ASN
1	A	3722	LYS
1	A	3813	ASN
1	A	3906	ASN
1	A	4131	GLN
1	A	4136	ARG
1	A	4170	LYS
1	A	4171	ARG

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Mol	Chain	Res	Type
1	A	4179	ASN
1	A	4499	ASN
1	A	4515	ASN
1	A	4652	ARG
1	A	4781	LEU
1	A	4875	ARG
1	A	4879	GLU
1	B	44	ASN
1	B	84	ASN
1	B	298	ARG
1	B	420	ARG
1	B	439	LYS
1	B	527	LYS
1	B	531	ASN
1	B	628	ASN
1	B	658	ASN
1	B	841	LYS
1	B	854	THR
1	B	925	PRO
1	B	990	PRO
1	B	1054	VAL
1	B	1089	ARG
1	B	1761	MET
1	B	2211	ASN
1	B	3722	LYS
1	B	3813	ASN
1	B	3906	ASN
1	B	4131	GLN
1	B	4136	ARG
1	B	4170	LYS
1	B	4171	ARG
1	B	4179	ASN
1	B	4499	ASN
1	B	4515	ASN
1	B	4652	ARG
1	B	4781	LEU
1	B	4875	ARG
1	B	4879	GLU
1	C	44	ASN
1	C	84	ASN
1	C	298	ARG
1	C	420	ARG

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Mol	Chain	Res	Type
1	C	439	LYS
1	C	527	LYS
1	C	531	ASN
1	C	628	ASN
1	C	658	ASN
1	C	841	LYS
1	C	854	THR
1	C	925	PRO
1	C	950	VAL
1	C	990	PRO
1	C	1054	VAL
1	C	1089	ARG
1	C	1761	MET
1	C	2211	ASN
1	C	3722	LYS
1	C	3813	ASN
1	C	3906	ASN
1	C	4131	GLN
1	C	4136	ARG
1	C	4170	LYS
1	C	4171	ARG
1	C	4179	ASN
1	C	4499	ASN
1	C	4515	ASN
1	C	4652	ARG
1	C	4781	LEU
1	C	4875	ARG
1	C	4879	GLU
1	D	44	ASN
1	D	84	ASN
1	D	298	ARG
1	D	420	ARG
1	D	439	LYS
1	D	527	LYS
1	D	531	ASN
1	D	628	ASN
1	D	658	ASN
1	D	841	LYS
1	D	854	THR
1	D	925	PRO
1	D	950	VAL
1	D	990	PRO

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Mol	Chain	Res	Type
1	D	1054	VAL
1	D	1089	ARG
1	D	1761	MET
1	D	2211	ASN
1	D	3722	LYS
1	D	3813	ASN
1	D	3906	ASN
1	D	4131	GLN
1	D	4136	ARG
1	D	4170	LYS
1	D	4171	ARG
1	D	4179	ASN
1	D	4499	ASN
1	D	4515	ASN
1	D	4652	ARG
1	D	4781	LEU
1	D	4875	ARG
1	D	4879	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (156) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	84	ASN
1	A	123	HIS
1	A	293	GLN
1	A	364	GLN
1	A	375	GLN
1	A	476	GLN
1	A	531	ASN
1	A	593	HIS
1	A	604	HIS
1	A	628	ASN
1	A	1267	HIS
1	A	1294	ASN
1	A	1602	GLN
1	A	1631	HIS
1	A	1684	GLN
1	A	1722	ASN
1	A	1835	HIS
1	A	2090	HIS
1	A	2212	GLN

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Mol	Chain	Res	Type
1	A	2225	ASN
1	A	2251	ASN
1	A	2310	ASN
1	A	3856	GLN
1	A	3906	ASN
1	A	3916	GLN
1	A	3926	GLN
1	A	3950	HIS
1	A	3956	GLN
1	A	3961	GLN
1	A	3976	GLN
1	A	3993	ASN
1	A	4179	ASN
1	A	4499	ASN
1	A	4515	ASN
1	A	4621	GLN
1	A	4914	HIS
1	A	4962	GLN
1	B	23	GLN
1	B	44	ASN
1	B	84	ASN
1	B	123	HIS
1	B	293	GLN
1	B	364	GLN
1	B	375	GLN
1	B	476	GLN
1	B	531	ASN
1	B	593	HIS
1	B	604	HIS
1	B	628	ASN
1	B	1267	HIS
1	B	1294	ASN
1	B	1440	ASN
1	B	1602	GLN
1	B	1631	HIS
1	B	1684	GLN
1	B	1722	ASN
1	B	1835	HIS
1	B	2090	HIS
1	B	2212	GLN
1	B	2225	ASN
1	B	2251	ASN

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Mol	Chain	Res	Type
1	B	2310	ASN
1	B	2730	HIS
1	B	3856	GLN
1	B	3906	ASN
1	B	3916	GLN
1	B	3926	GLN
1	B	3956	GLN
1	B	3961	GLN
1	B	3976	GLN
1	B	3993	ASN
1	B	4179	ASN
1	B	4499	ASN
1	B	4515	ASN
1	B	4621	GLN
1	B	4914	HIS
1	B	4962	GLN
1	C	23	GLN
1	C	44	ASN
1	C	84	ASN
1	C	123	HIS
1	C	293	GLN
1	C	364	GLN
1	C	375	GLN
1	C	476	GLN
1	C	531	ASN
1	C	593	HIS
1	C	604	HIS
1	C	628	ASN
1	C	1267	HIS
1	C	1294	ASN
1	C	1440	ASN
1	C	1602	GLN
1	C	1631	HIS
1	C	1684	GLN
1	C	1691	ASN
1	C	1722	ASN
1	C	1835	HIS
1	C	2090	HIS
1	C	2212	GLN
1	C	2225	ASN
1	C	2251	ASN
1	C	2310	ASN

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Mol	Chain	Res	Type
1	C	2730	HIS
1	C	3856	GLN
1	C	3906	ASN
1	C	3916	GLN
1	C	3926	GLN
1	C	3956	GLN
1	C	3961	GLN
1	C	3976	GLN
1	C	3993	ASN
1	C	4179	ASN
1	C	4499	ASN
1	C	4515	ASN
1	C	4621	GLN
1	C	4914	HIS
1	C	4962	GLN
1	D	44	ASN
1	D	84	ASN
1	D	123	HIS
1	D	293	GLN
1	D	364	GLN
1	D	375	GLN
1	D	476	GLN
1	D	531	ASN
1	D	593	HIS
1	D	604	HIS
1	D	628	ASN
1	D	1267	HIS
1	D	1294	ASN
1	D	1602	GLN
1	D	1631	HIS
1	D	1684	GLN
1	D	1722	ASN
1	D	1835	HIS
1	D	2090	HIS
1	D	2212	GLN
1	D	2225	ASN
1	D	2251	ASN
1	D	2730	HIS
1	D	3856	GLN
1	D	3906	ASN
1	D	3916	GLN
1	D	3926	GLN

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Mol	Chain	Res	Type
1	D	3956	GLN
1	D	3961	GLN
1	D	3976	GLN
1	D	3993	ASN
1	D	4179	ASN
1	D	4499	ASN
1	D	4515	ASN
1	D	4621	GLN
1	D	4914	HIS
1	D	4962	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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 ⓘ

There are no chain breaks in this entry.

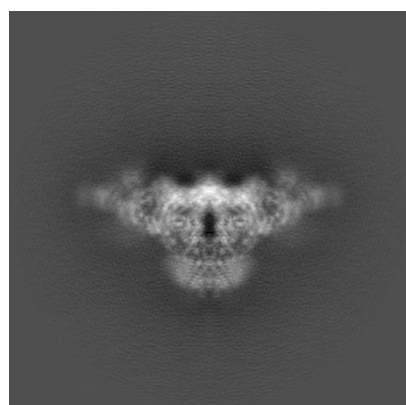
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9528. These allow visual inspection of the internal detail of the map and identification of artifacts.

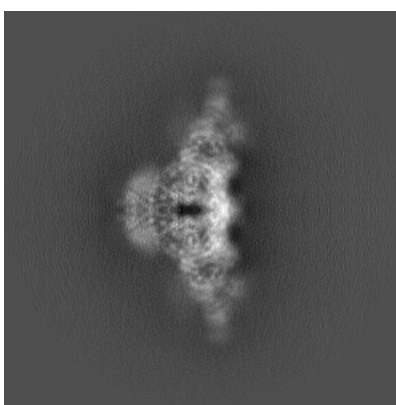
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

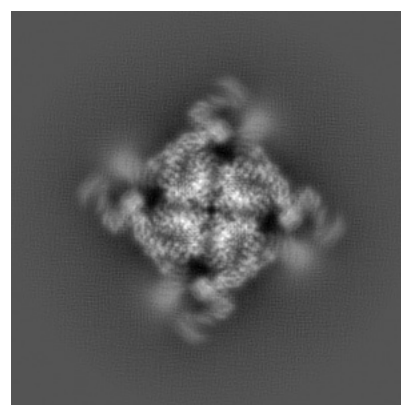
6.1.1 Primary map



X



Y

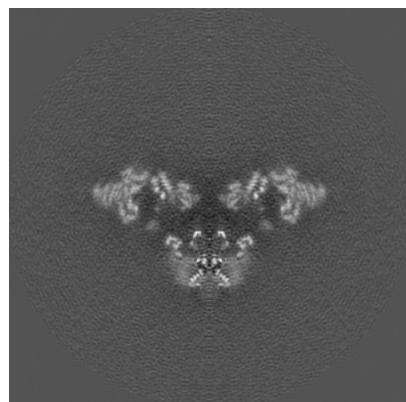


Z

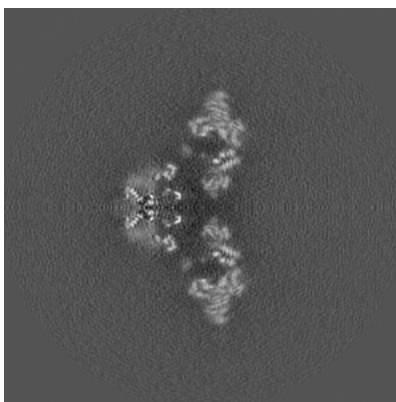
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

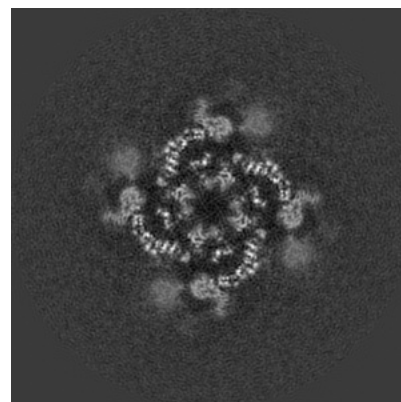
6.2.1 Primary map



X Index: 260



Y Index: 260

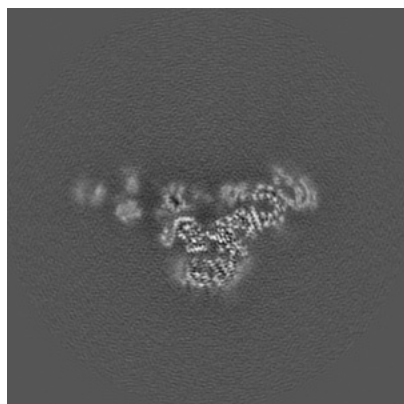


Z Index: 260

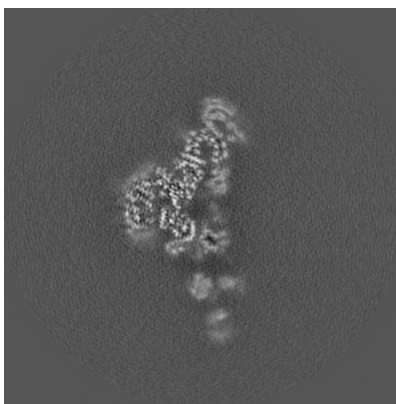
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

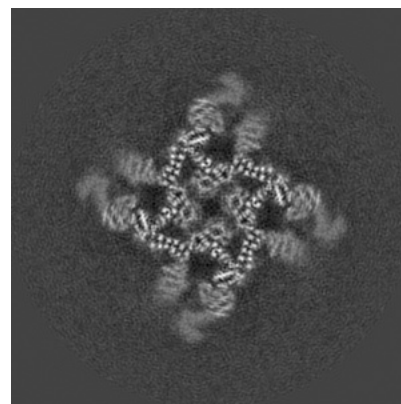
6.3.1 Primary map



X Index: 243



Y Index: 277



Z Index: 271

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

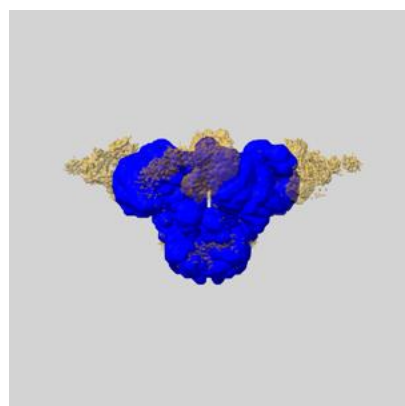
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

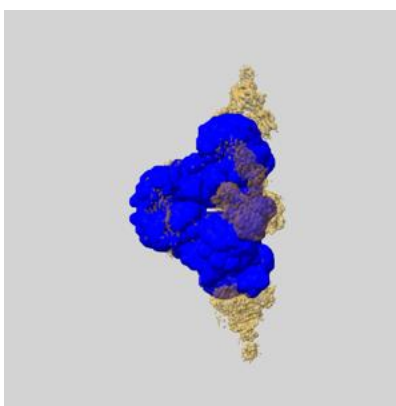
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

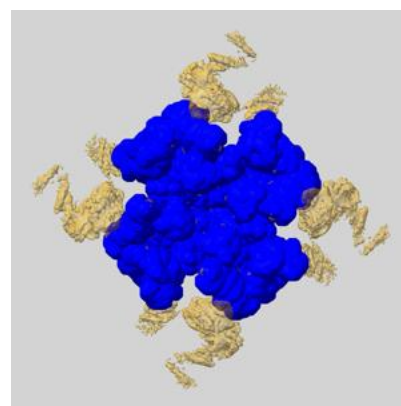
6.5.1 emd_9528_msk_1.map [i](#)



X



Y

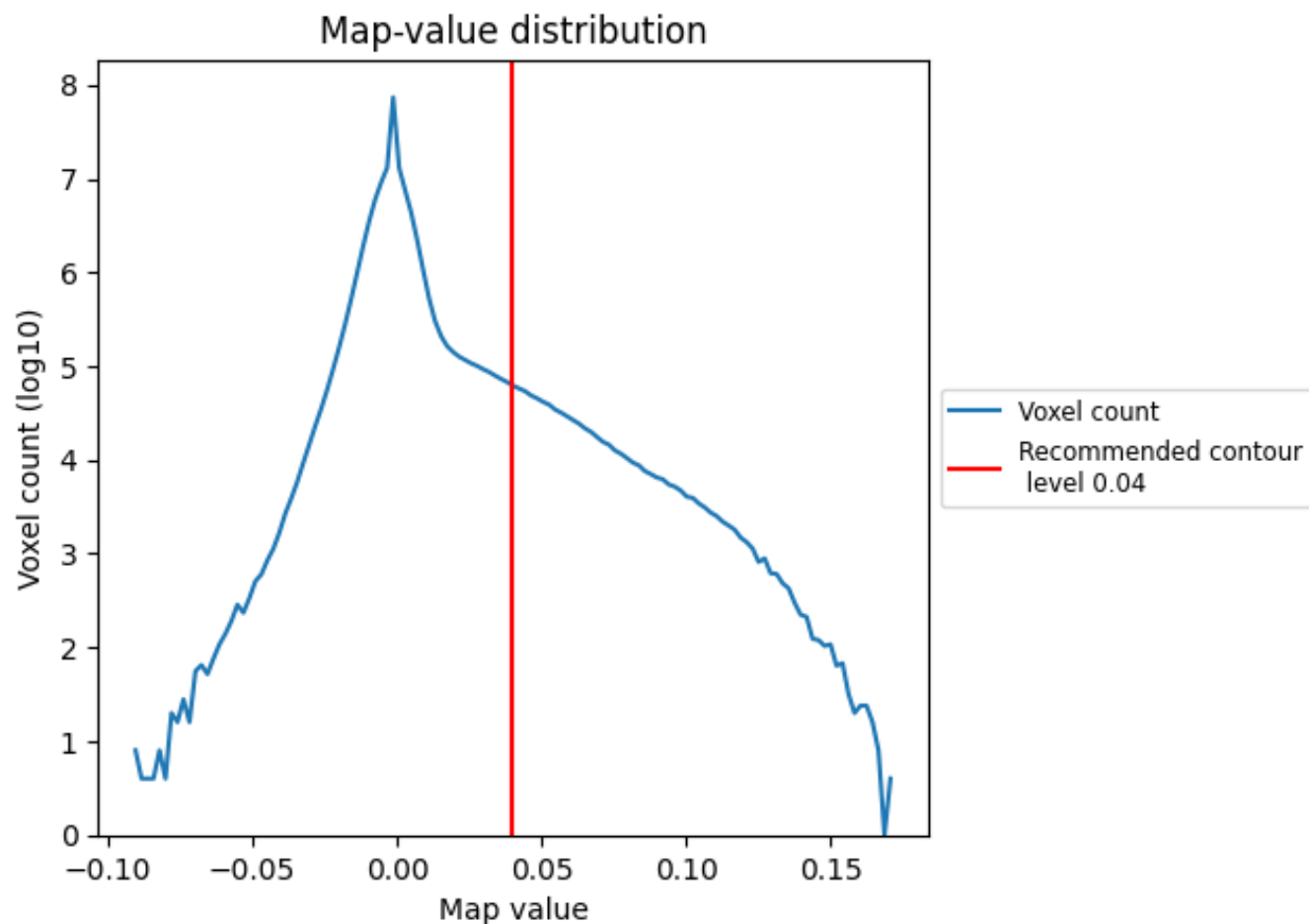


Z

7 Map analysis [i](#)

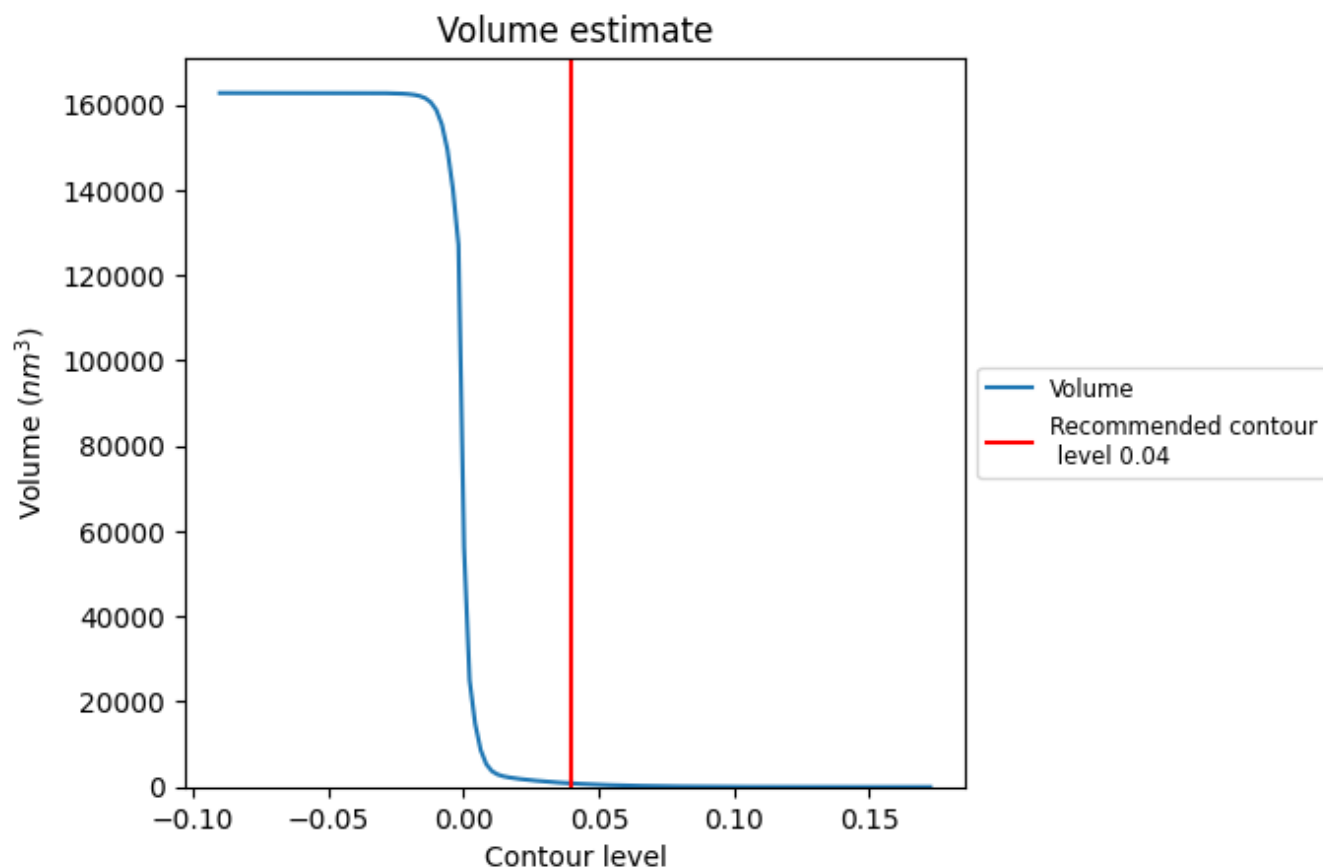
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

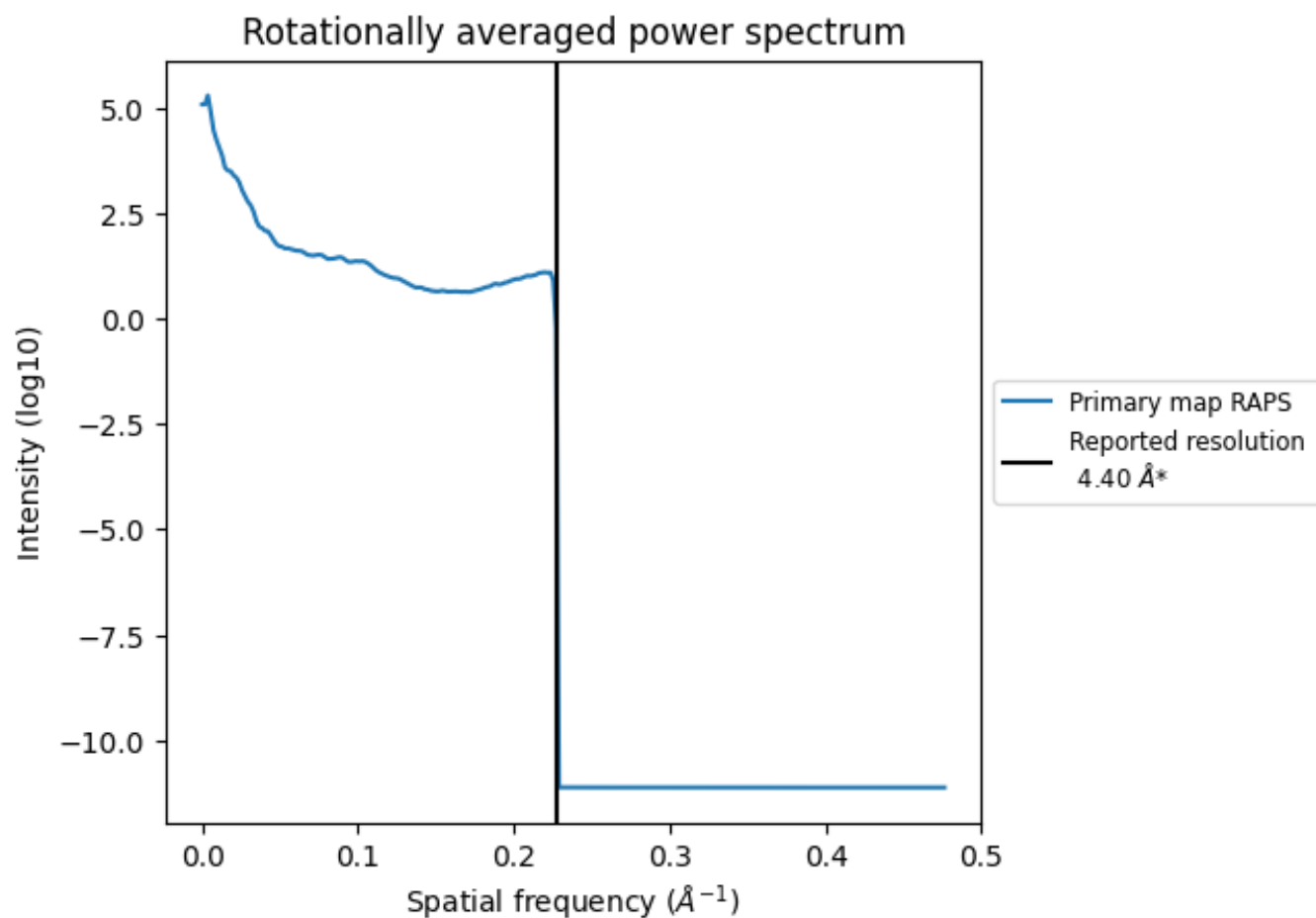
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 837 nm³; this corresponds to an approximate mass of 756 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

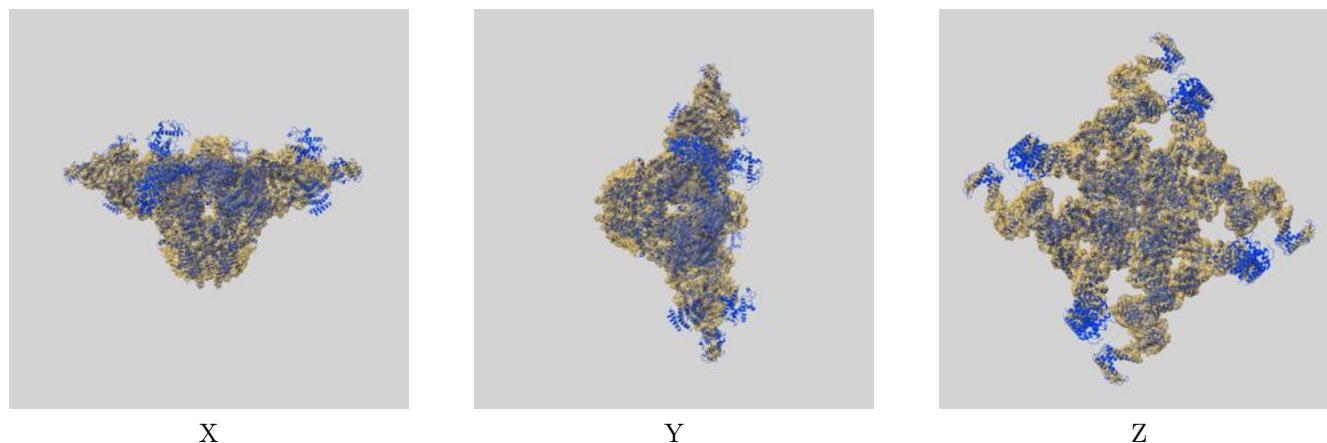
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

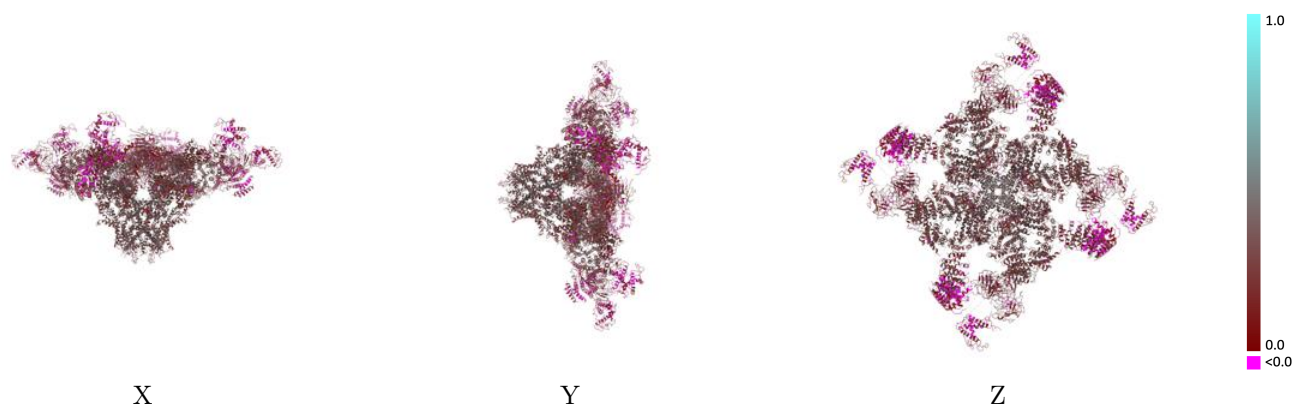
This section contains information regarding the fit between EMDB map EMD-9528 and PDB model 5GO9. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



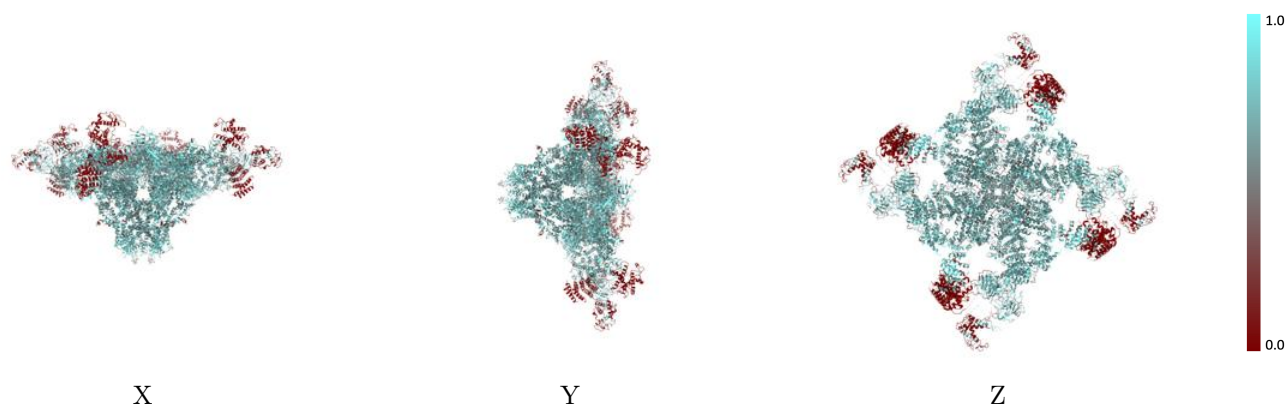
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



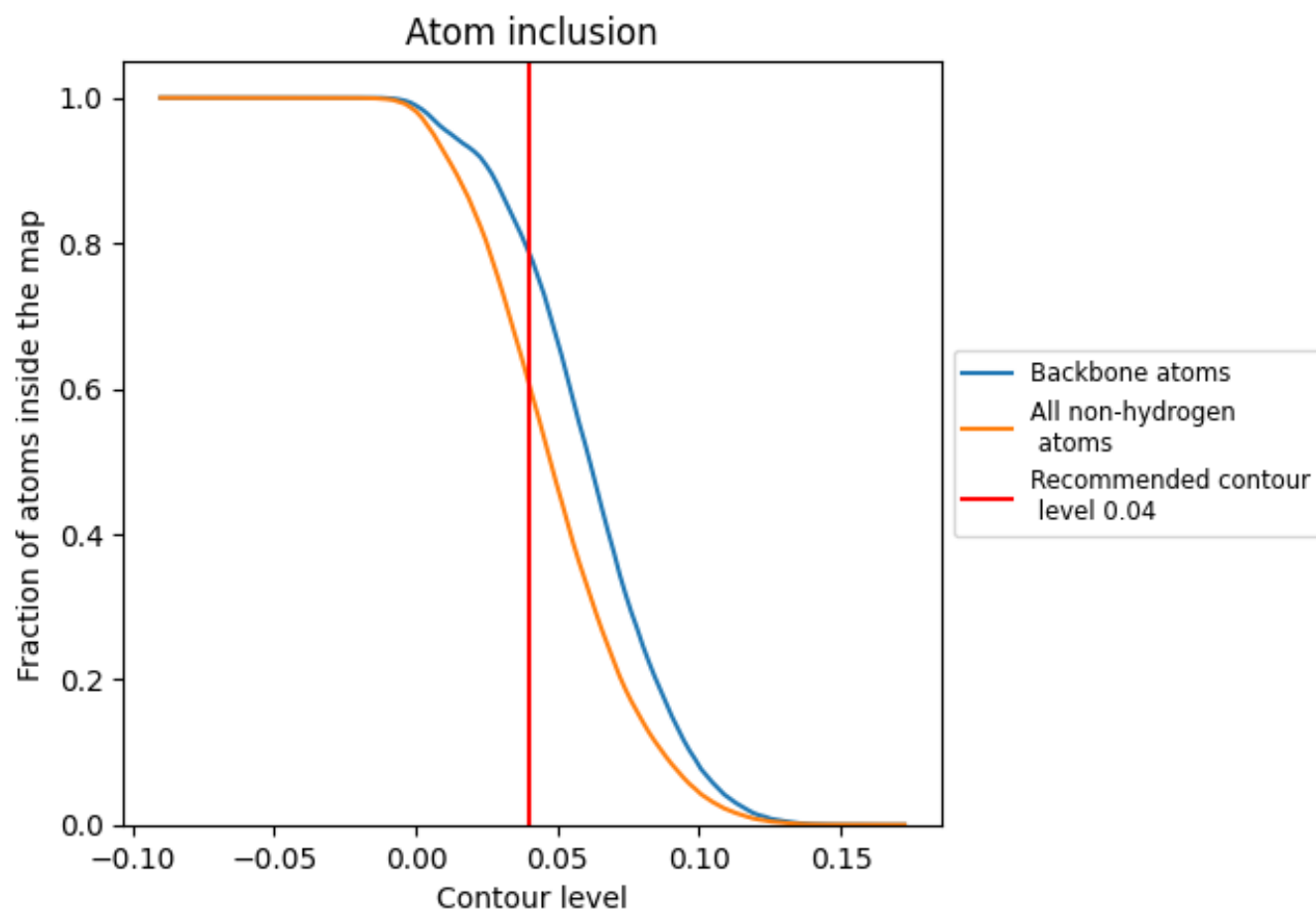
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6057	<div></div> 0.2520
A	<div></div> 0.6057	<div></div> 0.2520
B	<div></div> 0.6057	<div></div> 0.2530
C	<div></div> 0.6056	<div></div> 0.2520
D	<div></div> 0.6057	<div></div> 0.2520

