



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 03:44 PM UTC

PDB ID : 5L1D / pdb_00005l1d
EMDB ID : EMD-8303
Title : Structure of rabbit RyR2 in complex with FKBP12.6 in a closed state (conformation C1)
Authors : Dhindwal, S.; Lobo, J.J.; Samso, M.
Deposited on : 2016-07-29
Resolution : 11.00 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:

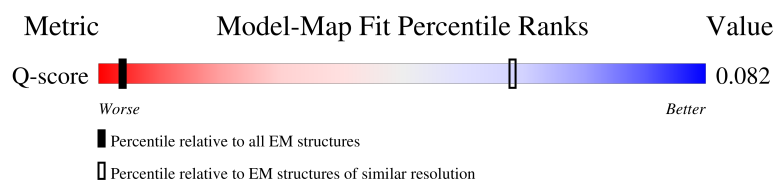
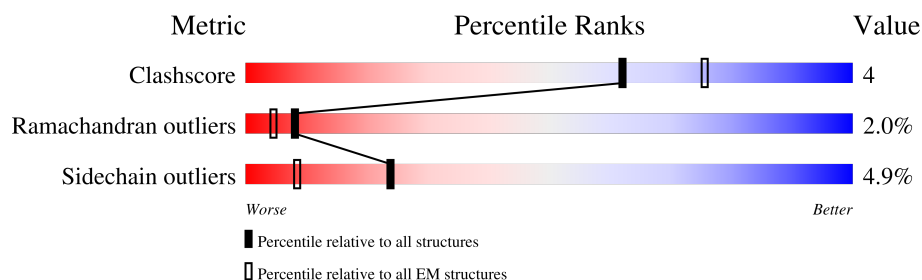
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 11.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	97 (10.50 - 11.50)

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	4387	9% 70% 11% 19%
1	C	4387	9% 69% 11% 19%
1	E	4387	9% 69% 11% 19%
1	G	4387	9% 69% 11% 19%

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Mol	Chain	Length	Quality of chain
2	B	158	8% 58% 10% 32%
2	D	158	8% 59% 8% 32%
2	F	158	8% 55% 13% 32%
2	H	158	8% 63% 5% 32%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 112936 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 Ryanodine Receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3570	Total	C	N	O	S	0	0
			27416	17427	4732	5102	155		
1	C	3570	Total	C	N	O	S	0	0
			27416	17427	4732	5102	155		
1	E	3570	Total	C	N	O	S	0	0
			27416	17427	4732	5102	155		
1	G	3570	Total	C	N	O	S	0	0
			27416	17427	4732	5102	155		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	D	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-50	MET	-	expression tag	UNP P68106
B	-49	ASN	-	expression tag	UNP P68106
B	-48	HIS	-	expression tag	UNP P68106
B	-47	LYS	-	expression tag	UNP P68106
B	-46	VAL	-	expression tag	UNP P68106
B	-45	HIS	-	expression tag	UNP P68106
B	-44	HIS	-	expression tag	UNP P68106
B	-43	HIS	-	expression tag	UNP P68106
B	-42	HIS	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-41	HIS	-	expression tag	UNP P68106
B	-40	HIS	-	expression tag	UNP P68106
B	-39	MET	-	expression tag	UNP P68106
B	-38	ASP	-	expression tag	UNP P68106
B	-37	GLU	-	expression tag	UNP P68106
B	-36	LYS	-	expression tag	UNP P68106
B	-35	THR	-	expression tag	UNP P68106
B	-34	THR	-	expression tag	UNP P68106
B	-33	GLY	-	expression tag	UNP P68106
B	-32	TRP	-	expression tag	UNP P68106
B	-31	ARG	-	expression tag	UNP P68106
B	-30	GLY	-	expression tag	UNP P68106
B	-29	GLY	-	expression tag	UNP P68106
B	-28	HIS	-	expression tag	UNP P68106
B	-27	VAL	-	expression tag	UNP P68106
B	-26	VAL	-	expression tag	UNP P68106
B	-25	GLU	-	expression tag	UNP P68106
B	-24	GLY	-	expression tag	UNP P68106
B	-23	LEU	-	expression tag	UNP P68106
B	-22	ALA	-	expression tag	UNP P68106
B	-21	GLY	-	expression tag	UNP P68106
B	-20	GLU	-	expression tag	UNP P68106
B	-19	LEU	-	expression tag	UNP P68106
B	-18	GLU	-	expression tag	UNP P68106
B	-17	GLN	-	expression tag	UNP P68106
B	-16	LEU	-	expression tag	UNP P68106
B	-15	ARG	-	expression tag	UNP P68106
B	-14	ALA	-	expression tag	UNP P68106
B	-13	ARG	-	expression tag	UNP P68106
B	-12	LEU	-	expression tag	UNP P68106
B	-11	GLU	-	expression tag	UNP P68106
B	-10	HIS	-	expression tag	UNP P68106
B	-9	HIS	-	expression tag	UNP P68106
B	-8	PRO	-	expression tag	UNP P68106
B	-7	GLN	-	expression tag	UNP P68106
B	-6	GLY	-	expression tag	UNP P68106
B	-5	GLN	-	expression tag	UNP P68106
B	-4	ARG	-	expression tag	UNP P68106
B	-3	GLU	-	expression tag	UNP P68106
B	-2	PRO	-	expression tag	UNP P68106
B	-1	GLU	-	expression tag	UNP P68106
B	0	LEU	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-50	MET	-	expression tag	UNP P68106
D	-49	ASN	-	expression tag	UNP P68106
D	-48	HIS	-	expression tag	UNP P68106
D	-47	LYS	-	expression tag	UNP P68106
D	-46	VAL	-	expression tag	UNP P68106
D	-45	HIS	-	expression tag	UNP P68106
D	-44	HIS	-	expression tag	UNP P68106
D	-43	HIS	-	expression tag	UNP P68106
D	-42	HIS	-	expression tag	UNP P68106
D	-41	HIS	-	expression tag	UNP P68106
D	-40	HIS	-	expression tag	UNP P68106
D	-39	MET	-	expression tag	UNP P68106
D	-38	ASP	-	expression tag	UNP P68106
D	-37	GLU	-	expression tag	UNP P68106
D	-36	LYS	-	expression tag	UNP P68106
D	-35	THR	-	expression tag	UNP P68106
D	-34	THR	-	expression tag	UNP P68106
D	-33	GLY	-	expression tag	UNP P68106
D	-32	TRP	-	expression tag	UNP P68106
D	-31	ARG	-	expression tag	UNP P68106
D	-30	GLY	-	expression tag	UNP P68106
D	-29	GLY	-	expression tag	UNP P68106
D	-28	HIS	-	expression tag	UNP P68106
D	-27	VAL	-	expression tag	UNP P68106
D	-26	VAL	-	expression tag	UNP P68106
D	-25	GLU	-	expression tag	UNP P68106
D	-24	GLY	-	expression tag	UNP P68106
D	-23	LEU	-	expression tag	UNP P68106
D	-22	ALA	-	expression tag	UNP P68106
D	-21	GLY	-	expression tag	UNP P68106
D	-20	GLU	-	expression tag	UNP P68106
D	-19	LEU	-	expression tag	UNP P68106
D	-18	GLU	-	expression tag	UNP P68106
D	-17	GLN	-	expression tag	UNP P68106
D	-16	LEU	-	expression tag	UNP P68106
D	-15	ARG	-	expression tag	UNP P68106
D	-14	ALA	-	expression tag	UNP P68106
D	-13	ARG	-	expression tag	UNP P68106
D	-12	LEU	-	expression tag	UNP P68106
D	-11	GLU	-	expression tag	UNP P68106
D	-10	HIS	-	expression tag	UNP P68106
D	-9	HIS	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	PRO	-	expression tag	UNP P68106
D	-7	GLN	-	expression tag	UNP P68106
D	-6	GLY	-	expression tag	UNP P68106
D	-5	GLN	-	expression tag	UNP P68106
D	-4	ARG	-	expression tag	UNP P68106
D	-3	GLU	-	expression tag	UNP P68106
D	-2	PRO	-	expression tag	UNP P68106
D	-1	GLU	-	expression tag	UNP P68106
D	0	LEU	-	expression tag	UNP P68106
F	-50	MET	-	expression tag	UNP P68106
F	-49	ASN	-	expression tag	UNP P68106
F	-48	HIS	-	expression tag	UNP P68106
F	-47	LYS	-	expression tag	UNP P68106
F	-46	VAL	-	expression tag	UNP P68106
F	-45	HIS	-	expression tag	UNP P68106
F	-44	HIS	-	expression tag	UNP P68106
F	-43	HIS	-	expression tag	UNP P68106
F	-42	HIS	-	expression tag	UNP P68106
F	-41	HIS	-	expression tag	UNP P68106
F	-40	HIS	-	expression tag	UNP P68106
F	-39	MET	-	expression tag	UNP P68106
F	-38	ASP	-	expression tag	UNP P68106
F	-37	GLU	-	expression tag	UNP P68106
F	-36	LYS	-	expression tag	UNP P68106
F	-35	THR	-	expression tag	UNP P68106
F	-34	THR	-	expression tag	UNP P68106
F	-33	GLY	-	expression tag	UNP P68106
F	-32	TRP	-	expression tag	UNP P68106
F	-31	ARG	-	expression tag	UNP P68106
F	-30	GLY	-	expression tag	UNP P68106
F	-29	GLY	-	expression tag	UNP P68106
F	-28	HIS	-	expression tag	UNP P68106
F	-27	VAL	-	expression tag	UNP P68106
F	-26	VAL	-	expression tag	UNP P68106
F	-25	GLU	-	expression tag	UNP P68106
F	-24	GLY	-	expression tag	UNP P68106
F	-23	LEU	-	expression tag	UNP P68106
F	-22	ALA	-	expression tag	UNP P68106
F	-21	GLY	-	expression tag	UNP P68106
F	-20	GLU	-	expression tag	UNP P68106
F	-19	LEU	-	expression tag	UNP P68106
F	-18	GLU	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-17	GLN	-	expression tag	UNP P68106
F	-16	LEU	-	expression tag	UNP P68106
F	-15	ARG	-	expression tag	UNP P68106
F	-14	ALA	-	expression tag	UNP P68106
F	-13	ARG	-	expression tag	UNP P68106
F	-12	LEU	-	expression tag	UNP P68106
F	-11	GLU	-	expression tag	UNP P68106
F	-10	HIS	-	expression tag	UNP P68106
F	-9	HIS	-	expression tag	UNP P68106
F	-8	PRO	-	expression tag	UNP P68106
F	-7	GLN	-	expression tag	UNP P68106
F	-6	GLY	-	expression tag	UNP P68106
F	-5	GLN	-	expression tag	UNP P68106
F	-4	ARG	-	expression tag	UNP P68106
F	-3	GLU	-	expression tag	UNP P68106
F	-2	PRO	-	expression tag	UNP P68106
F	-1	GLU	-	expression tag	UNP P68106
F	0	LEU	-	expression tag	UNP P68106
H	-50	MET	-	expression tag	UNP P68106
H	-49	ASN	-	expression tag	UNP P68106
H	-48	HIS	-	expression tag	UNP P68106
H	-47	LYS	-	expression tag	UNP P68106
H	-46	VAL	-	expression tag	UNP P68106
H	-45	HIS	-	expression tag	UNP P68106
H	-44	HIS	-	expression tag	UNP P68106
H	-43	HIS	-	expression tag	UNP P68106
H	-42	HIS	-	expression tag	UNP P68106
H	-41	HIS	-	expression tag	UNP P68106
H	-40	HIS	-	expression tag	UNP P68106
H	-39	MET	-	expression tag	UNP P68106
H	-38	ASP	-	expression tag	UNP P68106
H	-37	GLU	-	expression tag	UNP P68106
H	-36	LYS	-	expression tag	UNP P68106
H	-35	THR	-	expression tag	UNP P68106
H	-34	THR	-	expression tag	UNP P68106
H	-33	GLY	-	expression tag	UNP P68106
H	-32	TRP	-	expression tag	UNP P68106
H	-31	ARG	-	expression tag	UNP P68106
H	-30	GLY	-	expression tag	UNP P68106
H	-29	GLY	-	expression tag	UNP P68106
H	-28	HIS	-	expression tag	UNP P68106
H	-27	VAL	-	expression tag	UNP P68106

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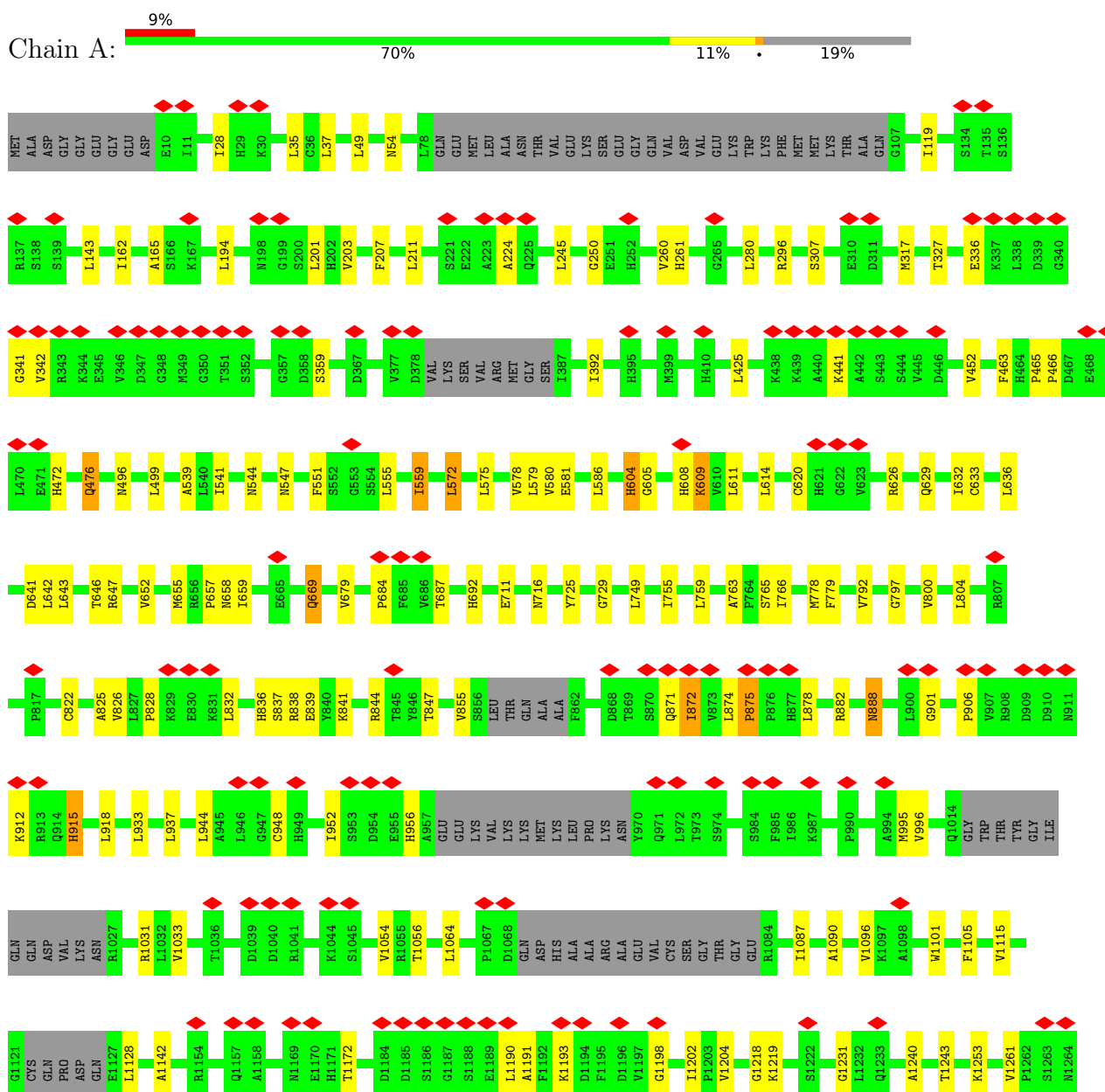
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Chain	Residue	Modelled	Actual	Comment	Reference
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H	-25	GLU	-	expression tag	UNP P68106
H	-24	GLY	-	expression tag	UNP P68106
H	-23	LEU	-	expression tag	UNP P68106
H	-22	ALA	-	expression tag	UNP P68106
H	-21	GLY	-	expression tag	UNP P68106
H	-20	GLU	-	expression tag	UNP P68106
H	-19	LEU	-	expression tag	UNP P68106
H	-18	GLU	-	expression tag	UNP P68106
H	-17	GLN	-	expression tag	UNP P68106
H	-16	LEU	-	expression tag	UNP P68106
H	-15	ARG	-	expression tag	UNP P68106
H	-14	ALA	-	expression tag	UNP P68106
H	-13	ARG	-	expression tag	UNP P68106
H	-12	LEU	-	expression tag	UNP P68106
H	-11	GLU	-	expression tag	UNP P68106
H	-10	HIS	-	expression tag	UNP P68106
H	-9	HIS	-	expression tag	UNP P68106
H	-8	PRO	-	expression tag	UNP P68106
H	-7	GLN	-	expression tag	UNP P68106
H	-6	GLY	-	expression tag	UNP P68106
H	-5	GLN	-	expression tag	UNP P68106
H	-4	ARG	-	expression tag	UNP P68106
H	-3	GLU	-	expression tag	UNP P68106
H	-2	PRO	-	expression tag	UNP P68106
H	-1	GLU	-	expression tag	UNP P68106
H	0	LEU	-	expression tag	UNP P68106

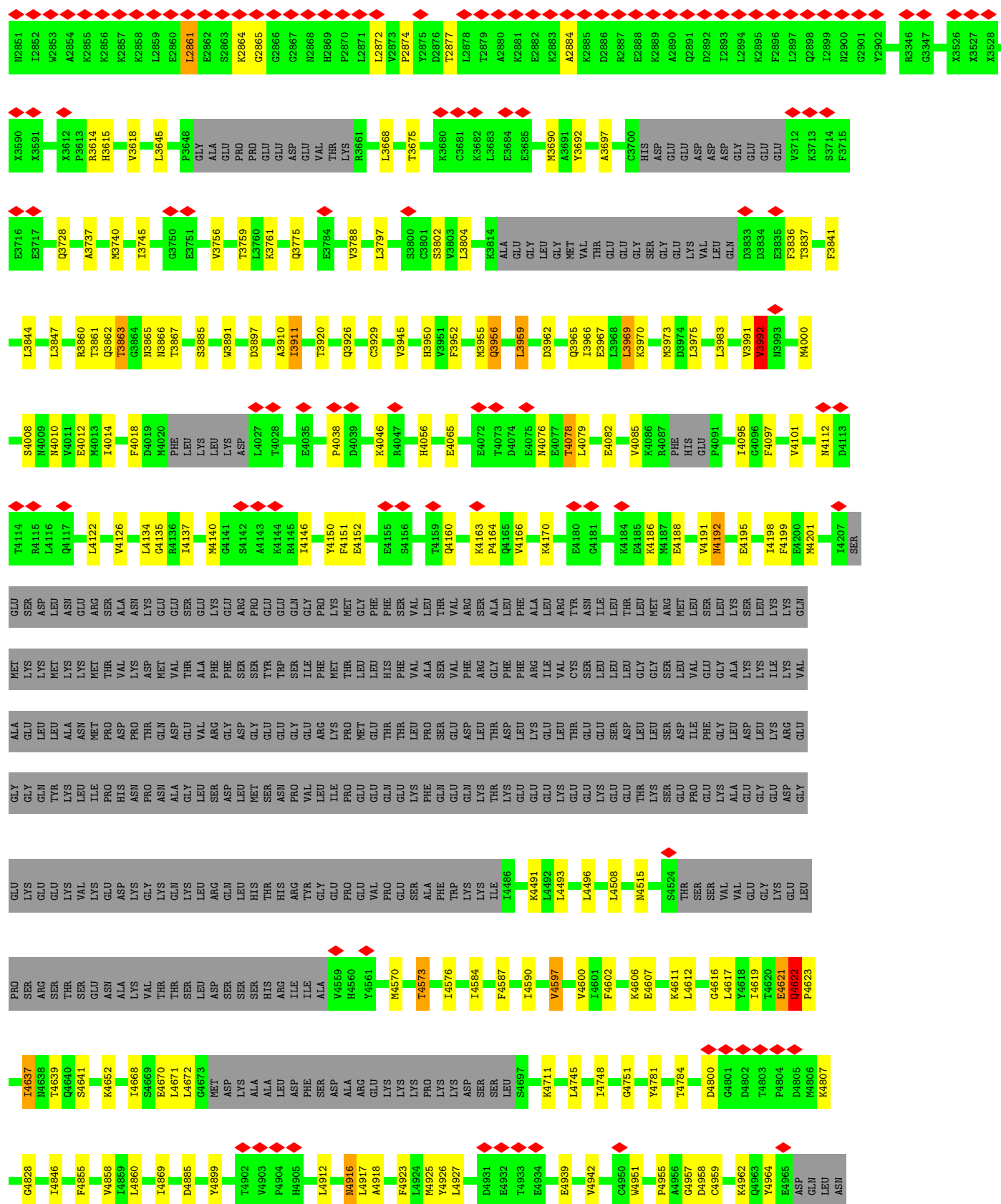
3 Residue-property plots [i](#)

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: Ryanodine Receptor

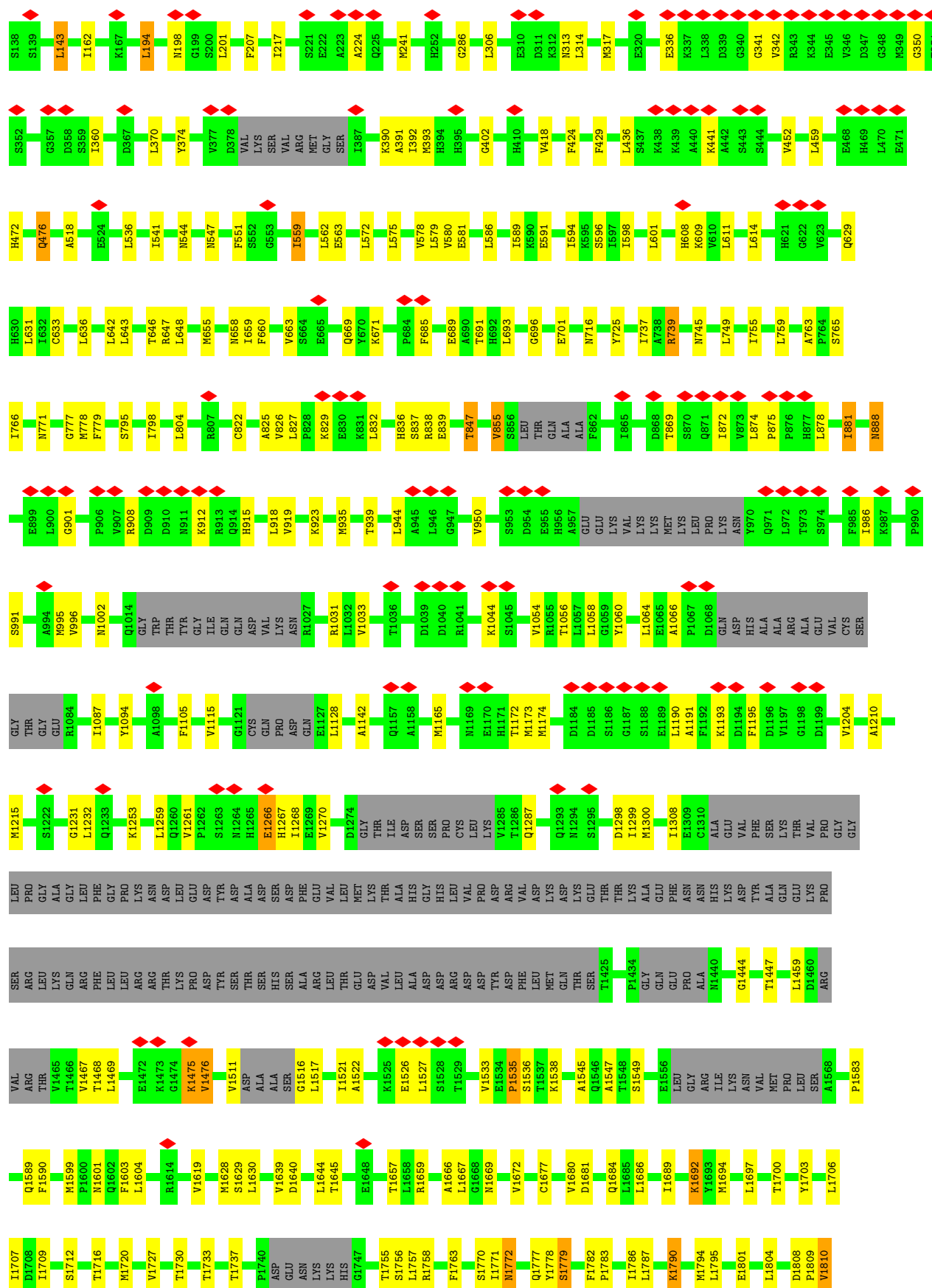


E2791	H2730	V2491	A2256	T2126	P1901	M1831	T1730	K1481	ASP	H1265
R2792	D2731	L2497	E2259	R2127	L1908	G1832	T1730	L1595	TYR	E1266
T2793	D2732	R2498	P2260	S2128	L1909	L1833	T1733	X1496	SER	H1267
R2794	K2733			L2129	L1910	F1834			THR	I1268
E2795	K2734	L2503	R2268	S2131	Q1911	L1843	I1736	I1507	HIS	E1269
Q2796	M2735	ASP	L2275	V2132	Y1912	Q1844	T1737	V1511	SER	V1270
D2797	D2736	THR	L2275	ARG	I1922	L1845		ASP	PHE	D1274
T2798	K2737	ALA	GLN	MET	K1935	P1848	P1740	ASP	GLY	
M2799	L2738	LEU	SER	GLY		SER	GLU	ALA	THR	THR
A2800	L2738	LEU	CYS	LYS		VAL	ASN	SER	LEU	ILE
L2801	K2739	SER	GLN	E2137	K1935	PHE	LYS	G1516	ASP	ASP
L2802	A2740	ALA	MET	P2159	X2022	L2023	LYS	V1639	THR	SER
K2803	G2741	T2511	VAL	P2162	T2024	ASP	HIS	D1630	ALA	PRO
		M2513	SER	M2162		ALA	G1747	L1644	ALA	CYS
			LYS	M2167	LEU	THR	L1748	E1648	ASP	LEU
			GLY	M2167	PRO	GLU	P1749	E1649	ASP	LYS
			TYR	T2170	LYS	GLU	T1755	E1526	ARG	V1285
			ASP	T2170	LYS	GLU	T1755	E1526	VAL	F1286
			ILE	V2174	LYS	GLU	R1758	L1527	PRO	Q1287
			GLY		GLN	GLY		S1528	ASP	
			TRP	V2178	THR	ASP	M1761	T1529	ARG	
			ASN	L2179	GLU	THR	Q1762	V1533	VAL	G1293
			P2293	G2180	LYS	LEU	F1763	E1534	LEU	M1294
				GLY	PRO	GLU	G1668	P1535	ASP	S1295
				VAL	VAL	GLU	N1669		THR	
			R2304	GLY	GLU	GLU	I1771	K1538	SER	
				GLU	GLU	GLU	Y1776	L1539	THR	
			V2307	SER	ASP	PRO	Q1777	P1434	LYS	
			G2311	LYS	SER	SER	Y1778	A1545	ALA	
				ILE	ARG	VAL	S1779	Q1546	GLU	
			L2326	THR	LYS	ASP	F1782	A1547	PHE	
				PHE	SER	THR	Q1684	T1548	ASN	
			E2330	P2190	SER	LYS	P1783	T1548	ASN	
			CYS	K2191	LEU	LEU	L1685	S1549	ASN	
			PHE	M2192	GLU	GLU	L1784	V1440	GLU	
			GLY		GLY	GLY	L1787	V1552	VAL	
			PRO	L2206	ALA	ALA	E1689	F1553	LYS	
			ALA	V2067	GLY	GLY	K1790	Q1554	PHE	
			LEU	V2074	GLU	GLU	M1794	F1555	LYS	
			ARG	I2075	LYS	GLU	G1802	E1556	GLN	
			GLY	E2076	ALA	GLU	S1803	LEU	GLY	
			GLY	D2077	VAL	VAL	L1804	ARG	PRO	
			ASN	L2080	GLY	GLY	L1804	ILE	GLY	
			G2343	MET	ALA	LYS	D1808	LYS	LEU	
				ARG	VAL	ARG	P1809	ASN	PRO	
			E2349	SER	GLY	PRO	Y1810	VAL	SER	
				T2238	THR	LYS	V1819	ARG	GLY	
			L2354		Y2105	GLU	P1820	THR	LEU	
			ALA	D2241	Y2106	G1892	S1712	E1472	ALA	
			GLU	V2242				T1468	GLY	
			ASP		L2119	M1896	T1716	K1473	PHE	
			PRO	M2248	L2120	K1897	L1827	G1474	LEU	
			SER	D2249		L1898	L1828	K1475	ARG	
			ARG			P1899	L1829	V1476	THR	
			ASP		L2123	E1900	I1830	H1583	LYS	
								V1594	PRO	

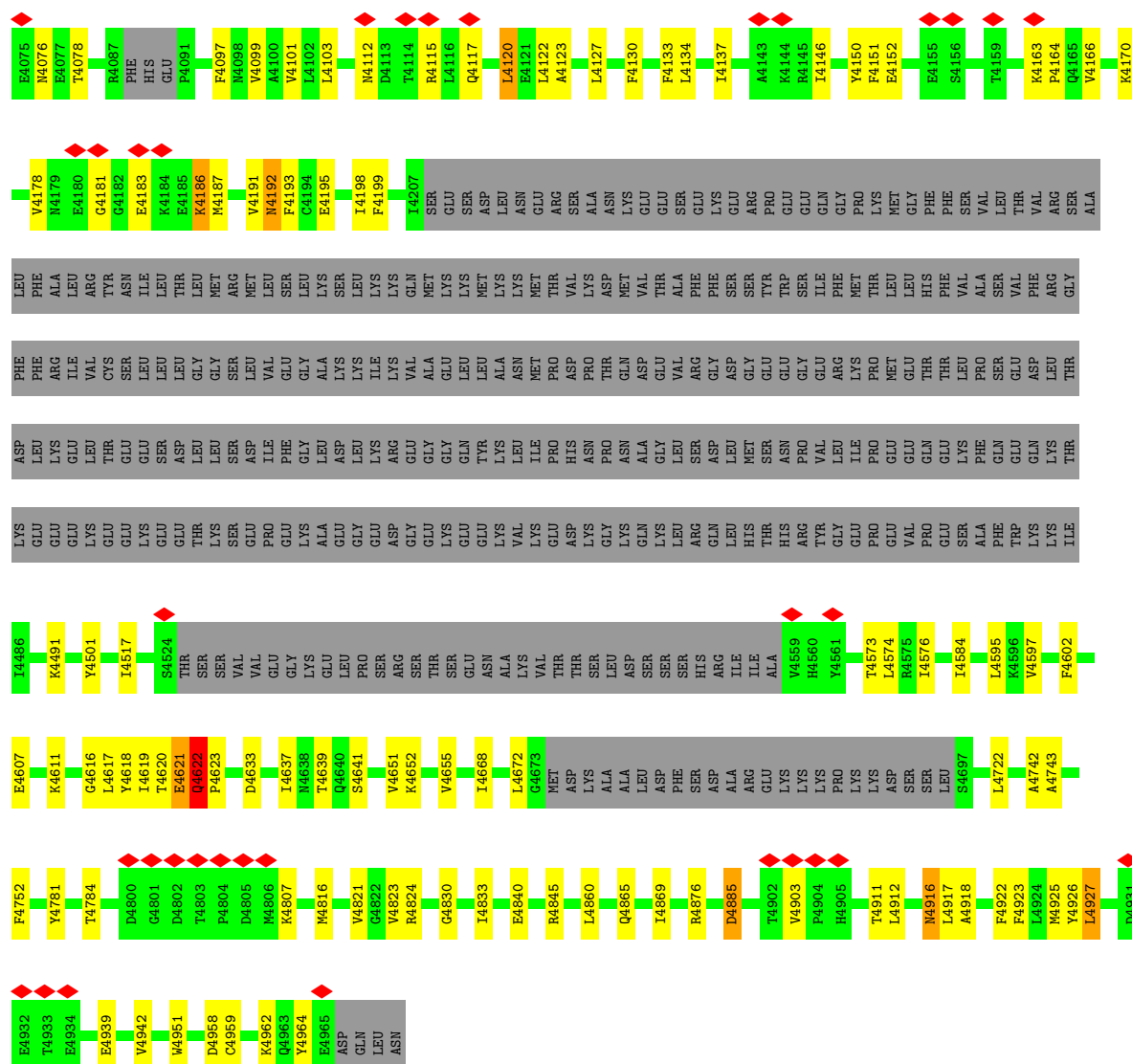




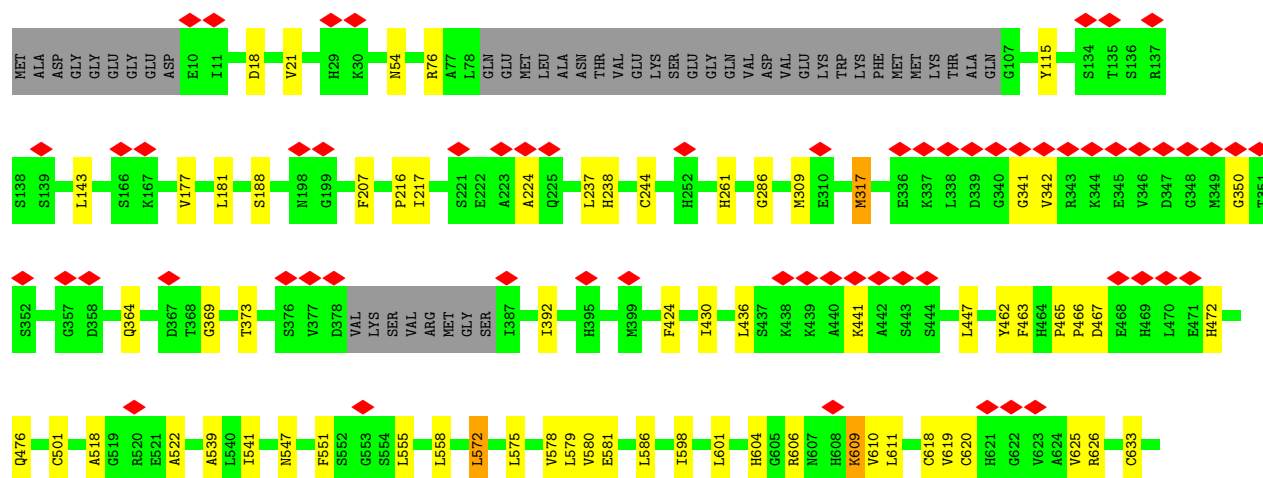


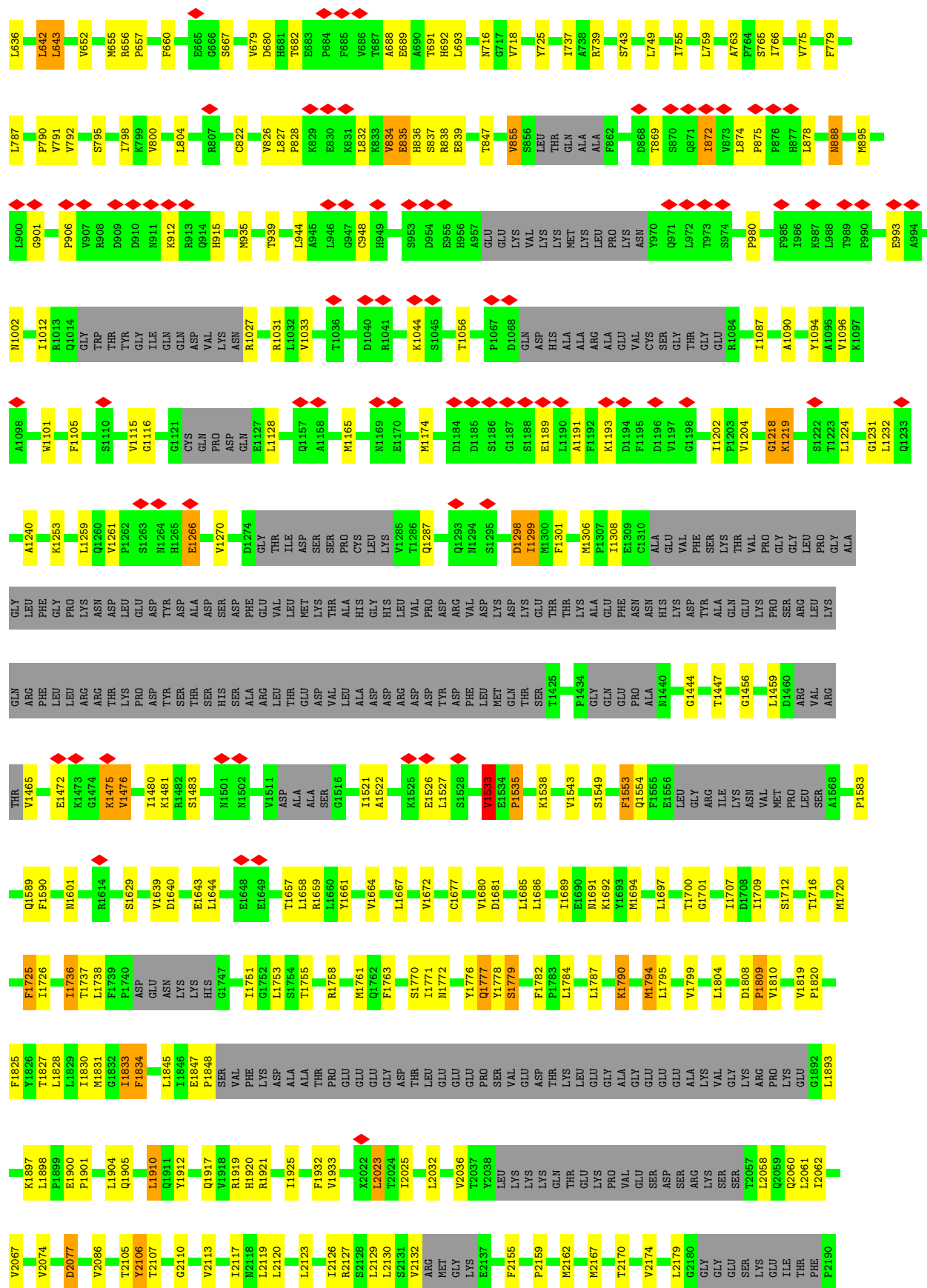






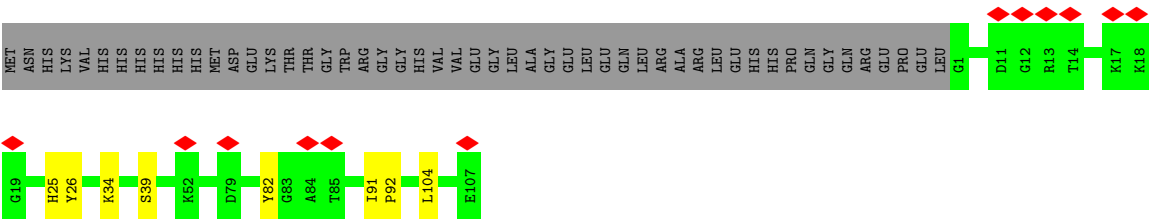
Molecule 1: Ryanodine Receptor







● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	13158	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	62000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.090	Depositor
Minimum map value	-0.046	Depositor
Average map value	-0.006	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	536.0, 536.0, 536.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality

5.1 Standard geometry

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	1.15	4/25831 (0.0%)	0.98	31/34865 (0.1%)
1	C	1.16	6/25831 (0.0%)	0.99	25/34865 (0.1%)
1	E	1.15	4/25831 (0.0%)	0.98	25/34865 (0.1%)
1	G	1.16	4/25831 (0.0%)	0.98	27/34865 (0.1%)
2	B	1.32	1/834 (0.1%)	1.02	2/1123 (0.2%)
2	D	1.33	0/834	1.00	0/1123
2	F	1.32	0/834	0.98	2/1123 (0.2%)
2	H	1.35	1/834 (0.1%)	1.01	0/1123
All	All	1.16	20/106660 (0.0%)	0.98	112/143952 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	G	0	1
All	All	0	3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	4183	GLU	CA-C	7.74	1.57	1.53
1	C	730	LEU	CA-C	6.51	1.55	1.52
1	G	4597	VAL	CA-CB	6.01	1.57	1.54
1	E	4597	VAL	CA-CB	5.85	1.57	1.54
1	C	1583	PRO	CA-C	5.81	1.57	1.52
1	C	4597	VAL	CA-CB	5.74	1.57	1.54
2	B	92	PRO	CA-C	5.73	1.55	1.52
1	A	1583	PRO	CA-C	5.71	1.57	1.52
1	E	1583	PRO	CA-C	5.66	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	92	PRO	CA-C	5.65	1.55	1.52
1	G	1583	PRO	CA-C	5.43	1.57	1.52
1	A	4597	VAL	CA-CB	5.33	1.57	1.54
1	G	915	HIS	CA-C	5.18	1.57	1.52
1	C	2869	HIS	CA-C	5.17	1.57	1.52
1	E	2869	HIS	CA-C	5.16	1.57	1.52
1	C	1632	ILE	N-CA	5.13	1.50	1.46
1	C	2714	ILE	CA-C	5.10	1.57	1.53
1	G	2869	HIS	CA-C	5.10	1.57	1.52
1	A	711	GLU	CA-C	5.10	1.57	1.53
1	A	915	HIS	CA-C	5.06	1.57	1.52

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2248	MET	N-CA-C	7.79	119.85	111.36
1	A	1444	GLY	N-CA-C	7.72	121.92	110.42
1	C	2248	MET	N-CA-C	7.48	119.07	111.07
1	E	2248	MET	N-CA-C	7.26	119.27	111.36
1	G	2248	MET	N-CA-C	7.16	119.16	111.36
1	C	2206	ILE	N-CA-C	7.01	117.77	110.62
1	C	1771	ILE	N-CA-C	6.92	117.04	110.53
1	A	4621	GLU	N-CA-C	6.90	118.88	111.36
1	E	4621	GLU	N-CA-C	6.87	118.85	111.36
1	G	4621	GLU	N-CA-C	6.79	118.76	111.36
1	G	2884	ALA	N-CA-C	6.75	118.29	111.07
1	A	2884	ALA	N-CA-C	6.68	118.57	111.28
1	A	1771	ILE	N-CA-C	6.57	116.73	110.42
1	C	2884	ALA	N-CA-C	6.55	118.07	111.07
1	E	2884	ALA	N-CA-C	6.54	118.07	111.07
1	E	2206	ILE	N-CA-C	6.52	117.27	110.62
1	A	1712	SER	N-CA-C	6.49	118.36	111.28
1	A	2307	VAL	N-CA-C	6.49	116.75	111.62
1	A	2206	ILE	N-CA-C	6.45	117.20	110.62
1	G	3863	THR	N-CA-C	6.30	118.15	111.28
1	A	2249	ASP	N-CA-C	6.21	117.72	111.07
1	A	2256	ALA	N-CA-C	6.17	120.27	112.87
1	A	2349	GLU	N-CA-C	6.13	117.76	111.14
1	C	4621	GLU	N-CA-C	6.13	118.04	111.36
1	E	4163	LYS	N-CA-C	6.09	121.03	112.75
1	C	841	LYS	N-CA-C	6.07	117.36	107.23
1	G	2206	ILE	N-CA-C	6.06	116.80	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	92	PRO	CA-C-N	6.04	126.06	119.90
2	B	92	PRO	C-N-CA	6.04	126.06	119.90
1	C	626	ARG	N-CA-C	5.98	118.32	111.02
1	A	1736	ILE	N-CA-C	5.94	116.72	110.72
1	C	301	THR	N-CA-C	5.92	117.82	111.36
1	A	3863	THR	N-CA-C	5.92	117.73	111.28
1	G	1444	GLY	N-CA-C	5.91	119.38	110.75
1	A	841	LYS	N-CA-C	5.91	117.24	107.20
1	A	2077	ASP	CA-C-N	5.88	125.42	119.19
1	A	2077	ASP	C-N-CA	5.88	125.42	119.19
1	C	2307	VAL	N-CA-C	5.81	116.21	111.62
1	A	1575	HIS	N-CA-C	5.80	117.28	111.07
1	A	626	ARG	N-CA-C	5.77	118.04	111.11
1	C	580	VAL	N-CA-C	5.77	116.50	110.62
1	A	4163	LYS	N-CA-C	5.75	120.57	112.75
1	C	2256	ALA	N-CA-C	5.74	119.38	112.38
1	A	1552	VAL	N-CA-C	5.73	116.51	110.72
1	C	2077	ASP	CA-C-N	5.70	125.56	119.28
1	C	2077	ASP	C-N-CA	5.70	125.56	119.28
1	C	4008	SER	N-CA-C	5.68	117.16	110.97
1	E	2256	ALA	N-CA-C	5.68	119.68	112.87
1	G	2307	VAL	N-CA-C	5.68	116.10	111.62
1	A	3615	HIS	N-CA-C	5.66	117.25	111.14
1	A	4166	VAL	N-CA-C	5.64	116.37	110.62
1	G	626	ARG	N-CA-C	5.61	117.85	111.11
1	E	4133	PHE	N-CA-C	5.59	119.28	111.56
1	G	2256	ALA	N-CA-C	5.58	119.57	112.87
1	E	4166	VAL	N-CA-C	5.52	116.91	110.62
1	E	875	PRO	CA-C-N	5.51	125.87	119.47
1	E	875	PRO	C-N-CA	5.51	125.87	119.47
1	C	4821	VAL	N-CA-C	5.51	115.98	111.62
1	A	836	HIS	N-CA-C	5.50	118.03	111.71
1	G	4008	SER	N-CA-C	5.48	116.94	110.97
1	G	261	HIS	N-CA-C	5.46	117.39	108.76
1	G	1712	SER	N-CA-C	5.42	117.19	111.28
1	A	875	PRO	CA-C-N	5.42	125.76	119.47
1	A	875	PRO	C-N-CA	5.42	125.76	119.47
1	C	1736	ILE	N-CA-C	5.40	116.18	110.72
1	E	1645	THR	N-CA-C	5.40	117.92	111.71
1	E	4008	SER	N-CA-C	5.40	116.86	110.97
1	G	1044	LYS	N-CA-C	5.40	117.92	111.71
1	G	1736	ILE	N-CA-C	5.39	116.12	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1712	SER	N-CA-C	5.39	117.85	111.33
1	C	4133	PHE	N-CA-C	5.38	118.98	111.56
1	G	4133	PHE	N-CA-C	5.36	118.96	111.56
1	E	4183	GLU	N-CA-C	5.36	113.89	108.75
1	A	4008	SER	N-CA-C	5.34	116.79	110.97
1	C	1645	THR	N-CA-C	5.34	117.85	111.71
1	C	1444	GLY	N-CA-C	5.26	118.26	110.63
1	C	836	HIS	N-CA-C	5.25	117.91	111.82
1	C	4918	ALA	N-CA-C	5.24	116.99	111.28
1	C	2266	VAL	N-CA-C	5.24	116.01	110.72
2	F	92	PRO	CA-C-N	5.24	125.24	119.90
2	F	92	PRO	C-N-CA	5.24	125.24	119.90
1	C	1712	SER	N-CA-C	5.23	116.98	111.28
1	A	261	HIS	N-CA-C	5.23	117.20	108.99
1	A	4828	GLY	N-CA-C	5.22	119.44	112.65
1	E	2077	ASP	CA-C-N	5.22	125.02	119.28
1	E	2077	ASP	C-N-CA	5.22	125.02	119.28
1	C	1545	ALA	N-CA-C	5.22	117.00	109.07
1	G	1553	PHE	N-CA-C	5.19	116.96	109.07
1	E	1444	GLY	N-CA-C	5.19	117.99	111.09
1	A	2747	ILE	N-CA-C	5.19	116.32	108.96
1	E	2307	VAL	N-CA-C	5.19	115.72	111.62
1	G	3677	LEU	N-CA-C	5.18	117.59	111.33
1	E	696	GLY	N-CA-C	5.17	118.09	110.80
1	G	2861	LEU	N-CA-C	5.17	116.99	111.36
1	A	605	GLY	N-CA-C	-5.15	103.56	111.24
1	G	1306	MET	CA-C-N	5.14	125.59	120.14
1	G	1306	MET	C-N-CA	5.14	125.59	120.14
1	G	3699	SER	N-CA-C	5.10	117.58	111.71
1	G	1266	GLU	N-CA-C	-5.10	105.63	111.14
1	E	1044	LYS	N-CA-C	5.08	118.74	112.54
1	A	1593	HIS	N-CA-C	5.08	116.79	108.76
1	G	4925	MET	CA-C-N	5.08	127.05	120.44
1	G	4925	MET	C-N-CA	5.08	127.05	120.44
1	E	1033	VAL	N-CA-C	5.06	114.53	108.96
1	E	1266	GLU	N-CA-C	-5.04	105.44	111.03
1	E	1603	PHE	N-CA-C	5.03	117.66	111.82
1	G	2077	ASP	CA-C-N	5.03	124.81	119.28
1	G	2077	ASP	C-N-CA	5.03	124.81	119.28
1	E	4821	VAL	N-CA-C	5.03	115.59	111.62
1	C	1575	HIS	N-CA-C	5.01	116.56	111.14
1	E	2761	TYR	N-CA-C	5.00	118.15	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1298	ASP	N-CA-C	5.00	114.84	108.24

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	604	HIS	Peptide
1	C	3614	ARG	Peptide
1	G	3614	ARG	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	27416	0	25487	220	0
1	C	27416	0	25485	239	0
1	E	27416	0	25489	241	0
1	G	27416	0	25485	225	0
2	B	818	0	824	10	0
2	D	818	0	824	6	0
2	F	818	0	824	9	0
2	H	818	0	824	4	0
All	All	112936	0	105242	937	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (937) 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:E:3945:VAL:HG11	1:E:3983:LEU:HD21	1.47	0.94
1:C:3778:MET:HE1	1:C:3847:LEU:HD22	1.49	0.94
1:A:874:LEU:HD23	1:A:878:LEU:HD13	1.50	0.94
1:G:4020:MET:HE3	1:G:4067:LEU:HD21	1.56	0.87
1:E:1172:THR:HG21	1:E:1190:LEU:HD13	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2783:MET:HE1	1:C:2897:LEU:HD11	1.59	0.84
1:G:874:LEU:HD23	1:G:878:LEU:HD13	1.60	0.82
1:E:4198:ILE:HG12	1:E:4925:MET:HE1	1.62	0.81
1:E:1261:VAL:HG11	1:E:1270:VAL:HG11	1.63	0.78
1:G:3945:VAL:HG11	1:G:3983:LEU:HD21	1.66	0.78
1:C:1172:THR:HG21	1:C:1190:LEU:HD13	1.66	0.77
1:G:1933:VAL:HG21	1:G:3618:VAL:HG22	1.66	0.76
1:A:1172:THR:HG21	1:A:1190:LEU:HD13	1.68	0.75
1:G:4617:LEU:O	1:G:4622:GLN:N	2.19	0.75
1:E:4617:LEU:O	1:E:4622:GLN:N	2.20	0.74
1:C:4617:LEU:O	1:C:4622:GLN:N	2.19	0.74
1:E:594:ILE:HD12	1:E:631:LEU:HD22	1.70	0.74
1:A:2119:LEU:HD21	1:A:2162:MET:HE1	1.68	0.74
1:A:1761:MET:HE2	1:A:1831:MET:HE3	1.71	0.72
1:G:1105:PHE:HB2	1:G:1115:VAL:HG21	1.72	0.71
1:A:2075:ILE:HG12	1:A:2080:LEU:HD23	1.74	0.69
1:C:314:LEU:HD12	1:C:391:ALA:HB1	1.73	0.69
1:G:1543:VAL:HG11	1:G:1553:PHE:CZ	2.27	0.69
1:A:4617:LEU:O	1:A:4622:GLN:N	2.20	0.69
1:C:633:CYS:HB3	1:C:1672:VAL:HG11	1.73	0.69
1:G:1691:ASN:HD21	1:G:1694:MET:HE3	1.57	0.69
1:C:874:LEU:HD23	1:C:878:LEU:HD13	1.75	0.68
1:A:3945:VAL:HG11	1:A:3983:LEU:HD21	1.74	0.68
1:G:655:MET:HE2	1:G:834:VAL:HG11	1.77	0.67
1:C:1105:PHE:HB2	1:C:1115:VAL:HG21	1.76	0.67
2:D:26:TYR:N	2:D:39:SER:OG	2.27	0.67
1:E:874:LEU:HD23	1:E:878:LEU:HD13	1.78	0.66
1:G:4198:ILE:CG1	1:G:4925:MET:HE1	2.25	0.66
1:E:1680:VAL:HG11	1:E:1709:ILE:HD13	1.78	0.66
1:C:26:ALA:HB3	1:C:35:LEU:HD13	1.77	0.65
1:E:314:LEU:HD12	1:E:391:ALA:HB1	1.77	0.65
1:G:633:CYS:HB3	1:G:1672:VAL:HG11	1.79	0.65
2:H:26:TYR:N	2:H:39:SER:OG	2.28	0.65
1:A:4192:ASN:HD22	1:A:4606:LYS:HE2	1.62	0.64
1:E:3778:MET:HE1	1:E:3847:LEU:HD22	1.78	0.64
1:G:2266:VAL:HG12	1:G:2303:LEU:HD11	1.79	0.64
1:A:143:LEU:HD11	1:A:207:PHE:CD2	2.32	0.64
1:A:1219:LYS:HA	1:A:1240:ALA:HB3	1.80	0.64
1:E:4517:ILE:HG21	1:E:4574:LEU:HD23	1.80	0.64
2:B:26:TYR:N	2:B:39:SER:OG	2.29	0.64
1:A:1261:VAL:HG11	1:A:1270:VAL:HG11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2123:LEU:HD12	1:A:2127:ARG:NH1	2.12	0.64
1:A:4097:PHE:CZ	1:A:4152:GLU:HB2	2.32	0.64
1:G:4198:ILE:HG12	1:G:4925:MET:HE1	1.80	0.63
1:A:1680:VAL:HG11	1:A:1709:ILE:HD13	1.80	0.63
1:E:4146:ILE:HD11	1:E:4958:ASP:HB3	1.80	0.63
1:G:1799:VAL:HG22	1:G:1893:LEU:HD22	1.80	0.63
1:A:4493:LEU:HD11	1:A:4590:ILE:HG21	1.81	0.63
1:C:1480:ILE:HG23	1:C:1481:LYS:HD2	1.81	0.63
1:E:2783:MET:HE1	1:E:2897:LEU:HD11	1.81	0.63
1:E:633:CYS:HB3	1:E:1672:VAL:HG11	1.79	0.63
1:E:591:GLU:HA	1:E:631:LEU:HD21	1.81	0.63
1:A:2178:VAL:HG11	1:A:2192:MET:HE2	1.80	0.62
1:A:3862:GLN:HE21	1:A:3865:ASN:HD22	1.48	0.62
1:C:4652:LYS:HG3	1:C:4672:LEU:HD23	1.82	0.62
1:G:3862:GLN:HE21	1:G:3865:ASN:HD22	1.48	0.62
1:A:888:ASN:ND2	1:A:1056:THR:HG21	2.15	0.61
1:A:1831:MET:HE1	1:A:1833:ILE:HD13	1.82	0.61
1:E:2266:VAL:HG21	1:E:2324:LEU:HB3	1.82	0.61
1:A:37:LEU:HD13	1:A:203:VAL:HG11	1.81	0.61
1:E:1831:MET:HE1	1:E:1833:ILE:HD13	1.82	0.61
1:E:1522:ALA:HB3	1:E:1527:LEU:HD11	1.81	0.61
1:A:1087:ILE:HD12	1:A:1128:LEU:HD23	1.82	0.61
1:A:4012:GLU:HG3	1:A:4122:LEU:HD21	1.82	0.61
1:C:1641:ILE:HG21	1:C:1694:MET:HE2	1.82	0.61
1:G:1522:ALA:HB3	1:G:1527:LEU:HD11	1.81	0.61
1:A:1522:ALA:HB3	1:A:1527:LEU:HD11	1.83	0.61
1:A:4146:ILE:HD11	1:A:4958:ASP:HB3	1.82	0.61
1:G:1261:VAL:HG11	1:G:1270:VAL:HG11	1.82	0.61
1:C:693:LEU:HG	1:C:749:LEU:HD12	1.83	0.60
1:E:2130:LEU:HA	1:E:2174:VAL:HG22	1.83	0.60
1:C:2130:LEU:HA	1:C:2174:VAL:HG22	1.82	0.60
1:C:28:ILE:HD11	1:C:201:LEU:HD11	1.83	0.60
1:C:4101:VAL:HG13	1:C:4150:TYR:HB2	1.84	0.60
1:G:1480:ILE:HG23	1:G:1481:LYS:HD2	1.82	0.60
1:G:766:ILE:HB	1:G:779:PHE:HB2	1.84	0.60
1:A:4916:ASN:O	1:A:4918:ALA:N	2.35	0.60
1:E:1727:VAL:HG11	1:E:1926:VAL:HG11	1.84	0.60
1:E:2067:VAL:HG21	1:E:3645:LEU:HD13	1.83	0.60
1:G:2130:LEU:HA	1:G:2174:VAL:HG22	1.84	0.59
1:A:4137:ILE:HG23	1:A:4151:PHE:CE2	2.37	0.59
1:C:3806:LEU:HD13	1:C:3889:PHE:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4101:VAL:HG13	1:E:4150:TYR:HB2	1.84	0.59
1:G:667:SER:HB2	1:G:1012:ILE:HD13	1.85	0.59
1:G:1707:ILE:HG23	1:G:1827:THR:HG21	1.84	0.59
1:E:4097:PHE:CZ	1:E:4152:GLU:HB2	2.37	0.59
1:C:2119:LEU:HD11	1:C:2162:MET:HE1	1.84	0.59
1:G:1219:LYS:HA	1:G:1240:ALA:HB3	1.85	0.59
1:A:1480:ILE:HG23	1:A:1481:LYS:HD2	1.83	0.59
1:A:1090:ALA:HB3	1:A:1202:ILE:CG2	2.33	0.58
1:C:1090:ALA:HB3	1:C:1202:ILE:CG2	2.33	0.58
1:G:1700:THR:HG22	1:G:1820:PRO:HG3	1.85	0.58
1:G:4203:LEU:HD13	1:G:4595:LEU:HD12	1.85	0.58
1:C:826:VAL:HG21	1:C:832:LEU:HD22	1.85	0.58
1:A:1922:ILE:HD13	1:A:2105:THR:HG21	1.84	0.58
1:C:4916:ASN:O	1:C:4918:ALA:N	2.36	0.58
1:C:869:THR:HG21	1:C:1002:ASN:HD21	1.68	0.58
1:E:4014:ILE:HG22	1:E:4018:PHE:CE2	2.39	0.58
2:F:26:TYR:N	2:F:39:SER:OG	2.29	0.58
1:G:4195:GLU:HA	1:G:4198:ILE:HD12	1.85	0.58
1:A:4869:ILE:HG23	1:G:4869:ILE:HG21	1.85	0.58
1:C:1830:ILE:HG22	1:C:1912:TYR:CD1	2.39	0.58
1:G:4916:ASN:O	1:G:4918:ALA:N	2.37	0.58
1:E:4076:ASN:HB3	1:E:4078:THR:HG22	1.86	0.58
1:C:3945:VAL:HG11	1:C:3983:LEU:HD21	1.86	0.57
1:C:4012:GLU:HG3	1:C:4122:LEU:HD21	1.84	0.57
1:E:4916:ASN:O	1:E:4918:ALA:N	2.37	0.57
1:A:4101:VAL:HG13	1:A:4150:TYR:HB2	1.87	0.57
1:C:4869:ILE:HG21	1:E:4869:ILE:HG23	1.86	0.57
1:E:3983:LEU:HD22	1:E:4000:MET:HE2	1.87	0.57
1:A:2498:ARG:HB3	1:A:2517:LEU:HD11	1.86	0.57
1:C:611:LEU:HD22	1:C:1659:ARG:HD2	1.87	0.57
1:C:2159:PRO:HB3	1:C:2206:ILE:HD12	1.86	0.57
1:E:1087:ILE:HD12	1:E:1128:LEU:HD23	1.85	0.57
1:E:3945:VAL:HG13	1:E:3979:MET:HE3	1.85	0.57
1:C:3879:LEU:HD11	1:C:3921:LEU:HD12	1.85	0.57
1:G:4014:ILE:HG22	1:G:4018:PHE:CE2	2.40	0.56
1:C:1519:THR:HG22	1:C:1529:THR:HG22	1.87	0.56
1:C:1680:VAL:HG11	1:C:1709:ILE:HD13	1.88	0.56
1:C:4618:TYR:OH	1:C:4633:ASP:HB2	2.05	0.56
1:A:2130:LEU:HA	1:A:2174:VAL:HG22	1.88	0.56
1:E:4618:TYR:OH	1:E:4633:ASP:HB2	2.06	0.56
2:D:25:HIS:CD2	2:D:104:LEU:HD11	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1534:GLU:HG2	1:A:1539:LEU:HD11	1.87	0.56
1:A:3959:LEU:HD22	1:A:3965:GLN:HB3	1.87	0.56
1:C:673:TRP:CH2	1:C:825:ALA:HB2	2.40	0.56
1:G:4652:LYS:HG3	1:G:4672:LEU:HD23	1.88	0.56
1:G:3911:ILE:HD11	1:G:3975:LEU:HB2	1.88	0.55
1:A:4137:ILE:HG23	1:A:4151:PHE:HE2	1.71	0.55
1:E:2159:PRO:HB3	1:E:2206:ILE:HD12	1.89	0.55
1:A:1105:PHE:HB2	1:A:1115:VAL:HG21	1.87	0.55
2:B:25:HIS:CD2	2:B:104:LEU:HD11	2.41	0.55
1:C:4097:PHE:CZ	1:C:4152:GLU:HB2	2.41	0.55
1:G:4146:ILE:HD11	1:G:4958:ASP:HB3	1.87	0.55
1:A:749:LEU:HD22	1:A:755:ILE:HD11	1.88	0.55
1:A:1521:ILE:HG22	1:A:1526:GLU:HA	1.88	0.55
1:A:2861:LEU:HD22	1:A:2872:LEU:HD11	1.88	0.55
1:A:4191:VAL:HG21	1:A:4951:TRP:CH2	2.42	0.55
1:C:2067:VAL:HG11	1:C:3645:LEU:HD22	1.88	0.55
1:C:2067:VAL:HG21	1:C:3645:LEU:HD13	1.89	0.55
1:C:3690:MET:N	1:C:3690:MET:HE3	2.21	0.55
1:C:4146:ILE:HD11	1:C:4958:ASP:HB3	1.88	0.55
1:E:4137:ILE:HG23	1:E:4151:PHE:HE2	1.72	0.55
1:C:1261:VAL:HG11	1:C:1270:VAL:HG11	1.87	0.55
1:E:207:PHE:CE2	1:G:2326:ILE:HD12	2.42	0.55
1:E:655:MET:HE1	1:E:1619:VAL:HG21	1.89	0.55
1:A:2162:MET:HE3	1:A:2167:MET:SD	2.46	0.55
1:C:4014:ILE:HG22	1:C:4018:PHE:CE2	2.42	0.55
1:C:1911:GLN:HB2	1:C:2087:LEU:HD11	1.88	0.55
1:C:3911:ILE:HD11	1:C:3975:LEU:HB2	1.88	0.55
1:E:3614:ARG:O	1:E:3618:VAL:HG23	2.06	0.55
1:E:4192:ASN:C	1:E:4192:ASN:HD22	2.14	0.55
1:G:2192:MET:HE3	1:G:2193:VAL:HG22	1.88	0.55
1:G:2861:LEU:HD22	1:G:2872:LEU:HD11	1.87	0.55
1:C:436:LEU:HD22	1:C:518:ALA:HA	1.89	0.55
1:C:872:ILE:HD13	1:C:873:VAL:N	2.21	0.55
1:E:2497:LEU:HD11	1:E:2873:VAL:HG12	1.90	0.55
1:G:3924:TYR:HB2	1:G:3925:ILE:HD12	1.89	0.55
1:C:1522:ALA:HB3	1:C:1527:LEU:HD11	1.87	0.54
1:C:4191:VAL:HG11	1:C:4951:TRP:CH2	2.43	0.54
2:F:25:HIS:CD2	2:F:104:LEU:HD11	2.42	0.54
1:G:3614:ARG:O	1:G:3618:VAL:HG23	2.07	0.54
1:A:1511:VAL:HA	1:A:1517:LEU:HD13	1.89	0.54
1:A:544:ASN:HB2	1:A:547:ASN:HD22	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4199:PHE:CZ	1:A:4602:PHE:CD1	2.96	0.54
2:B:82:TYR:CD2	2:B:91:ILE:HG21	2.42	0.54
1:E:2175:MET:HE2	1:E:2193:VAL:HG13	1.89	0.54
1:G:1736:ILE:HG13	1:G:1753:LEU:HD23	1.89	0.54
1:A:1268:ILE:HD11	1:A:1302:TYR:CE1	2.43	0.54
1:E:1173:MET:HE3	1:E:1195:PHE:CZ	2.43	0.54
2:H:26:TYR:H	2:H:39:SER:HG	1.51	0.54
1:C:3614:ARG:O	1:C:3618:VAL:HG23	2.07	0.54
1:A:3614:ARG:O	1:A:3618:VAL:HG23	2.06	0.54
1:A:4014:ILE:HG22	1:A:4018:PHE:CE2	2.42	0.54
1:A:2067:VAL:HG21	1:A:3645:LEU:HD13	1.90	0.54
1:C:74:LEU:HD11	1:C:117:HIS:CE1	2.43	0.54
1:C:3804:LEU:HD13	1:C:3910:ALA:HB2	1.89	0.54
1:C:360:ILE:HD11	1:C:402:GLY:HA3	1.89	0.54
1:C:2266:VAL:HG21	1:C:2324:LEU:HD13	1.89	0.54
1:E:4619:ILE:HD12	1:E:4668:ILE:HD12	1.90	0.54
1:G:1096:VAL:HG11	1:G:1101:TRP:CD1	2.43	0.54
1:G:1218:GLY:HA2	1:G:1224:LEU:HD11	1.90	0.54
1:G:2470:VAL:HG21	1:G:2523:THR:CG2	2.38	0.53
1:E:1521:ILE:HG22	1:E:1526:GLU:HA	1.90	0.53
1:G:3693:ALA:HB1	1:G:3758:ALA:O	2.08	0.53
1:A:828:PRO:HG3	1:A:1033:VAL:HG11	1.91	0.53
1:C:1831:MET:HE1	1:C:1833:ILE:HD13	1.91	0.53
1:C:3862:GLN:HE21	1:C:3865:ASN:HD22	1.55	0.53
1:G:601:LEU:HD23	1:G:642:LEU:HD21	1.89	0.53
1:G:1831:MET:HE1	1:G:1833:ILE:HD13	1.91	0.53
1:G:4618:TYR:OH	1:G:4633:ASP:HB2	2.08	0.53
1:A:1460:ASP:HA	1:A:1496:UNK:H2	1.74	0.53
1:A:4570:MET:HA	1:A:4573:THR:HG22	1.91	0.53
1:E:4198:ILE:CG1	1:E:4925:MET:HE1	2.38	0.53
1:G:618:CYS:SG	1:G:619:VAL:HG23	2.49	0.53
1:G:749:LEU:HD22	1:G:755:ILE:HD11	1.90	0.53
1:C:591:GLU:HA	1:C:631:LEU:HD21	1.90	0.53
1:A:4191:VAL:HG21	1:A:4951:TRP:CZ3	2.43	0.53
1:A:611:LEU:HD22	1:A:1659:ARG:HD2	1.91	0.53
1:A:4076:ASN:HB3	1:A:4078:THR:HG22	1.91	0.53
1:C:309:MET:HE2	1:C:317:MET:HE2	1.91	0.53
1:E:360:ILE:HD11	1:E:402:GLY:HA3	1.91	0.53
1:G:828:PRO:HG3	1:G:1033:VAL:HG11	1.90	0.52
1:G:1680:VAL:HG11	1:G:1709:ILE:HD13	1.90	0.52
1:E:4195:GLU:HA	1:E:4198:ILE:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4101:VAL:HG13	1:G:4150:TYR:HB2	1.91	0.52
1:C:688:ALA:HB1	1:C:691:THR:CB	2.39	0.52
1:G:4199:PHE:CZ	1:G:4602:PHE:CD1	2.97	0.52
1:C:688:ALA:HB1	1:C:691:THR:HB	1.91	0.52
1:C:2178:VAL:HG11	1:C:2192:MET:HE2	1.91	0.52
1:E:2790:ILE:HG12	1:E:2904:VAL:HG12	1.92	0.52
1:E:2178:VAL:HG11	1:E:2192:MET:HE2	1.91	0.52
1:G:3911:ILE:O	1:G:3911:ILE:HD13	2.09	0.52
1:A:35:LEU:HD22	1:A:49:LEU:HD13	1.91	0.52
1:E:4199:PHE:CZ	1:E:4602:PHE:CD1	2.97	0.52
1:E:4617:LEU:HA	1:E:4621:GLU:HB3	1.92	0.52
1:C:995:MET:HE1	1:C:1064:LEU:HD13	1.92	0.52
1:C:1894:LEU:HD12	1:C:2069:TRP:CZ2	2.44	0.52
1:G:1725:PHE:HB3	1:G:2105:THR:HG22	1.92	0.52
2:H:25:HIS:CD2	2:H:104:LEU:HD11	2.44	0.52
1:C:119:ILE:HG21	1:C:162:ILE:HD11	1.92	0.52
1:E:2718:LEU:HD22	1:E:2780:LEU:HD22	1.92	0.52
1:G:21:VAL:HG13	1:G:217:ILE:HD11	1.92	0.52
1:A:872:ILE:HD11	1:A:944:LEU:HD13	1.92	0.52
1:E:778:MET:O	1:E:1468:THR:OG1	2.28	0.52
1:E:1105:PHE:HB2	1:E:1115:VAL:HG21	1.91	0.52
1:G:1689:ILE:HD11	1:G:1790:LYS:HD3	1.91	0.52
1:E:633:CYS:SG	1:E:1669:ASN:ND2	2.83	0.52
1:G:935:MET:O	1:G:939:THR:HG23	2.10	0.52
1:G:2159:PRO:HB3	1:G:2206:ILE:HD12	1.92	0.52
1:C:572:LEU:HD13	1:C:609:LYS:HB2	1.90	0.51
1:E:611:LEU:HD22	1:E:1659:ARG:CD	2.40	0.51
1:G:1794:MET:HA	1:G:1794:MET:HE2	1.93	0.51
1:A:307:SER:HB3	1:A:327:THR:HG22	1.93	0.51
1:A:2159:PRO:HB3	1:A:2206:ILE:HD12	1.92	0.51
1:C:3693:ALA:HB1	1:C:3758:ALA:O	2.10	0.51
1:E:804:LEU:HD22	1:E:822:CYS:HB3	1.92	0.51
1:G:2119:LEU:HD11	1:G:2162:MET:HE1	1.92	0.51
1:A:3891:TRP:CZ2	1:G:76:ARG:HB2	2.45	0.51
2:B:26:TYR:N	2:B:39:SER:HG	2.08	0.51
1:C:4137:ILE:HG23	1:C:4151:PHE:CE2	2.45	0.51
1:C:3778:MET:CE	1:C:3847:LEU:HD22	2.34	0.51
1:E:4130:PHE:O	1:E:4134:LEU:N	2.43	0.51
1:A:633:CYS:SG	1:A:1669:ASN:ND2	2.83	0.51
1:E:991:SER:HB3	1:E:1066:ALA:HB2	1.93	0.51
1:G:436:LEU:HD11	1:G:447:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:541:ILE:HD12	1:E:578:VAL:HG22	1.93	0.51
1:E:659:ILE:HG23	1:E:825:ALA:HB1	1.92	0.51
1:E:745:ASN:HB2	1:E:771:ASN:HD21	1.75	0.51
1:G:1726:ILE:HG21	1:G:2120:LEU:HD21	1.92	0.51
1:C:436:LEU:HD13	1:C:518:ALA:HB2	1.91	0.51
1:C:4619:ILE:HD12	1:C:4668:ILE:HD12	1.93	0.51
1:G:4187:MET:HE3	1:G:4954:PHE:HB3	1.93	0.51
1:E:888:ASN:ND2	1:E:1056:THR:HG21	2.25	0.51
1:E:1105:PHE:CB	1:E:1115:VAL:HG21	2.41	0.51
1:A:4958:ASP:O	1:A:4962:LYS:HB2	2.11	0.51
1:E:693:LEU:HD22	1:E:798:ILE:HD13	1.92	0.51
1:E:4191:VAL:HG21	1:E:4951:TRP:CZ3	2.46	0.51
1:E:143:LEU:HD21	1:E:207:PHE:CE2	2.47	0.50
1:E:2170:THR:O	1:E:2174:VAL:HG23	2.11	0.50
1:G:888:ASN:ND2	1:G:1056:THR:HG21	2.26	0.50
1:A:1830:ILE:HG22	1:A:1912:TYR:CD1	2.46	0.50
1:E:436:LEU:HD22	1:E:518:ALA:HA	1.94	0.50
1:G:660:PHE:CD2	1:G:827:LEU:HD11	2.45	0.50
1:G:3689:TYR:OH	1:G:3744:THR:HG21	2.11	0.50
2:F:82:TYR:CD2	2:F:91:ILE:HG21	2.47	0.50
1:C:677:LEU:HD22	1:C:695:VAL:HG21	1.93	0.50
1:E:633:CYS:CB	1:E:1672:VAL:HG11	2.40	0.50
2:B:26:TYR:H	2:B:39:SER:HG	1.59	0.50
1:E:4103:LEU:HD12	1:E:4127:LEU:HD11	1.94	0.50
1:G:2067:VAL:HG21	1:G:3645:LEU:HD13	1.93	0.50
1:G:3745:ILE:HG13	1:G:3759:THR:HG21	1.93	0.50
1:C:2470:VAL:HG21	1:C:2523:THR:CG2	2.42	0.50
1:E:915:HIS:HB3	1:E:918:LEU:HD13	1.93	0.50
1:G:688:ALA:HB3	1:G:795:SER:OG	2.12	0.50
1:C:633:CYS:CB	1:C:1672:VAL:HG11	2.41	0.50
1:C:655:MET:HE2	1:C:834:VAL:CG1	2.41	0.50
1:G:872:ILE:HD11	1:G:944:LEU:HD13	1.92	0.50
1:C:1116:GLY:O	1:C:1204:VAL:HG12	2.11	0.50
1:C:4927:LEU:HD11	1:C:4942:VAL:HG13	1.94	0.50
1:G:4097:PHE:CZ	1:G:4152:GLU:HB2	2.46	0.50
1:A:759:LEU:HD13	1:A:766:ILE:CG1	2.41	0.49
1:A:4617:LEU:HD13	1:A:4621:GLU:HB3	1.94	0.49
1:C:72:SER:C	1:C:73:LEU:HD22	2.37	0.49
1:C:177:VAL:HG13	1:C:216:PRO:HD3	1.94	0.49
1:C:1794:MET:HA	1:C:1794:MET:HE2	1.94	0.49
1:E:3941:LEU:HD21	1:E:3982:MET:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:HIS:HB3	1:A:918:LEU:HD13	1.93	0.49
1:A:1507:ILE:HB	1:A:1521:ILE:HG13	1.94	0.49
1:A:2718:LEU:HD22	1:A:2780:LEU:HD22	1.94	0.49
1:C:4912:LEU:HA	1:C:4916:ASN:HB3	1.93	0.49
1:E:4912:LEU:HA	1:E:4916:ASN:HB3	1.94	0.49
1:G:2423:ILE:HD13	1:G:2423:ILE:O	2.10	0.49
1:G:3890:TYR:HD1	1:G:3955:MET:HE3	1.77	0.49
1:E:648:LEU:HD23	1:E:1684:GLN:HA	1.95	0.49
1:E:826:VAL:HG21	1:E:832:LEU:HD22	1.95	0.49
1:G:177:VAL:HG13	1:G:216:PRO:HD3	1.94	0.49
1:G:2159:PRO:CB	1:G:2206:ILE:HD12	2.43	0.49
1:G:2497:LEU:CD1	1:G:2873:VAL:HG12	2.43	0.49
1:A:4912:LEU:HA	1:A:4916:ASN:HB3	1.94	0.49
1:C:181:LEU:HD12	1:C:214:VAL:HG21	1.94	0.49
1:E:1259:LEU:HD13	1:E:1599:MET:HE1	1.94	0.49
1:E:3899:ILE:HD12	1:E:3959:LEU:HD23	1.93	0.49
1:E:4191:VAL:HG11	1:E:4951:TRP:CH2	2.46	0.49
1:A:165:ALA:HB1	1:A:211:LEU:HD11	1.94	0.49
1:A:2473:LEU:HD21	1:A:2484:PHE:CE2	2.47	0.49
1:C:4046:LYS:HG2	1:C:4079:LEU:HD21	1.93	0.49
1:E:1782:PHE:CE2	1:E:1787:LEU:HD22	2.47	0.49
1:G:1689:ILE:HD11	1:G:1790:LYS:CD	2.43	0.49
1:C:3911:ILE:HD13	1:C:3911:ILE:O	2.12	0.49
2:F:78:PRO:HA	2:F:81:ALA:HB3	1.93	0.49
1:G:826:VAL:HG21	1:G:832:LEU:HD22	1.94	0.49
1:G:4912:LEU:HA	1:G:4916:ASN:HB3	1.94	0.49
1:G:4958:ASP:O	1:G:4962:LYS:HB2	2.11	0.49
1:A:2304:ARG:HB2	1:A:2399:LEU:HD21	1.94	0.49
1:C:1445:TRP:CD1	1:C:1518:LEU:HD22	2.47	0.49
1:C:1826:TYR:CZ	1:C:1908:LEU:HD22	2.47	0.49
1:E:4617:LEU:HD13	1:E:4621:GLU:HB3	1.93	0.49
1:A:2470:VAL:HG11	1:A:2523:THR:HG22	1.94	0.49
1:C:28:ILE:CG1	1:C:201:LEU:HD11	2.42	0.49
1:C:1105:PHE:CB	1:C:1115:VAL:HG21	2.42	0.49
1:C:4958:ASP:O	1:C:4962:LYS:HB2	2.13	0.49
1:E:766:ILE:HB	1:E:779:PHE:HB2	1.95	0.49
1:G:660:PHE:CE2	1:G:827:LEU:HD11	2.48	0.49
1:G:3802:SER:HB2	1:G:3837:THR:HG21	1.95	0.49
1:A:3861:THR:HG23	1:A:3863:THR:HG23	1.94	0.48
1:G:1782:PHE:CE2	1:G:1787:LEU:HD22	2.47	0.48
1:E:601:LEU:HD23	1:E:642:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:881:ILE:HD11	1:E:1060:TYR:CD2	2.47	0.48
1:G:759:LEU:HD13	1:G:766:ILE:HG12	1.95	0.48
1:E:1087:ILE:HD12	1:E:1128:LEU:CD2	2.43	0.48
1:E:4099:VAL:O	1:E:4103:LEU:HG	2.13	0.48
1:G:1830:ILE:HG22	1:G:1912:TYR:CD1	2.48	0.48
1:E:2172:MET:HE3	1:E:2214:MET:HE1	1.95	0.48
1:E:2861:LEU:HD22	1:E:2872:LEU:HD11	1.94	0.48
1:E:3806:LEU:HD13	1:E:3889:PHE:HA	1.96	0.48
1:G:1475:LYS:O	1:G:1476:VAL:HG22	2.12	0.48
1:G:1483:SER:HB2	1:G:1533:VAL:HG23	1.94	0.48
1:G:4922:PHE:HA	1:G:4925:MET:HG2	1.93	0.48
1:A:2473:LEU:HD21	1:A:2484:PHE:HE2	1.78	0.48
1:C:579:LEU:HD22	1:C:586:LEU:HD23	1.95	0.48
1:C:3683:LEU:HD21	1:C:3747:ALA:HB1	1.95	0.48
1:C:3690:MET:HE2	1:C:3755:MET:HA	1.95	0.48
1:E:2783:MET:HE1	1:E:2897:LEU:CD1	2.43	0.48
1:E:3926:GLN:HA	1:E:3926:GLN:HE21	1.77	0.48
2:F:4:ILE:CD1	2:F:74:LEU:HD22	2.43	0.48
1:G:579:LEU:HD22	1:G:586:LEU:HD23	1.94	0.48
1:G:4496:LEU:HD22	1:G:4591:GLY:HA3	1.95	0.48
1:A:496:ASN:HA	1:A:499:LEU:HD12	1.95	0.48
2:B:4:ILE:CD1	2:B:74:LEU:HD22	2.44	0.48
1:C:73:LEU:C	1:C:74:LEU:HD12	2.39	0.48
1:C:541:ILE:HD12	1:C:578:VAL:HG22	1.95	0.48
1:E:1094:TYR:OH	1:E:1808:ASP:OD1	2.26	0.48
1:E:4192:ASN:HD22	1:E:4193:PHE:N	2.11	0.48
2:F:56:ILE:HD13	2:F:82:TYR:CZ	2.48	0.48
1:G:869:THR:HG21	1:G:1002:ASN:HD21	1.77	0.48
1:A:1726:ILE:HG21	1:A:2120:LEU:HD21	1.95	0.48
1:E:986:ILE:HD13	1:E:1058:LEU:HB3	1.96	0.48
1:G:309:MET:HE2	1:G:317:MET:HE2	1.96	0.48
1:C:2123:LEU:HD12	1:C:2127:ARG:NE	2.29	0.48
1:C:3737:ALA:HA	1:C:3740:MET:HG2	1.96	0.48
1:E:4922:PHE:HA	1:E:4925:MET:HG2	1.94	0.48
1:G:759:LEU:HD13	1:G:766:ILE:CG1	2.44	0.48
1:G:1105:PHE:CB	1:G:1115:VAL:HG21	2.42	0.48
1:C:3775:GLN:NE2	1:C:3847:LEU:O	2.47	0.48
1:C:76:ARG:CB	1:E:3891:TRP:CZ2	2.97	0.48
1:C:3778:MET:HE1	1:C:3847:LEU:CD2	2.35	0.48
1:C:4137:ILE:HG23	1:C:4151:PHE:HE2	1.78	0.48
1:C:4570:MET:HA	1:C:4573:THR:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1686:LEU:HD22	1:E:1790:LYS:HE3	1.95	0.48
1:G:4521:TYR:CZ	1:G:4562:VAL:HG22	2.49	0.48
1:C:230:GLY:HA3	1:C:289:ILE:HD11	1.95	0.47
1:C:4617:LEU:HD13	1:C:4621:GLU:HB3	1.96	0.47
1:E:4652:LYS:HG3	1:E:4672:LEU:HD23	1.95	0.47
1:G:237:LEU:HD23	1:G:244:CYS:SG	2.53	0.47
1:G:436:LEU:HD13	1:G:518:ALA:HB2	1.95	0.47
1:C:559:ILE:HG21	1:C:593:HIS:HA	1.96	0.47
1:C:3802:SER:HB2	1:C:3837:THR:HG21	1.96	0.47
1:E:2497:LEU:CD1	1:E:2873:VAL:HG12	2.45	0.47
1:E:2861:LEU:HD22	1:E:2872:LEU:CD1	2.45	0.47
1:E:4869:ILE:HG21	1:G:4869:ILE:HG23	1.95	0.47
1:E:4923:PHE:HZ	1:E:4942:VAL:HG11	1.79	0.47
1:G:4619:ILE:HD12	1:G:4668:ILE:HD12	1.96	0.47
1:A:3745:ILE:HG13	1:A:3759:THR:HG21	1.96	0.47
1:C:652:VAL:HG11	1:C:692:HIS:CD2	2.49	0.47
1:C:2498:ARG:CB	1:C:2517:LEU:HD11	2.45	0.47
1:E:1707:ILE:HG23	1:E:1827:THR:HG21	1.97	0.47
1:G:4104:THR:HG21	1:G:4134:LEU:HD11	1.97	0.47
1:A:4515:ASN:HD22	1:A:4745:LEU:HD21	1.80	0.47
1:C:935:MET:O	1:C:939:THR:HG23	2.14	0.47
1:C:52:THR:HG22	1:C:60:PRO:CB	2.45	0.47
1:C:1521:ILE:HG22	1:C:1526:GLU:HA	1.96	0.47
1:A:614:LEU:HD13	1:A:636:LEU:HD11	1.95	0.47
1:A:1686:LEU:HD22	1:A:1790:LYS:HE3	1.97	0.47
1:A:4619:ILE:HD12	1:A:4668:ILE:HD12	1.97	0.47
1:C:943:LEU:HD23	1:C:999:LEU:HD11	1.95	0.47
1:C:1303:ARG:HG2	1:C:1542:ALA:HB2	1.97	0.47
1:E:4923:PHE:CZ	1:E:4942:VAL:HG11	2.50	0.47
1:G:430:ILE:HD11	1:G:501:CYS:SG	2.55	0.47
1:G:1658:LEU:HD23	1:G:1701:GLY:HA3	1.96	0.47
1:C:2779:SER:OG	1:C:2849:TYR:OH	2.31	0.47
1:E:3752:THR:HG23	1:E:3836:PHE:CE2	2.50	0.47
1:G:826:VAL:HG13	1:G:832:LEU:HD13	1.97	0.47
1:G:1521:ILE:HG22	1:G:1526:GLU:HA	1.97	0.47
1:G:3911:ILE:HG12	1:G:3975:LEU:HD22	1.97	0.47
1:A:559:ILE:HG12	1:A:575:LEU:HD11	1.97	0.47
1:A:995:MET:HE1	1:A:1064:LEU:HD13	1.96	0.47
1:A:3866:ASN:OD1	1:A:3867:THR:HG23	2.14	0.47
1:A:4652:LYS:HG3	1:A:4672:LEU:HD23	1.97	0.47
1:C:655:MET:HE2	1:C:834:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2259:GLU:N	1:C:2260:PRO:HD2	2.30	0.47
1:C:3911:ILE:HG12	1:C:3975:LEU:HD22	1.97	0.47
1:E:660:PHE:CD2	1:E:827:LEU:HD11	2.50	0.47
1:E:749:LEU:HD22	1:E:755:ILE:HD11	1.97	0.47
1:G:1090:ALA:HB3	1:G:1202:ILE:CG2	2.45	0.47
1:G:3804:LEU:HD13	1:G:3910:ALA:HB2	1.97	0.47
1:A:629:GLN:CD	1:A:1666:ALA:HB1	2.40	0.47
1:A:4160:GLN:HG2	1:A:4201:MET:HA	1.97	0.47
1:C:1910:LEU:HG	1:C:2062:ILE:HD12	1.97	0.47
1:E:919:VAL:HG21	1:E:923:LYS:HD3	1.96	0.47
1:G:436:LEU:HD22	1:G:518:ALA:HA	1.96	0.47
1:C:1087:ILE:HD12	1:C:1128:LEU:CD2	2.45	0.46
1:C:1118:SER:CB	1:C:1204:VAL:HG11	2.45	0.46
1:G:737:ILE:HG21	1:G:1481:LYS:HG2	1.98	0.46
1:G:4137:ILE:HG23	1:G:4151:PHE:HE2	1.78	0.46
1:C:1118:SER:HB3	1:C:1204:VAL:HG11	1.98	0.46
2:D:16:PRO:HG3	2:D:106:LEU:HD21	1.97	0.46
1:E:580:VAL:HG23	1:E:581:GLU:HG2	1.97	0.46
1:E:1831:MET:CE	1:E:1833:ILE:HD13	2.43	0.46
1:E:4607:GLU:O	1:E:4611:LYS:HG2	2.15	0.46
1:C:618:CYS:SG	1:C:1666:ALA:HA	2.55	0.46
1:C:1218:GLY:O	1:C:1240:ALA:HB3	2.15	0.46
1:C:2023:LEU:N	1:C:2023:LEU:HD23	2.31	0.46
1:G:2493:PHE:O	1:G:2497:LEU:HG	2.15	0.46
1:G:2498:ARG:HB3	1:G:2517:LEU:HD11	1.98	0.46
1:A:496:ASN:HD22	1:A:499:LEU:HD12	1.79	0.46
1:A:4611:LYS:O	1:A:4616:GLY:N	2.49	0.46
1:C:2075:ILE:HD11	1:C:2080:LEU:HD23	1.97	0.46
1:C:3756:VAL:HG13	1:C:3836:PHE:CE1	2.51	0.46
1:E:2491:VAL:O	1:E:2495:PRO:HD2	2.16	0.46
1:E:3737:ALA:HA	1:E:3740:MET:HG2	1.96	0.46
1:G:804:LEU:HD22	1:G:822:CYS:HB3	1.96	0.46
1:G:3737:ALA:HA	1:G:3740:MET:HG2	1.98	0.46
1:G:3899:ILE:HD12	1:G:3959:LEU:HD23	1.97	0.46
1:A:572:LEU:HD13	1:A:609:LYS:HB2	1.98	0.46
1:A:1794:MET:HE2	1:A:1794:MET:HA	1.97	0.46
1:A:2783:MET:HE3	1:A:2845:MET:HE2	1.98	0.46
1:A:4939:GLU:HA	1:A:4942:VAL:HG12	1.98	0.46
1:C:4611:LYS:O	1:C:4616:GLY:N	2.49	0.46
1:E:1475:LYS:O	1:E:1476:VAL:HG22	2.16	0.46
1:E:4927:LEU:HD11	1:E:4942:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:778:MET:O	1:A:1468:THR:OG1	2.33	0.46
1:A:3737:ALA:HA	1:A:3740:MET:HG2	1.98	0.46
1:C:944:LEU:HD21	1:C:950:VAL:HG22	1.97	0.46
1:E:579:LEU:HD22	1:E:586:LEU:HD23	1.98	0.46
1:E:996:VAL:HG12	1:E:1054:VAL:HG11	1.97	0.46
1:E:1300:MET:HE2	1:E:1545:ALA:HB3	1.97	0.46
1:E:3693:ALA:HB1	1:E:3758:ALA:O	2.15	0.46
1:G:4617:LEU:HD13	1:G:4621:GLU:HB3	1.98	0.46
1:A:541:ILE:HG22	1:A:547:ASN:HB3	1.97	0.46
1:C:601:LEU:HD23	1:C:642:LEU:HD21	1.96	0.46
1:C:3983:LEU:HD22	1:C:4000:MET:HE2	1.98	0.46
1:E:739:ARG:CZ	1:E:1467:VAL:HG13	2.45	0.46
1:E:4501:TYR:OH	1:E:4595:LEU:HD21	2.15	0.46
1:G:633:CYS:CB	1:G:1672:VAL:HG11	2.46	0.46
1:G:1253:LYS:NZ	1:G:1601:ASN:HD22	2.14	0.46
1:C:2485:LEU:HD11	1:C:2527:PRO:HB3	1.98	0.46
1:G:1738:LEU:HD12	1:G:1921:ARG:HA	1.97	0.46
1:A:194:LEU:HD11	1:A:201:LEU:HD13	1.98	0.46
1:C:4198:ILE:HG23	1:C:4925:MET:CE	2.46	0.46
1:E:3797:LEU:HD21	1:E:3836:PHE:HE2	1.80	0.46
2:F:75:THR:HG23	2:F:98:ILE:CD1	2.46	0.46
1:G:2170:THR:O	1:G:2174:VAL:HG23	2.15	0.46
1:C:230:GLY:CA	1:C:289:ILE:HD11	2.46	0.46
1:C:743:SER:OG	1:C:775:VAL:HG22	2.16	0.46
1:C:4794:PHE:HB2	1:C:4833:ILE:HD11	1.98	0.46
1:A:1105:PHE:CB	1:A:1115:VAL:HG21	2.46	0.45
1:A:2170:THR:O	1:A:2174:VAL:HG23	2.16	0.45
1:A:2521:LEU:HD11	1:A:2601:UNK:CB	2.46	0.45
2:B:75:THR:HG23	2:B:98:ILE:CD1	2.46	0.45
1:E:611:LEU:HD22	1:E:1659:ARG:CG	2.45	0.45
1:E:4958:ASP:O	1:E:4962:LYS:HB2	2.16	0.45
1:G:541:ILE:HG22	1:G:547:ASN:HB3	1.97	0.45
1:G:3966:ILE:O	1:G:3969:LEU:N	2.49	0.45
1:A:2086:VAL:HG13	1:A:2087:LEU:HD12	1.98	0.45
1:C:670:TYR:O	1:C:673:TRP:NE1	2.49	0.45
1:C:1782:PHE:CE2	1:C:1787:LEU:HD22	2.51	0.45
1:C:3992:VAL:HG13	1:C:4964:TYR:CE2	2.51	0.45
1:E:476:GLN:HE21	1:E:476:GLN:HA	1.81	0.45
1:E:559:ILE:HD12	1:E:596:SER:HB2	1.98	0.45
1:E:3966:ILE:O	1:E:3969:LEU:N	2.48	0.45
1:G:3844:LEU:HD13	1:G:3847:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:PRO:HD2	1:A:878:LEU:HD12	1.98	0.45
1:C:3955:MET:HE2	1:C:3955:MET:HA	1.99	0.45
1:C:4617:LEU:HA	1:C:4621:GLU:HB3	1.98	0.45
1:G:4165:GLN:HG3	1:G:4501:TYR:CZ	2.52	0.45
1:C:112:THR:HG21	1:C:174:LYS:HD3	1.99	0.45
1:C:2423:ILE:HD13	1:C:2423:ILE:O	2.16	0.45
1:G:1094:TYR:OH	1:G:1808:ASP:OD1	2.33	0.45
1:A:3983:LEU:HD22	1:A:4000:MET:HE2	1.98	0.45
1:E:1253:LYS:NZ	1:E:1601:ASN:HD22	2.14	0.45
1:E:3952:PHE:HZ	1:E:3975:LEU:HD23	1.82	0.45
1:E:4152:GLU:HB3	1:E:4926:TYR:CD1	2.50	0.45
1:G:611:LEU:HD22	1:G:1659:ARG:HD2	1.98	0.45
1:A:996:VAL:HG12	1:A:1054:VAL:HG11	1.99	0.45
1:E:2023:LEU:N	1:E:2023:LEU:HD23	2.30	0.45
1:G:1299:ILE:HG23	1:G:1301:PHE:CE1	2.52	0.45
1:G:4130:PHE:O	1:G:4134:LEU:N	2.50	0.45
1:C:2513:MET:O	1:C:2517:LEU:HD13	2.17	0.45
1:G:689:GLU:O	1:G:691:THR:HG22	2.16	0.45
1:G:2896:PHE:HA	1:G:2899:ILE:HG12	1.98	0.45
1:E:459:LEU:HB3	1:E:536:LEU:HD13	1.99	0.45
1:E:1692:LYS:HG2	1:E:1810:VAL:HG13	1.97	0.45
1:E:1914:CYS:HB2	1:E:2091:GLN:HE22	1.82	0.45
1:E:2259:GLU:N	1:E:2260:PRO:HD2	2.32	0.45
1:G:598:ILE:HG23	1:G:642:LEU:HD22	1.99	0.45
1:G:2259:GLU:N	1:G:2260:PRO:HD2	2.31	0.45
1:A:1782:PHE:CE2	1:A:1787:LEU:HD22	2.52	0.45
1:C:2095:ILE:HD11	1:C:3630:ILE:HG22	1.99	0.45
1:C:2176:VAL:HG22	1:C:2224:ASN:HD21	1.81	0.45
1:A:804:LEU:HD22	1:A:822:CYS:HB3	1.98	0.45
1:C:4496:LEU:HD22	1:C:4591:GLY:HA3	1.99	0.45
1:E:739:ARG:NE	1:E:1467:VAL:HG13	2.32	0.45
1:E:935:MET:O	1:E:939:THR:HG23	2.17	0.45
1:E:4137:ILE:HG23	1:E:4151:PHE:CE2	2.50	0.45
1:E:4939:GLU:HA	1:E:4942:VAL:HG12	1.99	0.45
1:G:217:ILE:HG22	1:G:286:GLY:HA3	2.00	0.45
1:G:4611:LYS:O	1:G:4616:GLY:N	2.50	0.45
1:A:633:CYS:CB	1:A:1672:VAL:HG11	2.47	0.44
1:A:759:LEU:HD13	1:A:766:ILE:HG12	1.98	0.44
1:A:826:VAL:HG21	1:A:832:LEU:HD22	1.99	0.44
1:A:2473:LEU:HD13	1:A:2473:LEU:O	2.17	0.44
1:A:3911:ILE:HD11	1:A:3975:LEU:HD22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4195:GLU:HA	1:A:4198:ILE:HD12	2.00	0.44
1:E:2067:VAL:HG11	1:E:3645:LEU:HD22	1.99	0.44
1:G:2266:VAL:HG21	1:G:2324:LEU:HB3	1.99	0.44
1:A:4607:GLU:O	1:A:4611:LYS:HG2	2.17	0.44
1:C:1639:VAL:HG21	1:C:1644:LEU:HD23	1.99	0.44
1:E:1629:SER:HA	1:E:1640:ASP:HA	1.99	0.44
1:G:743:SER:OG	1:G:775:VAL:HG22	2.17	0.44
1:A:3956:GLN:HE21	1:A:4014:ILE:HG23	1.83	0.44
1:C:76:ARG:HB3	1:E:3891:TRP:CZ2	2.51	0.44
1:C:598:ILE:HG23	1:C:642:LEU:HD22	1.98	0.44
1:E:944:LEU:HD21	1:E:950:VAL:HG22	1.99	0.44
1:E:2473:LEU:HD21	1:E:2484:PHE:CE2	2.51	0.44
1:G:1847:GLU:CD	1:G:2061:LEU:HD22	2.43	0.44
1:G:2718:LEU:HD22	1:G:2780:LEU:HD22	1.99	0.44
1:G:4164:PRO:HG2	1:G:4166:VAL:HG22	2.00	0.44
1:G:679:VAL:HA	1:G:800:VAL:HG12	2.00	0.44
1:A:687:THR:HG22	1:A:797:GLY:C	2.42	0.44
1:A:2023:LEU:N	1:A:2023:LEU:HD23	2.32	0.44
1:A:4617:LEU:HA	1:A:4621:GLU:HB3	1.98	0.44
1:E:1689:ILE:HD11	1:E:1790:LYS:CD	2.47	0.44
1:E:2838:LEU:HD23	1:E:2841:MET:SD	2.57	0.44
1:A:4612:LEU:HD11	1:A:4637:ILE:HG12	2.00	0.44
1:C:2106:TYR:CG	1:C:2107:THR:N	2.85	0.44
1:E:2130:LEU:CA	1:E:2174:VAL:HG22	2.46	0.44
1:A:1253:LYS:NZ	1:A:1601:ASN:HD22	2.15	0.44
1:A:2259:GLU:N	1:A:2260:PRO:HD2	2.31	0.44
1:A:3992:VAL:HG13	1:A:4964:TYR:CE2	2.53	0.44
1:C:28:ILE:CD1	1:C:201:LEU:HD11	2.46	0.44
1:C:4191:VAL:HG21	1:C:4951:TRP:CZ3	2.52	0.44
1:C:4817:PHE:O	1:C:4821:VAL:HG22	2.18	0.44
1:C:4823:VAL:HG23	1:C:4824:ARG:HG3	1.99	0.44
1:E:826:VAL:CG2	1:E:832:LEU:HD13	2.48	0.44
1:E:3966:ILE:O	1:E:3967:GLU:C	2.61	0.44
1:G:1116:GLY:O	1:G:1204:VAL:HG12	2.18	0.44
1:G:3690:MET:HE3	1:G:3690:MET:N	2.32	0.44
1:G:3966:ILE:HD12	1:G:3969:LEU:HD23	1.99	0.44
1:G:3986:MET:SD	1:G:3996:ILE:HD11	2.57	0.44
1:A:1703:TYR:HB2	1:A:1820:PRO:HB3	1.99	0.44
1:A:1730:THR:O	1:A:1733:THR:OG1	2.33	0.44
1:A:4617:LEU:HA	1:A:4621:GLU:CB	2.48	0.44
1:C:4164:PRO:HG2	1:C:4166:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4611:LYS:O	1:E:4616:GLY:N	2.51	0.44
1:G:3697:ALA:HB2	1:G:3761:LYS:HB3	2.00	0.44
1:A:280:LEU:HD13	1:A:296:ARG:NH1	2.33	0.44
1:A:3775:GLN:NE2	1:A:3847:LEU:O	2.51	0.44
1:C:1090:ALA:HB3	1:C:1202:ILE:HG22	2.00	0.44
1:C:4846:ILE:CD1	1:E:4816:MET:HG3	2.47	0.44
1:E:759:LEU:HD13	1:E:766:ILE:CG1	2.48	0.44
1:G:737:ILE:HD13	1:G:1535:PRO:HG3	2.00	0.44
1:G:3879:LEU:HA	1:G:3882:VAL:HG22	2.00	0.44
1:A:655:MET:SD	1:A:1619:VAL:HG21	2.58	0.43
1:C:633:CYS:SG	1:C:1669:ASN:ND2	2.91	0.43
1:C:4191:VAL:HG21	1:C:4951:TRP:CH2	2.53	0.43
1:C:4607:GLU:O	1:C:4611:LYS:HG2	2.18	0.43
1:G:580:VAL:HG23	1:G:581:GLU:HG2	2.00	0.43
1:A:952:ILE:HD12	1:A:956:HIS:CE1	2.53	0.43
1:A:1090:ALA:HB3	1:A:1202:ILE:HG22	1.99	0.43
1:A:2075:ILE:CG1	1:A:2080:LEU:HD23	2.46	0.43
1:A:3802:SER:HB2	1:A:3837:THR:HG21	2.00	0.43
1:A:3804:LEU:HB3	1:A:3885:SER:HB3	2.00	0.43
1:C:1808:ASP:HB3	1:C:1809:PRO:HA	2.00	0.43
1:E:429:PHE:CD1	1:E:452:VAL:HG21	2.53	0.43
1:E:3916:GLN:O	1:E:3920:THR:HG23	2.19	0.43
1:G:895:MET:HE1	1:G:980:PRO:HD2	2.00	0.43
1:G:2874:PRO:O	1:G:2877:THR:OG1	2.36	0.43
1:G:3797:LEU:HD21	1:G:3836:PHE:CE2	2.53	0.43
1:A:463:PHE:HB3	1:A:539:ALA:HB1	2.00	0.43
1:A:611:LEU:HD22	1:A:1659:ARG:CD	2.48	0.43
1:A:2119:LEU:HD11	1:A:2162:MET:HE1	2.00	0.43
1:A:4496:LEU:HD12	1:A:4587:PHE:CZ	2.53	0.43
1:E:739:ARG:HG3	1:E:1469:LEU:HD21	2.01	0.43
1:E:1830:ILE:HG22	1:E:1912:TYR:CD1	2.53	0.43
1:E:1847:GLU:HB2	1:E:1848:PRO:HD3	2.00	0.43
1:A:580:VAL:HG23	1:A:581:GLU:HG2	2.00	0.43
1:A:2497:LEU:HD13	1:A:2874:PRO:HD2	1.99	0.43
1:A:4152:GLU:HB3	1:A:4926:TYR:CE1	2.53	0.43
1:A:4508:LEU:HD21	1:A:4748:ILE:HD13	2.00	0.43
1:A:4858:VAL:CG1	1:C:4864:ILE:HG21	2.49	0.43
1:C:2172:MET:HE3	1:C:2214:MET:HE1	1.99	0.43
1:C:2498:ARG:HB3	1:C:2517:LEU:HD11	1.99	0.43
1:C:4668:ILE:HD13	1:C:4671:LEU:HD12	2.00	0.43
1:C:4899:TYR:CE2	1:C:4962:LYS:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:629:GLN:CD	1:E:1666:ALA:HB1	2.43	0.43
1:E:1268:ILE:HG23	1:E:1268:ILE:O	2.18	0.43
1:E:4005:VAL:HG21	1:E:4115:ARG:HD3	2.00	0.43
1:G:364:GLN:HE21	1:G:369:GLY:HA2	1.83	0.43
1:G:656:ARG:NH2	1:G:835:GLU:OE2	2.51	0.43
1:G:4939:GLU:HA	1:G:4942:VAL:HG12	2.00	0.43
1:C:4651:VAL:O	1:C:4655:VAL:HG23	2.18	0.43
1:G:2155:PHE:HD1	1:G:2162:MET:HE2	1.83	0.43
1:A:2178:VAL:CG1	1:A:2192:MET:HE2	2.47	0.43
1:E:663:VAL:HG13	1:E:671:LYS:HD3	2.00	0.43
1:E:847:THR:HG21	1:E:1215:MET:O	2.18	0.43
1:E:1783:PRO:HB2	1:E:1786:ILE:HG22	2.01	0.43
1:E:1925:ILE:HD13	1:E:2032:LEU:HD21	2.00	0.43
1:G:2110:GLY:O	1:G:2113:VAL:HG13	2.18	0.43
1:G:2497:LEU:HD12	1:G:2873:VAL:HG12	2.01	0.43
1:A:4082:GLU:HA	1:A:4085:VAL:HG22	2.00	0.43
1:C:983:LEU:HD21	1:C:1056:THR:HG23	2.01	0.43
1:C:1783:PRO:HB2	1:C:1786:ILE:HG22	2.01	0.43
1:C:1894:LEU:HD11	1:C:2065:THR:HG21	2.01	0.43
1:C:3843:PHE:O	1:C:3847:LEU:HG	2.19	0.43
1:E:869:THR:HG21	1:E:1002:ASN:HD21	1.84	0.43
1:E:4178:VAL:HG21	1:E:4885:ASP:CG	2.44	0.43
1:E:4186:LYS:HE3	1:E:4187:MET:HE2	2.01	0.43
1:G:21:VAL:CG1	1:G:217:ILE:HD11	2.48	0.43
1:G:1808:ASP:HB3	1:G:1809:PRO:HA	2.00	0.43
1:G:2713:ILE:HD13	1:G:2714:ILE:N	2.34	0.43
1:G:4781:TYR:HA	1:G:4784:THR:HG22	2.00	0.43
1:C:2192:MET:HE3	1:C:2193:VAL:HA	2.00	0.43
1:E:1511:VAL:HA	1:E:1517:LEU:HD13	2.01	0.43
1:E:2497:LEU:HD13	1:E:2874:PRO:HD3	2.00	0.43
1:G:2023:LEU:N	1:G:2023:LEU:HD23	2.34	0.43
1:A:1808:ASP:HB3	1:A:1809:PRO:HA	2.00	0.43
1:A:1826:TYR:CZ	1:A:1908:LEU:HD22	2.54	0.43
1:A:4597:VAL:HA	1:A:4600:VAL:HG22	2.00	0.43
1:C:544:ASN:HB2	1:C:547:ASN:HD22	1.84	0.43
1:C:1641:ILE:CG2	1:C:1694:MET:HE2	2.46	0.43
1:E:2058:LEU:HA	1:E:2061:LEU:HD23	2.01	0.43
1:E:2266:VAL:HG21	1:E:2324:LEU:HD13	2.00	0.43
1:G:693:LEU:HD13	1:G:798:ILE:HD13	2.00	0.43
1:G:4192:ASN:HD22	1:G:4192:ASN:C	2.26	0.43
1:A:3697:ALA:HB2	1:A:3761:LYS:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3973:MET:O	1:A:4095:ILE:HD11	2.19	0.43
1:E:2130:LEU:CB	1:E:2174:VAL:HG22	2.49	0.43
1:E:4103:LEU:HD12	1:E:4127:LEU:CD1	2.49	0.43
1:G:611:LEU:HD22	1:G:1659:ARG:CG	2.49	0.43
1:G:643:LEU:HD22	1:G:1661:TYR:CZ	2.53	0.43
1:G:2513:MET:O	1:G:2517:LEU:HD13	2.18	0.43
1:A:633:CYS:HB3	1:A:1672:VAL:HG11	2.01	0.42
1:A:1802:GLY:O	1:A:1896:MET:HE2	2.19	0.42
1:A:2874:PRO:O	1:A:2877:THR:OG1	2.30	0.42
1:C:1802:GLY:O	1:C:1896:MET:HE2	2.19	0.42
1:C:2266:VAL:HG21	1:C:2324:LEU:HB3	2.01	0.42
1:C:4781:TYR:HA	1:C:4784:THR:HG22	2.01	0.42
1:E:763:ALA:HB3	1:E:765:SER:N	2.34	0.42
1:G:763:ALA:HB3	1:G:765:SER:N	2.33	0.42
1:G:1686:LEU:HD22	1:G:1790:LYS:HD2	2.01	0.42
1:G:1799:VAL:HG11	1:G:1845:LEU:HD11	2.01	0.42
1:A:1691:ASN:HD21	1:A:1694:MET:HE3	1.84	0.42
1:A:2326:ILE:HG23	1:G:207:PHE:CD1	2.54	0.42
1:A:4046:LYS:HG2	1:A:4079:LEU:HD21	2.00	0.42
1:A:4493:LEU:HD21	1:A:4590:ILE:CG2	2.48	0.42
1:A:4846:ILE:CD1	1:C:4816:MET:HG3	2.48	0.42
1:C:207:PHE:CG	1:E:2326:ILE:HG23	2.54	0.42
1:C:1928:PHE:CG	1:C:2032:LEU:HD22	2.53	0.42
1:C:2896:PHE:HA	1:C:2899:ILE:HG12	2.01	0.42
1:E:611:LEU:HD22	1:E:1659:ARG:HG3	2.01	0.42
1:E:614:LEU:HD13	1:E:636:LEU:HD11	2.00	0.42
1:E:3911:ILE:CD1	1:E:3975:LEU:HD22	2.49	0.42
1:G:636:LEU:HD13	1:G:1664:VAL:HG21	2.01	0.42
1:G:1087:ILE:HD12	1:G:1128:LEU:HD23	2.01	0.42
1:G:2470:VAL:HG21	1:G:2523:THR:HG23	2.01	0.42
1:A:646:THR:HG23	1:A:1684:GLN:NE2	2.34	0.42
1:A:763:ALA:HB3	1:A:765:SER:N	2.34	0.42
1:A:1300:MET:HE2	1:A:1545:ALA:HB3	2.01	0.42
1:A:1749:PRO:HB2	1:A:1843:LEU:HD21	2.01	0.42
1:A:1761:MET:HE2	1:A:1831:MET:CE	2.45	0.42
1:A:4899:TYR:CE2	1:A:4962:LYS:HG2	2.54	0.42
2:B:16:PRO:HG3	2:B:106:LEU:HD21	2.01	0.42
1:C:289:ILE:HG22	1:C:354:ILE:HD12	2.01	0.42
1:C:591:GLU:CA	1:C:631:LEU:HD21	2.49	0.42
1:C:875:PRO:HD2	1:C:878:LEU:HD12	2.01	0.42
1:C:2874:PRO:O	1:C:2877:THR:OG1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4939:GLU:HA	1:C:4942:VAL:HG12	2.01	0.42
1:E:4617:LEU:HA	1:E:4621:GLU:CB	2.49	0.42
1:G:652:VAL:HG11	1:G:692:HIS:CD2	2.54	0.42
1:G:3797:LEU:HD21	1:G:3836:PHE:HE2	1.84	0.42
1:G:3924:TYR:HB3	1:G:3932:ASN:HD21	1.85	0.42
1:C:1680:VAL:HG21	1:C:1685:LEU:HD13	2.01	0.42
1:C:4195:GLU:HA	1:C:4198:ILE:HD12	2.00	0.42
1:E:1932:PHE:CE2	1:E:2025:ILE:HG13	2.54	0.42
1:G:606:ARG:HG2	1:G:610:VAL:HG21	2.00	0.42
1:G:1253:LYS:HZ1	1:G:1601:ASN:HD22	1.68	0.42
1:A:629:GLN:HA	1:A:632:ILE:HD12	2.00	0.42
1:A:1459:LEU:HD13	1:A:1459:LEU:N	2.35	0.42
1:A:1828:LEU:HD23	1:A:1834:PHE:CZ	2.54	0.42
1:A:3911:ILE:CD1	1:A:3975:LEU:HD22	2.49	0.42
1:C:2420:ILE:O	1:C:2424:LEU:HD13	2.20	0.42
1:C:4082:GLU:HA	1:C:4085:VAL:HG22	2.01	0.42
1:E:370:LEU:O	1:E:393:MET:HE3	2.19	0.42
1:E:611:LEU:HD22	1:E:1659:ARG:HD2	2.00	0.42
1:E:3950:HIS:N	1:E:4010:ASN:HD21	2.18	0.42
1:E:4097:PHE:O	1:E:4101:VAL:HG23	2.19	0.42
1:E:4781:TYR:HA	1:E:4784:THR:HG22	2.00	0.42
2:F:66:MET:SD	2:F:74:LEU:HD21	2.59	0.42
1:G:682:THR:HG22	1:G:798:ILE:HG12	2.01	0.42
1:G:3644:ASP:HA	1:G:3647:LYS:HD2	2.02	0.42
1:G:3775:GLN:NE2	1:G:3847:LEU:O	2.53	0.42
1:G:3861:THR:HG23	1:G:3863:THR:HG23	2.00	0.42
1:A:245:LEU:HD11	1:A:260:VAL:CG1	2.49	0.42
1:A:652:VAL:HG11	1:A:692:HIS:CD2	2.55	0.42
1:A:996:VAL:CG1	1:A:1054:VAL:HG11	2.49	0.42
1:A:3668:LEU:HD21	1:A:3692:TYR:CD1	2.54	0.42
1:A:4923:PHE:CZ	1:A:4942:VAL:HG11	2.55	0.42
1:C:4043:ILE:HD12	1:C:4078:THR:HG21	2.01	0.42
1:C:4204:ALA:HA	1:C:4207:ILE:HG22	2.01	0.42
1:E:194:LEU:HD11	1:E:201:LEU:HD13	2.00	0.42
1:E:3775:GLN:NE2	1:E:3847:LEU:O	2.52	0.42
1:G:1932:PHE:CD2	1:G:2025:ILE:HD11	2.54	0.42
1:G:3740:MET:O	1:G:3744:THR:HG22	2.19	0.42
1:A:659:ILE:HG23	1:A:825:ALA:HB1	2.02	0.42
1:A:792:VAL:HG13	1:A:792:VAL:O	2.19	0.42
1:A:4191:VAL:HG11	1:A:4951:TRP:CH2	2.55	0.42
1:E:544:ASN:HB2	1:E:547:ASN:HD22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:689:GLU:O	1:E:691:THR:HG22	2.19	0.42
1:E:1516:GLY:C	1:E:1517:LEU:HD12	2.44	0.42
1:E:4639:THR:HG22	1:E:4641:SER:H	1.84	0.42
1:G:625:VAL:HG13	1:G:2132:VAL:HG23	2.01	0.42
1:G:875:PRO:HD2	1:G:878:LEU:HD12	2.00	0.42
1:A:3950:HIS:N	1:A:4010:ASN:HD21	2.17	0.42
1:C:892:LEU:C	1:C:892:LEU:HD13	2.45	0.42
1:E:559:ILE:HG12	1:E:575:LEU:HD11	2.02	0.42
1:E:2493:PHE:O	1:E:2497:LEU:HG	2.19	0.42
1:E:3883:GLN:HE22	1:E:3947:GLY:HA3	1.84	0.42
1:E:3956:GLN:NE2	1:E:4014:ILE:HG23	2.35	0.42
1:E:3992:VAL:HG13	1:E:4964:TYR:CE2	2.55	0.42
1:G:115:TYR:HE1	1:G:181:LEU:HD22	1.85	0.42
1:G:555:LEU:HD13	1:G:578:VAL:HG11	2.02	0.42
1:G:1910:LEU:HD12	1:G:2062:ILE:HD12	2.01	0.42
1:G:2250:ASN:HB2	1:G:2253:LEU:HB2	2.01	0.42
1:G:2420:ILE:O	1:G:2424:LEU:HD13	2.19	0.42
1:G:3966:ILE:O	1:G:3967:GLU:C	2.63	0.42
1:A:874:LEU:HD22	1:A:882:ARG:NH2	2.34	0.42
1:A:1819:VAL:HG21	1:A:1901:PRO:HB2	2.02	0.42
1:A:1911:GLN:HB2	1:A:2087:LEU:HD11	2.01	0.42
1:A:3862:GLN:HE21	1:A:3865:ASN:ND2	2.15	0.42
1:C:1596:TRP:HB2	1:C:1599:MET:HE2	2.02	0.42
1:C:1847:GLU:HB2	1:C:1848:PRO:HD3	2.02	0.42
1:C:4576:ILE:HD13	1:C:4576:ILE:O	2.20	0.42
1:E:119:ILE:HD13	1:E:162:ILE:HD11	2.02	0.42
1:G:718:VAL:HG22	1:G:791:VAL:HG13	2.00	0.42
1:G:2119:LEU:HD11	1:G:2167:MET:HE1	2.01	0.42
1:G:2123:LEU:HD12	1:G:2127:ARG:NH1	2.35	0.42
1:G:2192:MET:HE3	1:G:2193:VAL:CG2	2.50	0.42
1:A:1516:GLY:C	1:A:1517:LEU:HD12	2.45	0.42
1:A:2513:MET:O	1:A:2517:LEU:HD13	2.20	0.42
1:A:3756:VAL:HG13	1:A:3836:PHE:CE1	2.54	0.42
1:E:2420:ILE:O	1:E:2424:LEU:HD13	2.20	0.42
1:G:1165:MET:HE3	1:G:1174:MET:CB	2.50	0.42
1:G:1819:VAL:HG21	1:G:1901:PRO:HB2	2.01	0.42
1:G:2106:TYR:CG	1:G:2107:THR:N	2.88	0.42
1:A:766:ILE:HB	1:A:779:PHE:HB2	2.02	0.41
1:C:646:THR:HG23	1:C:1684:GLN:NE2	2.35	0.41
1:C:4147:GLU:OE1	1:C:4938:GLN:NE2	2.53	0.41
1:E:647:ARG:HA	1:E:1684:GLN:CD	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1795:LEU:HD11	1:E:1825:PHE:HB2	2.01	0.41
1:E:3907:PHE:HE2	1:E:3972:LEU:HD21	1.85	0.41
1:A:207:PHE:CE2	1:C:2326:ILE:HD12	2.54	0.41
1:E:658:ASN:C	1:E:659:ILE:HD12	2.44	0.41
1:E:3742:LEU:HD11	1:E:3778:MET:HG2	2.02	0.41
1:E:3911:ILE:HD11	1:E:3975:LEU:HD22	2.02	0.41
1:A:119:ILE:HG21	1:A:162:ILE:HD11	2.00	0.41
1:A:1096:VAL:HG13	1:A:1101:TRP:CD1	2.55	0.41
1:A:3952:PHE:HZ	1:A:3975:LEU:HD23	1.84	0.41
1:A:4140:MET:HE3	1:A:4955:PRO:HA	2.02	0.41
1:C:1629:SER:HA	1:C:1640:ASP:HA	2.02	0.41
1:C:1707:ILE:HD11	1:C:1824:LEU:HA	2.02	0.41
1:C:1828:LEU:HD23	1:C:1834:PHE:HZ	1.84	0.41
2:D:29:MET:HE2	2:D:98:ILE:HB	2.03	0.41
1:E:4833:ILE:HD13	1:E:4845:ARG:NH1	2.35	0.41
1:G:1761:MET:HB2	1:G:1776:TYR:CD2	2.55	0.41
1:G:2354:ILE:HG23	1:G:2386:GLY:HA3	2.02	0.41
1:G:4097:PHE:O	1:G:4101:VAL:HG23	2.20	0.41
1:A:28:ILE:CG1	1:A:201:LEU:HD11	2.50	0.41
1:A:49:LEU:HD11	1:A:194:LEU:HD21	2.03	0.41
1:A:657:PRO:CB	1:A:804:LEU:HD11	2.50	0.41
1:A:3966:ILE:O	1:A:3969:LEU:N	2.54	0.41
1:C:679:VAL:HA	1:C:800:VAL:HG12	2.02	0.41
1:C:1604:LEU:HD21	1:C:1627:PHE:HE1	1.86	0.41
1:E:1703:TYR:HB2	1:E:1820:PRO:HB3	2.02	0.41
1:E:1819:VAL:HG21	1:E:1901:PRO:HB2	2.02	0.41
1:E:3862:GLN:HG2	1:E:3865:ASN:HD22	1.85	0.41
1:G:1847:GLU:HB2	1:G:1848:PRO:HD3	2.03	0.41
1:A:476:GLN:HA	1:A:476:GLN:HE21	1.84	0.41
1:A:4639:THR:HG22	1:A:4641:SER:H	1.85	0.41
1:C:594:ILE:HD12	1:C:631:LEU:HD22	2.02	0.41
1:E:306:LEU:HD11	1:E:314:LEU:HD22	2.03	0.41
1:E:1165:MET:SD	1:E:1174:MET:HE3	2.60	0.41
1:E:2106:TYR:CG	1:E:2107:THR:N	2.88	0.41
1:E:4049:PHE:HE2	1:E:4067:LEU:HD13	1.85	0.41
1:G:1685:LEU:HD22	1:G:1709:ILE:HD11	2.01	0.41
1:G:3862:GLN:HE21	1:G:3865:ASN:ND2	2.14	0.41
1:A:425:LEU:HD13	1:A:452:VAL:HG22	2.03	0.41
1:A:579:LEU:HD22	1:A:586:LEU:HD23	2.02	0.41
1:A:1629:SER:HA	1:A:1640:ASP:HA	2.03	0.41
1:A:4869:ILE:HG21	1:C:4869:ILE:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:MET:SD	2:B:74:LEU:HD21	2.60	0.41
1:C:648:LEU:HD23	1:C:1684:GLN:HA	2.02	0.41
1:C:3693:ALA:HB3	1:C:3758:ALA:HB1	2.02	0.41
1:E:4012:GLU:HG3	1:E:4122:LEU:HD21	2.03	0.41
1:E:4823:VAL:HG23	1:E:4824:ARG:HG3	2.02	0.41
1:G:4135:GLY:HA3	1:G:4151:PHE:CZ	2.55	0.41
1:A:1300:MET:HE1	1:A:1547:ALA:HA	2.01	0.41
1:A:3966:ILE:O	1:A:3967:GLU:C	2.63	0.41
1:A:4097:PHE:O	1:A:4101:VAL:HG23	2.21	0.41
1:A:4135:GLY:HA3	1:A:4151:PHE:CZ	2.56	0.41
1:C:21:VAL:CG1	1:C:217:ILE:HD11	2.51	0.41
1:C:165:ALA:HB3	1:C:211:LEU:HD21	2.02	0.41
1:C:2081:VAL:HG23	1:C:3671:LEU:HD12	2.03	0.41
1:E:42:PHE:CG	1:E:418:VAL:HG22	2.56	0.41
1:E:996:VAL:CG1	1:E:1054:VAL:HG11	2.51	0.41
1:G:1795:LEU:HD11	1:G:1825:PHE:CD1	2.55	0.41
1:G:2861:LEU:HD22	1:G:2872:LEU:CD1	2.51	0.41
1:G:3908:SER:HA	1:G:3911:ILE:HG22	2.01	0.41
1:A:4781:TYR:HA	1:A:4784:THR:HG22	2.02	0.41
1:C:572:LEU:HD13	1:C:609:LYS:CB	2.51	0.41
1:E:1253:LYS:HZ1	1:E:1601:ASN:HD22	1.68	0.41
1:E:1730:THR:O	1:E:1733:THR:OG1	2.37	0.41
1:E:1772:ASN:N	1:E:1772:ASN:HD22	2.19	0.41
1:A:555:LEU:HD13	1:A:578:VAL:HG11	2.03	0.41
1:A:679:VAL:HA	1:A:800:VAL:HG12	2.02	0.41
1:A:933:LEU:O	1:A:937:LEU:HB2	2.21	0.41
1:A:3841:PHE:HB3	1:A:3920:THR:HG21	2.02	0.41
1:C:888:ASN:ND2	1:C:1056:THR:HG21	2.35	0.41
1:C:1749:PRO:HB3	1:C:2058:LEU:HD23	2.02	0.41
1:C:1795:LEU:HD11	1:C:1825:PHE:CG	2.55	0.41
1:C:3950:HIS:N	1:C:4010:ASN:HD21	2.19	0.41
1:E:598:ILE:HG23	1:E:642:LEU:HD22	2.02	0.41
1:E:995:MET:HE1	1:E:1064:LEU:HD13	2.02	0.41
1:E:2172:MET:HE3	1:E:2214:MET:CE	2.51	0.41
2:F:55:VAL:HG21	2:F:59:PHE:HD1	1.86	0.41
1:G:657:PRO:HG2	1:G:790:PRO:HG2	2.02	0.41
1:G:792:VAL:O	1:G:792:VAL:HG13	2.21	0.41
1:G:1751:ILE:HD13	1:G:1920:HIS:CE1	2.56	0.41
1:G:3956:GLN:HE21	1:G:4014:ILE:HG23	1.84	0.41
1:G:4911:THR:O	1:G:4916:ASN:N	2.50	0.41
1:A:1910:LEU:HG	1:A:2062:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:PHE:CZ	1:E:2423:ILE:HD12	2.56	0.41
1:C:570:GLY:O	1:C:574:VAL:HG23	2.21	0.41
1:C:828:PRO:HG2	1:C:1037:LEU:HB3	2.03	0.41
1:C:4015:LEU:HD13	1:C:4123:ALA:HA	2.03	0.41
1:E:2029:LEU:HD21	1:E:3629:TRP:CE3	2.56	0.41
1:E:4120:LEU:HA	1:E:4123:ALA:HB3	2.03	0.41
1:E:4611:LYS:HB3	1:E:4617:LEU:HD23	2.03	0.41
1:E:4911:THR:O	1:E:4916:ASN:N	2.51	0.41
1:G:3896:LYS:O	1:G:3898:VAL:N	2.54	0.41
1:A:3992:VAL:HG13	1:A:4964:TYR:CZ	2.56	0.40
1:C:496:ASN:HA	1:C:499:LEU:HD12	2.02	0.40
1:C:1828:LEU:HD23	1:C:1834:PHE:CZ	2.56	0.40
1:C:2103:PRO:O	1:C:2164:ALA:HB1	2.20	0.40
1:C:3875:THR:HG21	1:C:3924:TYR:HE2	1.86	0.40
1:C:4148:ARG:NH2	1:C:4914:GLU:OE2	2.54	0.40
1:C:4785:VAL:HG21	1:E:4742:ALA:CB	2.50	0.40
1:C:4923:PHE:HZ	1:C:4942:VAL:HG11	1.86	0.40
1:E:241:MET:HA	1:E:241:MET:HE2	2.04	0.40
1:E:646:THR:HG23	1:E:1684:GLN:NE2	2.36	0.40
1:E:881:ILE:HD11	1:E:1060:TYR:CE2	2.56	0.40
1:E:1628:MET:HG2	1:E:1694:MET:HE1	2.02	0.40
1:E:2894:LEU:CD1	1:E:2897:LEU:HD12	2.52	0.40
1:G:143:LEU:C	1:G:143:LEU:HD13	2.45	0.40
1:G:463:PHE:HB3	1:G:539:ALA:HB1	2.03	0.40
1:G:465:PRO:HA	1:G:466:PRO:HD3	1.96	0.40
1:G:1686:LEU:HD22	1:G:1790:LYS:HE3	2.02	0.40
1:A:207:PHE:CD2	1:C:2326:ILE:HD12	2.56	0.40
1:A:4134:LEU:HD13	1:A:4134:LEU:C	2.46	0.40
1:C:652:VAL:HG13	1:C:794:PHE:C	2.46	0.40
1:C:1686:LEU:HD22	1:C:1790:LYS:HE3	2.04	0.40
1:C:2159:PRO:CB	1:C:2206:ILE:HD12	2.49	0.40
1:C:2221:LEU:HD21	1:C:2242:VAL:HB	2.03	0.40
1:C:2735:MET:HE1	1:C:2826:ALA:HA	2.02	0.40
1:C:3966:ILE:O	1:C:3969:LEU:N	2.54	0.40
2:D:75:THR:HG23	2:D:98:ILE:CD1	2.51	0.40
1:E:1756:SER:C	1:E:1757:LEU:HD22	2.46	0.40
1:E:2874:PRO:O	1:E:2877:THR:OG1	2.33	0.40
1:E:3841:PHE:HB3	1:E:3920:THR:HG21	2.04	0.40
1:G:447:LEU:HD21	1:G:522:ALA:HB2	2.03	0.40
1:G:572:LEU:HD13	1:G:609:LYS:CB	2.51	0.40
1:G:1629:SER:HA	1:G:1640:ASP:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1828:LEU:HD23	1:G:1834:PHE:HZ	1.86	0.40
1:A:647:ARG:HA	1:A:1684:GLN:CD	2.47	0.40
1:A:658:ASN:C	1:A:659:ILE:HD12	2.46	0.40
1:C:572:LEU:HD22	1:C:609:LYS:HB3	2.04	0.40
1:E:1828:LEU:HD23	1:E:1834:PHE:HZ	1.87	0.40
1:A:465:PRO:HA	1:A:466:PRO:HD3	1.97	0.40
1:A:1268:ILE:O	1:A:1268:ILE:HG23	2.21	0.40
1:A:3804:LEU:HD13	1:A:3910:ALA:HB2	2.03	0.40
1:C:611:LEU:HB2	1:C:1659:ARG:HG3	2.02	0.40
1:C:1686:LEU:HD22	1:C:1790:LYS:HD2	2.02	0.40
1:C:2713:ILE:HD13	1:C:2714:ILE:N	2.36	0.40
1:C:2894:LEU:HD11	1:C:2904:VAL:HG21	2.04	0.40
1:C:3908:SER:HA	1:C:3911:ILE:HG22	2.02	0.40
1:C:4097:PHE:O	1:C:4101:VAL:HG23	2.22	0.40
1:C:4165:GLN:HG3	1:C:4501:TYR:CZ	2.57	0.40
1:C:4794:PHE:CB	1:C:4833:ILE:HD11	2.52	0.40
1:E:763:ALA:HB3	1:E:765:SER:H	1.86	0.40
2:H:82:TYR:CD2	2:H:91:ILE:HG21	2.56	0.40
1:A:1782:PHE:CZ	1:A:1787:LEU:HD22	2.57	0.40
1:A:2241:ASP:OD1	1:A:2242:VAL:N	2.55	0.40
1:A:2713:ILE:HD13	1:A:2714:ILE:N	2.36	0.40
2:B:4:ILE:HD12	2:B:74:LEU:HD22	2.03	0.40
1:C:4843:ILE:O	1:C:4846:ILE:HG22	2.22	0.40
2:D:30:LEU:O	2:D:32:ASN:N	2.55	0.40
1:E:217:ILE:HG22	1:E:286:GLY:HA3	2.03	0.40
1:E:737:ILE:HD13	1:E:1535:PRO:HG3	2.04	0.40
1:E:1706:LEU:O	1:E:1706:LEU:HD13	2.22	0.40
1:E:2175:MET:HE1	1:E:2239:PRO:HB3	2.04	0.40
1:E:4651:VAL:O	1:E:4655:VAL:HG23	2.22	0.40
1:G:4573:THR:HA	1:G:4576:ILE:HG22	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	3065/4387 (70%)	2784 (91%)	217 (7%)	64 (2%)	5	30
1	C	3065/4387 (70%)	2773 (90%)	236 (8%)	56 (2%)	6	34
1	E	3065/4387 (70%)	2765 (90%)	238 (8%)	62 (2%)	6	31
1	G	3065/4387 (70%)	2789 (91%)	211 (7%)	65 (2%)	5	30
2	B	105/158 (66%)	97 (92%)	7 (7%)	1 (1%)	12	49
2	D	105/158 (66%)	96 (91%)	8 (8%)	1 (1%)	12	49
2	F	105/158 (66%)	97 (92%)	6 (6%)	2 (2%)	6	32
2	H	105/158 (66%)	97 (92%)	8 (8%)	0	100	100
All	All	12680/18180 (70%)	11498 (91%)	931 (7%)	251 (2%)	8	31

All (251) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	472	HIS
1	A	1476	VAL
1	A	1549	SER
1	A	1779	SER
1	A	3897	ASP
1	A	3992	VAL
1	A	4916	ASN
1	A	4917	LEU
1	C	472	HIS
1	C	1476	VAL
1	C	1549	SER
1	C	1779	SER
1	C	3897	ASP
1	C	4916	ASN
2	D	31	GLN
1	E	837	SER
1	E	855	VAL
1	E	1549	SER
1	E	1590	PHE
1	E	1779	SER
1	E	3897	ASP
1	E	3992	VAL
1	E	4916	ASN
1	E	4917	LEU

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Mol	Chain	Res	Type
1	E	4959	CYS
1	G	472	HIS
1	G	837	SER
1	G	855	VAL
1	G	1549	SER
1	G	1639	VAL
1	G	1779	SER
1	G	3897	ASP
1	G	4916	ASN
1	G	4917	LEU
1	G	4959	CYS
1	A	250	GLY
1	A	838	ARG
1	A	855	VAL
1	A	901	GLY
1	A	1191	ALA
1	A	1535	PRO
1	A	1639	VAL
1	A	1737	THR
1	A	4751	GLY
1	A	4959	CYS
1	C	855	VAL
1	C	901	GLY
1	C	906	PRO
1	C	1267	HIS
1	C	1535	PRO
1	C	1639	VAL
1	C	1681	ASP
1	C	1737	THR
1	C	1755	THR
1	C	2795	GLU
1	C	2797	ASP
1	C	3992	VAL
1	C	4917	LEU
1	C	4959	CYS
1	E	350	GLY
1	E	836	HIS
1	E	838	ARG
1	E	1191	ALA
1	E	1476	VAL
1	E	1667	LEU
1	E	1681	ASP

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Mol	Chain	Res	Type
1	E	1737	THR
1	E	1755	THR
1	E	4038	PRO
1	G	188	SER
1	G	350	GLY
1	G	716	ASN
1	G	838	ARG
1	G	901	GLY
1	G	1191	ALA
1	G	1218	GLY
1	G	1456	GLY
1	G	1476	VAL
1	G	1535	PRO
1	G	1681	ASP
1	G	1755	THR
1	G	3992	VAL
1	A	359	SER
1	A	716	ASN
1	A	1667	LEU
1	A	1681	ASP
1	A	1755	THR
1	A	2106	TYR
1	A	2864	LYS
1	A	4038	PRO
1	A	4112	ASN
1	C	224	ALA
1	C	838	ARG
1	C	1191	ALA
1	C	1590	PHE
1	C	1667	LEU
1	C	2106	TYR
1	C	4112	ASN
1	C	4957	GLY
1	E	716	ASN
1	E	901	GLY
1	E	1639	VAL
1	E	4112	ASN
2	F	31	GLN
1	G	224	ALA
1	G	906	PRO
1	G	1219	LYS
1	G	1231	GLY

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Mol	Chain	Res	Type
1	G	1590	PHE
1	G	1667	LEU
1	G	2106	TYR
1	G	2797	ASP
1	G	4112	ASN
1	A	224	ALA
1	A	641	ASP
1	A	642	LEU
1	A	669	GLN
1	A	837	SER
1	A	1218	GLY
1	A	1472	GLU
1	A	1725	PHE
1	A	1758	ARG
1	A	1834	PHE
1	A	2074	VAL
1	A	2077	ASP
1	A	4056	HIS
1	C	350	GLY
1	C	620	CYS
1	C	847	THR
1	C	1231	GLY
1	C	1604	LEU
1	C	1758	ARG
1	C	2077	ASP
1	C	2710	SER
1	E	63	SER
1	E	224	ALA
1	E	472	HIS
1	E	1210	ALA
1	E	1535	PRO
1	E	1536	SER
1	E	1758	ARG
1	E	1770	SER
1	E	2074	VAL
1	E	2077	ASP
1	E	2106	TYR
1	E	2797	ASP
1	E	3686	ASP
2	F	32	ASN
1	G	467	ASP
1	G	642	LEU

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Mol	Chain	Res	Type
1	G	836	HIS
1	G	847	THR
1	G	1725	PHE
1	G	1737	THR
1	G	2074	VAL
1	G	2077	ASP
1	G	2710	SER
1	G	3681	CYS
1	G	4056	HIS
1	G	4802	ASP
1	A	620	CYS
1	A	839	GLU
1	A	847	THR
1	A	871	GLN
1	A	1142	ALA
1	A	1267	HIS
1	A	2311	GLY
1	A	4164	PRO
1	A	4622	GLN
1	C	641	ASP
1	C	642	LEU
1	C	837	SER
1	C	839	GLU
1	C	1210	ALA
1	C	1299	ILE
1	C	2074	VAL
1	C	3991	VAL
1	C	4622	GLN
1	E	685	PHE
1	E	829	LYS
1	E	839	GLU
1	E	1142	ALA
1	E	1231	GLY
1	E	1547	ALA
1	E	1604	LEU
1	E	3788	VAL
1	E	4056	HIS
1	E	4164	PRO
1	E	4181	GLY
1	E	4743	ALA
1	G	341	GLY
1	G	620	CYS

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Mol	Chain	Res	Type
1	G	839	GLU
1	G	1299	ILE
1	G	1472	GLU
1	G	1758	ARG
1	G	1770	SER
1	G	1777	GLN
1	G	1834	PHE
1	G	4622	GLN
1	G	4751	GLY
1	G	4800	ASP
1	A	1299	ILE
1	A	4800	ASP
2	B	31	GLN
1	C	341	GLY
1	C	467	ASP
1	C	670	TYR
1	C	1194	ASP
1	C	1777	GLN
1	C	1810	VAL
1	C	2311	GLY
1	E	777	GLY
1	E	847	THR
1	E	1267	HIS
1	E	1299	ILE
1	E	2311	GLY
1	E	3681	CYS
1	E	4622	GLN
1	G	1810	VAL
1	A	341	GLY
1	A	1231	GLY
1	A	1810	VAL
1	E	341	GLY
1	E	3991	VAL
1	G	2866	GLY
1	A	906	PRO
1	A	3991	VAL
1	A	4623	PRO
1	E	1810	VAL
1	G	3991	VAL
1	A	729	GLY
1	A	1198	GLY
1	A	4957	GLY

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Mol	Chain	Res	Type
1	C	1218	GLY
1	C	4623	PRO
1	E	4623	PRO
1	G	4164	PRO
1	A	684	PRO
1	C	3788	VAL
1	E	4830	GLY
1	G	834	VAL
1	G	1533	VAL
1	G	4895	ILE
1	A	2865	GLY
1	A	3788	VAL
1	G	2311	GLY
1	G	1809	PRO
1	C	1809	PRO
1	A	1809	PRO
1	E	1809	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2774/3480 (80%)	2654 (96%)	120 (4%)	26	47
1	C	2774/3480 (80%)	2629 (95%)	145 (5%)	21	42
1	E	2774/3480 (80%)	2628 (95%)	146 (5%)	20	41
1	G	2774/3480 (80%)	2631 (95%)	143 (5%)	21	42
2	B	88/131 (67%)	87 (99%)	1 (1%)	65	76
2	D	88/131 (67%)	87 (99%)	1 (1%)	65	76
2	F	88/131 (67%)	87 (99%)	1 (1%)	65	76
2	H	88/131 (67%)	87 (99%)	1 (1%)	65	76
All	All	11448/14444 (79%)	10890 (95%)	558 (5%)	24	43

All (558) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	317	MET
1	A	336	GLU
1	A	342	VAL
1	A	392	ILE
1	A	441	LYS
1	A	476	GLN
1	A	551	PHE
1	A	559	ILE
1	A	572	LEU
1	A	604	HIS
1	A	608	HIS
1	A	609	LYS
1	A	643	LEU
1	A	669	GLN
1	A	725	TYR
1	A	844	ARG
1	A	872	ILE
1	A	888	ASN
1	A	912	LYS
1	A	948	CYS
1	A	1031	ARG
1	A	1193	LYS
1	A	1204	VAL
1	A	1243	THR
1	A	1266	GLU
1	A	1287	GLN
1	A	1294	ASN
1	A	1298	ASP
1	A	1302	TYR
1	A	1308	ILE
1	A	1447	THR
1	A	1459	LEU
1	A	1475	LYS
1	A	1533	VAL
1	A	1538	LYS
1	A	1554	GLN
1	A	1595	LEU
1	A	1630	LEU
1	A	1644	LEU
1	A	1657	THR
1	A	1689	ILE
1	A	1692	LYS

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Mol	Chain	Res	Type
1	A	1697	LEU
1	A	1700	THR
1	A	1716	THR
1	A	1720	MET
1	A	1763	PHE
1	A	1771	ILE
1	A	1776	TYR
1	A	1777	GLN
1	A	1778	TYR
1	A	1779	SER
1	A	1784	LEU
1	A	1790	LYS
1	A	1794	MET
1	A	1804	LEU
1	A	1833	ILE
1	A	1845	LEU
1	A	1897	LYS
1	A	1898	LEU
1	A	1900	GLU
1	A	1910	LEU
1	A	1935	LYS
1	A	2023	LEU
1	A	2088	LEU
1	A	2126	ILE
1	A	2129	LEU
1	A	2179	LEU
1	A	2192	MET
1	A	2354	ILE
1	A	2423	ILE
1	A	2466	LYS
1	A	2473	LEU
1	A	2517	LEU
1	A	2713	ILE
1	A	2717	LYS
1	A	2723	ASN
1	A	2746	GLU
1	A	2747	ILE
1	A	2770	GLU
1	A	2861	LEU
1	A	3675	THR
1	A	3690	MET
1	A	3728	GLN

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Mol	Chain	Res	Type
1	A	3797	LEU
1	A	3844	LEU
1	A	3860	ARG
1	A	3911	ILE
1	A	3926	GLN
1	A	3929	CYS
1	A	3955	MET
1	A	3956	GLN
1	A	3959	LEU
1	A	3962	ASP
1	A	3969	LEU
1	A	3970	LYS
1	A	3992	VAL
1	A	4065	GLU
1	A	4078	THR
1	A	4126	VAL
1	A	4170	LYS
1	A	4186	LYS
1	A	4188	GLU
1	A	4192	ASN
1	A	4491	LYS
1	A	4573	THR
1	A	4576	ILE
1	A	4584	ILE
1	A	4622	GLN
1	A	4637	ILE
1	A	4670	GLU
1	A	4671	LEU
1	A	4711	LYS
1	A	4807	LYS
1	A	4855	PHE
1	A	4860	LEU
1	A	4885	ASP
1	A	4925	MET
1	A	4927	LEU
2	B	34	LYS
1	C	28	ILE
1	C	32	GLN
1	C	54	ASN
1	C	190	ARG
1	C	317	MET
1	C	321	LYS

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Mol	Chain	Res	Type
1	C	336	GLU
1	C	342	VAL
1	C	392	ILE
1	C	441	LYS
1	C	476	GLN
1	C	558	LEU
1	C	572	LEU
1	C	575	LEU
1	C	608	HIS
1	C	609	LYS
1	C	643	LEU
1	C	669	GLN
1	C	725	TYR
1	C	787	LEU
1	C	829	LYS
1	C	835	GLU
1	C	844	ARG
1	C	872	ILE
1	C	880	ARG
1	C	888	ASN
1	C	912	LYS
1	C	918	LEU
1	C	948	CYS
1	C	1028	ARG
1	C	1031	ARG
1	C	1193	LYS
1	C	1243	THR
1	C	1265	HIS
1	C	1287	GLN
1	C	1308	ILE
1	C	1447	THR
1	C	1450	PHE
1	C	1459	LEU
1	C	1465	VAL
1	C	1475	LYS
1	C	1533	VAL
1	C	1538	LYS
1	C	1554	GLN
1	C	1589	GLN
1	C	1625	LEU
1	C	1637	ARG
1	C	1644	LEU

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Mol	Chain	Res	Type
1	C	1657	THR
1	C	1660	LEU
1	C	1692	LYS
1	C	1697	LEU
1	C	1720	MET
1	C	1763	PHE
1	C	1771	ILE
1	C	1772	ASN
1	C	1777	GLN
1	C	1778	TYR
1	C	1790	LYS
1	C	1794	MET
1	C	1804	LEU
1	C	1833	ILE
1	C	1897	LYS
1	C	1908	LEU
1	C	1909	LEU
1	C	1910	LEU
1	C	1925	ILE
1	C	1935	LYS
1	C	2023	LEU
1	C	2032	LEU
1	C	2036	VAL
1	C	2088	LEU
1	C	2099	VAL
1	C	2117	ILE
1	C	2126	ILE
1	C	2129	LEU
1	C	2138	GLU
1	C	2139	GLU
1	C	2192	MET
1	C	2298	ARG
1	C	2354	ILE
1	C	2399	LEU
1	C	2423	ILE
1	C	2466	LYS
1	C	2517	LEU
1	C	2713	ILE
1	C	2717	LYS
1	C	2723	ASN
1	C	2747	ILE
1	C	2750	ASP

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Mol	Chain	Res	Type
1	C	2795	GLU
1	C	2861	LEU
1	C	3616	ARG
1	C	3662	VAL
1	C	3665	LEU
1	C	3675	THR
1	C	3690	MET
1	C	3728	GLN
1	C	3797	LEU
1	C	3801	CYS
1	C	3860	ARG
1	C	3866	ASN
1	C	3876	VAL
1	C	3887	SER
1	C	3911	ILE
1	C	3912	GLN
1	C	3926	GLN
1	C	3929	CYS
1	C	3951	VAL
1	C	3959	LEU
1	C	3962	ASP
1	C	3969	LEU
1	C	3970	LYS
1	C	3979	MET
1	C	3992	VAL
1	C	4014	ILE
1	C	4032	THR
1	C	4065	GLU
1	C	4086	LYS
1	C	4117	GLN
1	C	4120	LEU
1	C	4142	SER
1	C	4152	GLU
1	C	4170	LYS
1	C	4178	VAL
1	C	4186	LYS
1	C	4188	GLU
1	C	4192	ASN
1	C	4200	GLU
1	C	4491	LYS
1	C	4576	ILE
1	C	4584	ILE

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Mol	Chain	Res	Type
1	C	4622	GLN
1	C	4637	ILE
1	C	4752	PHE
1	C	4807	LYS
1	C	4840	GLU
1	C	4860	LEU
1	C	4865	GLN
1	C	4875	LEU
1	C	4876	ARG
1	C	4882	VAL
1	C	4885	ASP
1	C	4914	GLU
1	C	4925	MET
2	D	34	LYS
1	E	18	ASP
1	E	54	ASN
1	E	143	LEU
1	E	194	LEU
1	E	198	ASN
1	E	313	ASN
1	E	317	MET
1	E	336	GLU
1	E	342	VAL
1	E	374	TYR
1	E	390	LYS
1	E	392	ILE
1	E	424	PHE
1	E	441	LYS
1	E	476	GLN
1	E	551	PHE
1	E	559	ILE
1	E	562	LEU
1	E	563	GLU
1	E	572	LEU
1	E	589	ILE
1	E	608	HIS
1	E	609	LYS
1	E	643	LEU
1	E	669	GLN
1	E	701	GLU
1	E	725	TYR
1	E	739	ARG

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Mol	Chain	Res	Type
1	E	795	SER
1	E	855	VAL
1	E	872	ILE
1	E	881	ILE
1	E	888	ASN
1	E	908	ARG
1	E	912	LYS
1	E	1031	ARG
1	E	1193	LYS
1	E	1204	VAL
1	E	1232	LEU
1	E	1266	GLU
1	E	1287	GLN
1	E	1298	ASP
1	E	1308	ILE
1	E	1447	THR
1	E	1459	LEU
1	E	1475	LYS
1	E	1533	VAL
1	E	1538	LYS
1	E	1589	GLN
1	E	1630	LEU
1	E	1644	LEU
1	E	1657	THR
1	E	1677	CYS
1	E	1692	LYS
1	E	1697	LEU
1	E	1700	THR
1	E	1716	THR
1	E	1720	MET
1	E	1763	PHE
1	E	1771	ILE
1	E	1772	ASN
1	E	1777	GLN
1	E	1778	TYR
1	E	1779	SER
1	E	1790	LYS
1	E	1794	MET
1	E	1801	GLU
1	E	1804	LEU
1	E	1833	ILE
1	E	1845	LEU

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Mol	Chain	Res	Type
1	E	1897	LYS
1	E	1898	LEU
1	E	1916	CYS
1	E	1935	LYS
1	E	2023	LEU
1	E	2032	LEU
1	E	2058	LEU
1	E	2061	LEU
1	E	2081	VAL
1	E	2087	LEU
1	E	2098	LEU
1	E	2099	VAL
1	E	2126	ILE
1	E	2129	LEU
1	E	2175	MET
1	E	2179	LEU
1	E	2192	MET
1	E	2326	ILE
1	E	2354	ILE
1	E	2399	LEU
1	E	2423	ILE
1	E	2462	CYS
1	E	2466	LYS
1	E	2511	THR
1	E	2517	LEU
1	E	2713	ILE
1	E	2717	LYS
1	E	2719	GLU
1	E	2723	ASN
1	E	2746	GLU
1	E	2747	ILE
1	E	2750	ASP
1	E	2770	GLU
1	E	2795	GLU
1	E	2861	LEU
1	E	2864	LYS
1	E	3671	LEU
1	E	3675	THR
1	E	3728	GLN
1	E	3801	CYS
1	E	3844	LEU
1	E	3860	ARG

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Mol	Chain	Res	Type
1	E	3911	ILE
1	E	3912	GLN
1	E	3926	GLN
1	E	3929	CYS
1	E	3951	VAL
1	E	3959	LEU
1	E	3962	ASP
1	E	3969	LEU
1	E	3970	LYS
1	E	3979	MET
1	E	3992	VAL
1	E	4065	GLU
1	E	4117	GLN
1	E	4120	LEU
1	E	4170	LYS
1	E	4186	LYS
1	E	4192	ASN
1	E	4491	LYS
1	E	4573	THR
1	E	4576	ILE
1	E	4584	ILE
1	E	4620	THR
1	E	4622	GLN
1	E	4637	ILE
1	E	4722	LEU
1	E	4752	PHE
1	E	4807	LYS
1	E	4840	GLU
1	E	4860	LEU
1	E	4865	GLN
1	E	4876	ARG
1	E	4885	ASP
1	E	4903	VAL
1	E	4927	LEU
2	F	34	LYS
1	G	18	ASP
1	G	54	ASN
1	G	238	HIS
1	G	317	MET
1	G	342	VAL
1	G	373	THR
1	G	392	ILE

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Mol	Chain	Res	Type
1	G	424	PHE
1	G	441	LYS
1	G	462	TYR
1	G	476	GLN
1	G	551	PHE
1	G	558	LEU
1	G	572	LEU
1	G	575	LEU
1	G	604	HIS
1	G	609	LYS
1	G	643	LEU
1	G	680	ASP
1	G	725	TYR
1	G	739	ARG
1	G	787	LEU
1	G	835	GLU
1	G	855	VAL
1	G	872	ILE
1	G	888	ASN
1	G	912	LYS
1	G	948	CYS
1	G	993	GLU
1	G	1027	ARG
1	G	1031	ARG
1	G	1189	GLU
1	G	1193	LYS
1	G	1232	LEU
1	G	1259	LEU
1	G	1266	GLU
1	G	1287	GLN
1	G	1298	ASP
1	G	1308	ILE
1	G	1447	THR
1	G	1459	LEU
1	G	1465	VAL
1	G	1475	LYS
1	G	1533	VAL
1	G	1538	LYS
1	G	1554	GLN
1	G	1589	GLN
1	G	1643	GLU
1	G	1644	LEU

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Mol	Chain	Res	Type
1	G	1657	THR
1	G	1677	CYS
1	G	1692	LYS
1	G	1697	LEU
1	G	1716	THR
1	G	1720	MET
1	G	1763	PHE
1	G	1771	ILE
1	G	1772	ASN
1	G	1777	GLN
1	G	1778	TYR
1	G	1779	SER
1	G	1784	LEU
1	G	1790	LYS
1	G	1794	MET
1	G	1804	LEU
1	G	1833	ILE
1	G	1897	LYS
1	G	1898	LEU
1	G	1900	GLU
1	G	1904	LEU
1	G	1905	GLN
1	G	1910	LEU
1	G	1917	GLN
1	G	1919	ARG
1	G	1925	ILE
1	G	2023	LEU
1	G	2032	LEU
1	G	2036	VAL
1	G	2058	LEU
1	G	2060	GLN
1	G	2086	VAL
1	G	2117	ILE
1	G	2126	ILE
1	G	2129	LEU
1	G	2179	LEU
1	G	2192	MET
1	G	2220	TYR
1	G	2354	ILE
1	G	2399	LEU
1	G	2423	ILE
1	G	2426	SER

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Mol	Chain	Res	Type
1	G	2466	LYS
1	G	2511	THR
1	G	2517	LEU
1	G	2713	ILE
1	G	2717	LYS
1	G	2723	ASN
1	G	2724	LYS
1	G	2746	GLU
1	G	2747	ILE
1	G	2750	ASP
1	G	2770	GLU
1	G	2795	GLU
1	G	2838	LEU
1	G	2861	LEU
1	G	3675	THR
1	G	3690	MET
1	G	3728	GLN
1	G	3801	CYS
1	G	3860	ARG
1	G	3866	ASN
1	G	3911	ILE
1	G	3912	GLN
1	G	3926	GLN
1	G	3929	CYS
1	G	3951	VAL
1	G	3959	LEU
1	G	3962	ASP
1	G	3970	LYS
1	G	3992	VAL
1	G	4012	GLU
1	G	4050	HIS
1	G	4065	GLU
1	G	4117	GLN
1	G	4120	LEU
1	G	4126	VAL
1	G	4154	SER
1	G	4170	LYS
1	G	4171	ARG
1	G	4186	LYS
1	G	4188	GLU
1	G	4192	ASN
1	G	4196	ASP

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Mol	Chain	Res	Type
1	G	4576	ILE
1	G	4584	ILE
1	G	4620	THR
1	G	4622	GLN
1	G	4637	ILE
1	G	4671	LEU
1	G	4807	LYS
1	G	4860	LEU
1	G	4885	ASP
1	G	4927	LEU
2	H	34	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (243) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	202	HIS
1	A	270	HIS
1	A	375	GLN
1	A	388	GLN
1	A	404	ASN
1	A	409	GLN
1	A	472	HIS
1	A	476	GLN
1	A	487	ASN
1	A	496	ASN
1	A	544	ASN
1	A	547	ASN
1	A	692	HIS
1	A	888	ASN
1	A	890	HIS
1	A	914	GLN
1	A	930	ASN
1	A	932	ASN
1	A	949	HIS
1	A	956	HIS
1	A	1002	ASN
1	A	1004	HIS
1	A	1151	HIS
1	A	1211	GLN
1	A	1257	GLN
1	A	1287	GLN

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Mol	Chain	Res	Type
1	A	1451	HIS
1	A	1601	ASN
1	A	1684	GLN
1	A	1691	ASN
1	A	1722	ASN
1	A	1773	ASN
1	A	1905	GLN
1	A	2152	ASN
1	A	2158	HIS
1	A	2209	GLN
1	A	2755	GLN
1	A	2891	GLN
1	A	3666	HIS
1	A	3812	GLN
1	A	3845	GLN
1	A	3851	HIS
1	A	3865	ASN
1	A	3912	GLN
1	A	3926	GLN
1	A	3934	GLN
1	A	3938	HIS
1	A	3956	GLN
1	A	3990	ASN
1	A	4160	GLN
1	A	4192	ASN
1	A	4515	ASN
1	A	4631	GLN
1	A	4638	ASN
1	A	4708	GLN
1	A	4744	HIS
1	A	4765	ASN
1	A	4878	GLN
1	A	4879	GLN
1	A	4897	ASN
1	A	4919	ASN
1	A	4935	HIS
2	B	25	HIS
2	B	65	GLN
1	C	23	GLN
1	C	54	ASN
1	C	71	GLN
1	C	110	HIS

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Mol	Chain	Res	Type
1	C	168	GLN
1	C	193	HIS
1	C	388	GLN
1	C	398	HIS
1	C	404	ASN
1	C	427	ASN
1	C	476	GLN
1	C	487	ASN
1	C	496	ASN
1	C	547	ASN
1	C	635	ASN
1	C	669	GLN
1	C	692	HIS
1	C	745	ASN
1	C	771	ASN
1	C	890	HIS
1	C	932	ASN
1	C	956	HIS
1	C	1002	ASN
1	C	1211	GLN
1	C	1260	GLN
1	C	1293	GLN
1	C	1501	ASN
1	C	1602	GLN
1	C	1691	ASN
1	C	1772	ASN
1	C	1773	ASN
1	C	1905	GLN
1	C	1911	GLN
1	C	2118	ASN
1	C	2224	ASN
1	C	2387	ASN
1	C	2891	GLN
1	C	3743	GLN
1	C	3775	GLN
1	C	3812	GLN
1	C	3845	GLN
1	C	3862	GLN
1	C	3912	GLN
1	C	3926	GLN
1	C	3933	GLN
1	C	3976	GLN

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Mol	Chain	Res	Type
1	C	4009	ASN
1	C	4010	ASN
1	C	4192	ASN
1	C	4494	ASN
1	C	4581	HIS
1	C	4644	ASN
1	C	4708	GLN
1	C	4744	HIS
1	C	4818	HIS
1	C	4878	GLN
1	C	4897	ASN
1	C	4919	ASN
2	D	25	HIS
1	E	23	GLN
1	E	33	GLN
1	E	44	ASN
1	E	168	GLN
1	E	240	HIS
1	E	410	HIS
1	E	476	GLN
1	E	487	ASN
1	E	513	HIS
1	E	544	ASN
1	E	547	ASN
1	E	550	GLN
1	E	607	ASN
1	E	621	HIS
1	E	745	ASN
1	E	771	ASN
1	E	888	ASN
1	E	914	GLN
1	E	930	ASN
1	E	1002	ASN
1	E	1211	GLN
1	E	1293	GLN
1	E	1601	ASN
1	E	1691	ASN
1	E	1723	ASN
1	E	1772	ASN
1	E	1773	ASN
1	E	1905	GLN
1	E	2091	GLN

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Mol	Chain	Res	Type
1	E	2118	ASN
1	E	2160	ASN
1	E	2168	HIS
1	E	2195	ASN
1	E	2387	ASN
1	E	2465	HIS
1	E	2848	ASN
1	E	2891	GLN
1	E	3812	GLN
1	E	3845	GLN
1	E	3865	ASN
1	E	3912	GLN
1	E	3926	GLN
1	E	3954	HIS
1	E	3965	GLN
1	E	4009	ASN
1	E	4098	ASN
1	E	4179	ASN
1	E	4192	ASN
1	E	4515	ASN
1	E	4581	HIS
1	E	4631	GLN
1	E	4644	ASN
1	E	4865	GLN
1	E	4897	ASN
1	E	4919	ASN
1	E	4935	HIS
1	E	4963	GLN
2	F	25	HIS
2	F	31	GLN
1	G	33	GLN
1	G	44	ASN
1	G	54	ASN
1	G	168	GLN
1	G	193	HIS
1	G	409	GLN
1	G	476	GLN
1	G	487	ASN
1	G	490	GLN
1	G	513	HIS
1	G	544	ASN
1	G	547	ASN

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Mol	Chain	Res	Type
1	G	550	GLN
1	G	607	ASN
1	G	608	HIS
1	G	635	ASN
1	G	746	GLN
1	G	888	ASN
1	G	914	GLN
1	G	930	ASN
1	G	932	ASN
1	G	949	HIS
1	G	956	HIS
1	G	1002	ASN
1	G	1149	ASN
1	G	1242	ASN
1	G	1257	GLN
1	G	1451	HIS
1	G	1501	ASN
1	G	1601	ASN
1	G	1691	ASN
1	G	1772	ASN
1	G	2091	GLN
1	G	2118	ASN
1	G	2195	ASN
1	G	2387	ASN
1	G	2891	GLN
1	G	2898	GLN
1	G	2900	ASN
1	G	3623	GLN
1	G	3799	GLN
1	G	3812	GLN
1	G	3845	GLN
1	G	3865	ASN
1	G	3912	GLN
1	G	3926	GLN
1	G	3932	ASN
1	G	3956	GLN
1	G	3965	GLN
1	G	3976	GLN
1	G	4010	ASN
1	G	4192	ASN
1	G	4202	GLN
1	G	4638	ASN

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Mol	Chain	Res	Type
1	G	4879	GLN
1	G	4897	ASN
1	G	4919	ASN
1	G	4935	HIS
2	H	25	HIS
2	H	32	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	27
1	G	27
1	E	27
1	A	27

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	3612:UNK	C	3613:PRO	N	76.52
1	G	3612:UNK	C	3613:PRO	N	75.29
1	E	3612:UNK	C	3613:PRO	N	74.52
1	A	3612:UNK	C	3613:PRO	N	74.10
1	E	2701:UNK	C	2702:PHE	N	43.29
1	C	2701:UNK	C	2702:PHE	N	43.25
1	G	2701:UNK	C	2702:PHE	N	42.68
1	A	2701:UNK	C	2702:PHE	N	41.57
1	E	3589:UNK	C	3590:UNK	N	41.47
1	A	3589:UNK	C	3590:UNK	N	40.67
1	G	3589:UNK	C	3590:UNK	N	38.79
1	C	3589:UNK	C	3590:UNK	N	37.92
1	G	3436:UNK	C	3437:UNK	N	22.01
1	A	3347:GLY	C	3348:UNK	N	21.94
1	E	3347:GLY	C	3348:UNK	N	21.63
1	C	2529:LEU	C	2578:UNK	N	21.47
1	E	3436:UNK	C	3437:UNK	N	21.40
1	C	3347:GLY	C	3348:UNK	N	21.29
1	E	2529:LEU	C	2578:UNK	N	20.68
1	G	3347:GLY	C	3348:UNK	N	20.37
1	C	3436:UNK	C	3437:UNK	N	20.35
1	A	2529:LEU	C	2578:UNK	N	20.28
1	A	3436:UNK	C	3437:UNK	N	20.21
1	A	2659:UNK	C	2660:UNK	N	19.56
1	G	2529:LEU	C	2578:UNK	N	19.18
1	G	2659:UNK	C	2660:UNK	N	18.25
1	E	1943:ARG	C	2008:UNK	N	18.00
1	G	1943:ARG	C	2008:UNK	N	17.56
1	C	3414:UNK	C	3415:UNK	N	17.36
1	G	3496:UNK	C	3497:UNK	N	17.23
1	E	3371:UNK	C	3372:UNK	N	17.18
1	A	1943:ARG	C	2008:UNK	N	17.12
1	E	2659:UNK	C	2660:UNK	N	16.94
1	G	3478:UNK	C	3479:UNK	N	16.94
1	G	1500:UNK	C	1501:ASN	N	16.90
1	E	3478:UNK	C	3479:UNK	N	16.86
1	C	3478:UNK	C	3479:UNK	N	16.82
1	A	3414:UNK	C	3415:UNK	N	16.74
1	C	1500:UNK	C	1501:ASN	N	16.69
1	E	2597:UNK	C	2598:UNK	N	16.38
1	C	2659:UNK	C	2660:UNK	N	16.36
1	C	1943:ARG	C	2008:UNK	N	16.33
1	E	3414:UNK	C	3415:UNK	N	16.18

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	3496:UNK	C	3497:UNK	N	16.05
1	E	1500:UNK	C	1501:ASN	N	16.00
1	A	3510:UNK	C	3511:UNK	N	15.98
1	A	1500:UNK	C	1501:ASN	N	15.96
1	C	2597:UNK	C	2598:UNK	N	15.85
1	G	3414:UNK	C	3415:UNK	N	15.79
1	C	2679:UNK	C	2680:UNK	N	15.57
1	A	3478:UNK	C	3479:UNK	N	15.52
1	G	3510:UNK	C	3511:UNK	N	15.50
1	E	2636:UNK	C	2637:UNK	N	15.08
1	G	3371:UNK	C	3372:UNK	N	15.08
1	G	2022:UNK	C	2023:LEU	N	14.88
1	A	3496:UNK	C	3497:UNK	N	14.87
1	E	3510:UNK	C	3511:UNK	N	14.76
1	A	2022:UNK	C	2023:LEU	N	14.71
1	A	2597:UNK	C	2598:UNK	N	14.71
1	C	2022:UNK	C	2023:LEU	N	14.64
1	G	3548:UNK	C	3549:UNK	N	14.53
1	E	2022:UNK	C	2023:LEU	N	14.45
1	G	3571:UNK	C	3572:UNK	N	14.26
1	C	3510:UNK	C	3511:UNK	N	13.96
1	G	2679:UNK	C	2680:UNK	N	13.82
1	C	2636:UNK	C	2637:UNK	N	13.74
1	C	3571:UNK	C	3572:UNK	N	13.65
1	G	2636:UNK	C	2637:UNK	N	13.56
1	C	3371:UNK	C	3372:UNK	N	13.49
1	A	2679:UNK	C	2680:UNK	N	13.34
1	A	3548:UNK	C	3549:UNK	N	13.33
1	E	3496:UNK	C	3497:UNK	N	12.80
1	C	3528:UNK	C	3529:UNK	N	12.75
1	A	2636:UNK	C	2637:UNK	N	12.73
1	G	2597:UNK	C	2598:UNK	N	12.44
1	E	3528:UNK	C	3529:UNK	N	12.40
1	G	3391:UNK	C	3392:UNK	N	12.33
1	E	3571:UNK	C	3572:UNK	N	12.27
1	C	3548:UNK	C	3549:UNK	N	12.03
1	E	3457:UNK	C	3458:UNK	N	11.91
1	E	3391:UNK	C	3392:UNK	N	11.75
1	E	2679:UNK	C	2680:UNK	N	11.67
1	C	3457:UNK	C	3458:UNK	N	11.62
1	A	3528:UNK	C	3529:UNK	N	11.43
1	A	2460:UNK	C	2461:PHE	N	10.92

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3571:UNK	C	3572:UNK	N	10.38
1	A	3371:UNK	C	3372:UNK	N	10.05
1	E	2460:UNK	C	2461:PHE	N	9.63
1	G	2460:UNK	C	2461:PHE	N	9.03
1	C	2460:UNK	C	2461:PHE	N	9.00
1	G	3528:UNK	C	3529:UNK	N	8.96
1	A	3457:UNK	C	3458:UNK	N	8.73
1	A	3391:UNK	C	3392:UNK	N	8.48
1	E	2616:UNK	C	2617:UNK	N	8.34
1	G	3457:UNK	C	3458:UNK	N	8.29
1	E	3548:UNK	C	3549:UNK	N	6.74
1	C	2616:UNK	C	2617:UNK	N	6.50
1	G	2616:UNK	C	2617:UNK	N	6.26
1	C	1484:ASN	C	1496:UNK	N	5.85
1	A	1484:ASN	C	1496:UNK	N	5.47
1	C	2427:LEU	C	2447:UNK	N	5.34
1	E	2427:LEU	C	2447:UNK	N	5.15
1	G	1484:ASN	C	1496:UNK	N	4.71
1	A	2616:UNK	C	2617:UNK	N	4.70
1	C	3391:UNK	C	3392:UNK	N	4.48
1	A	2427:LEU	C	2447:UNK	N	4.21
1	E	1484:ASN	C	1496:UNK	N	4.12
1	G	2427:LEU	C	2447:UNK	N	3.84

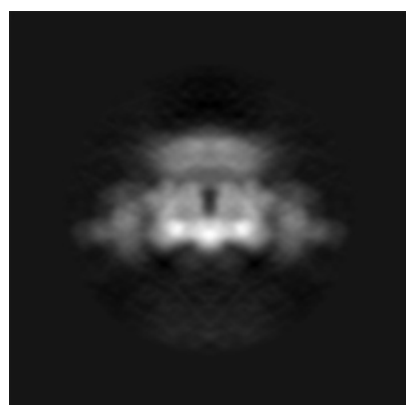
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8303. These allow visual inspection of the internal detail of the map and identification of artifacts.

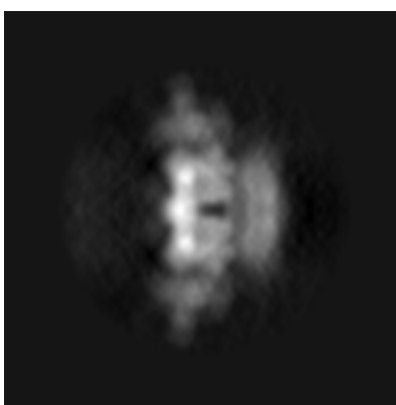
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

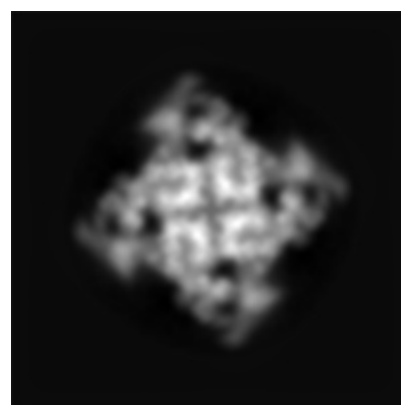
6.1.1 Primary map



X



Y

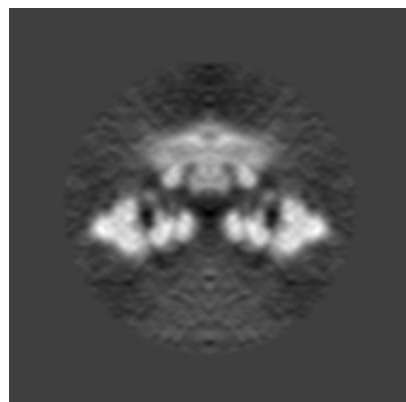


Z

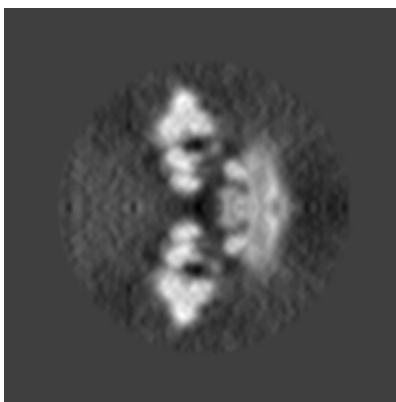
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

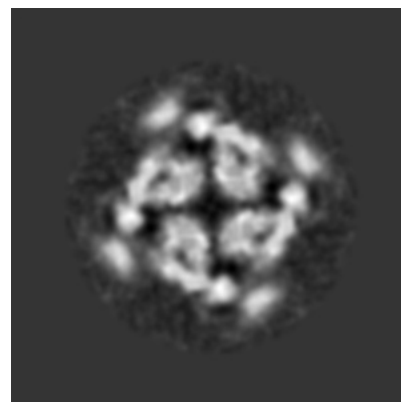
6.2.1 Primary map



X Index: 200



Y Index: 200

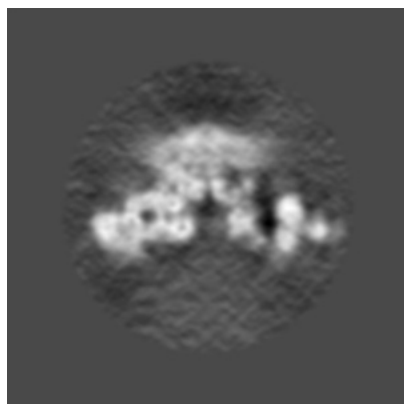


Z Index: 200

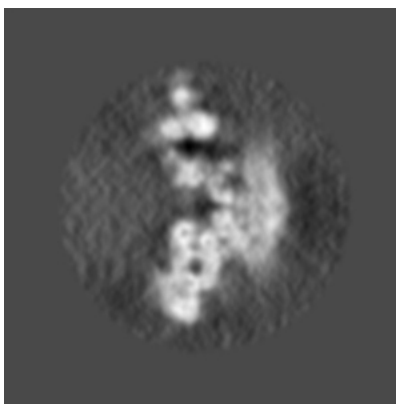
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

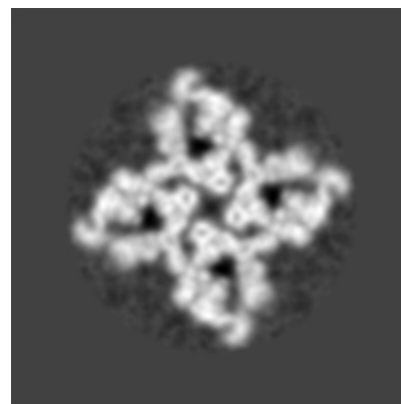
6.3.1 Primary map



X Index: 190



Y Index: 210

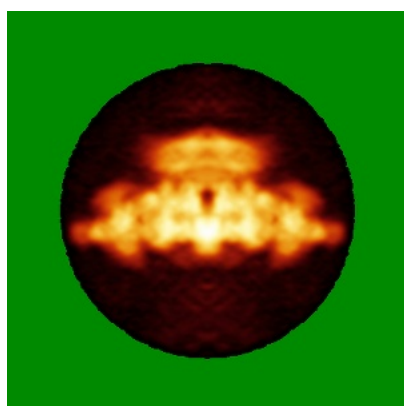


Z Index: 181

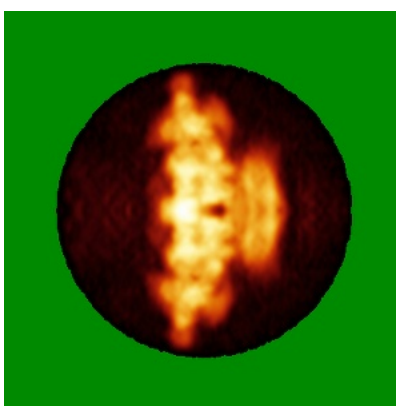
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

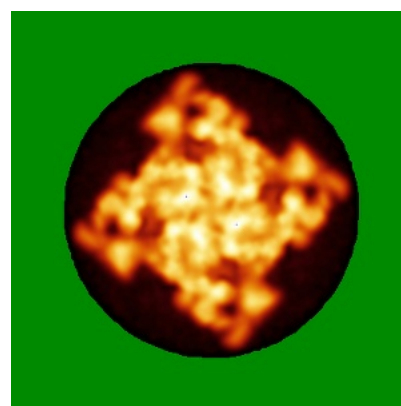
6.4.1 Primary map



X



Y

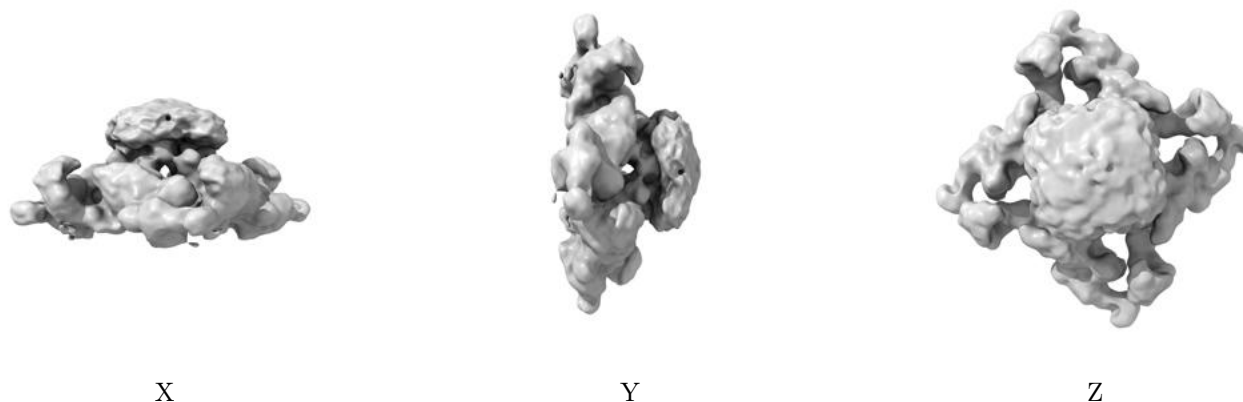


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

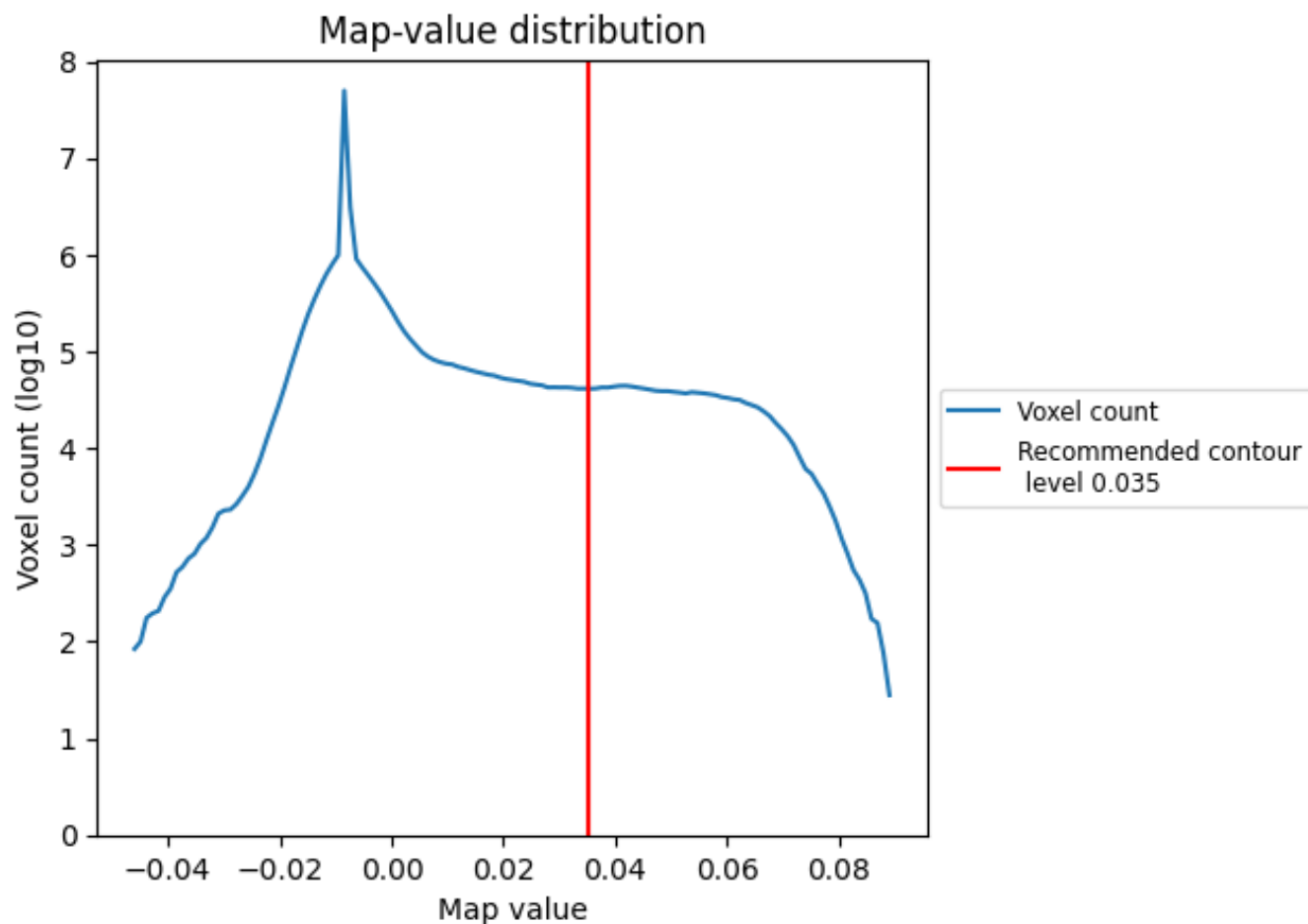
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

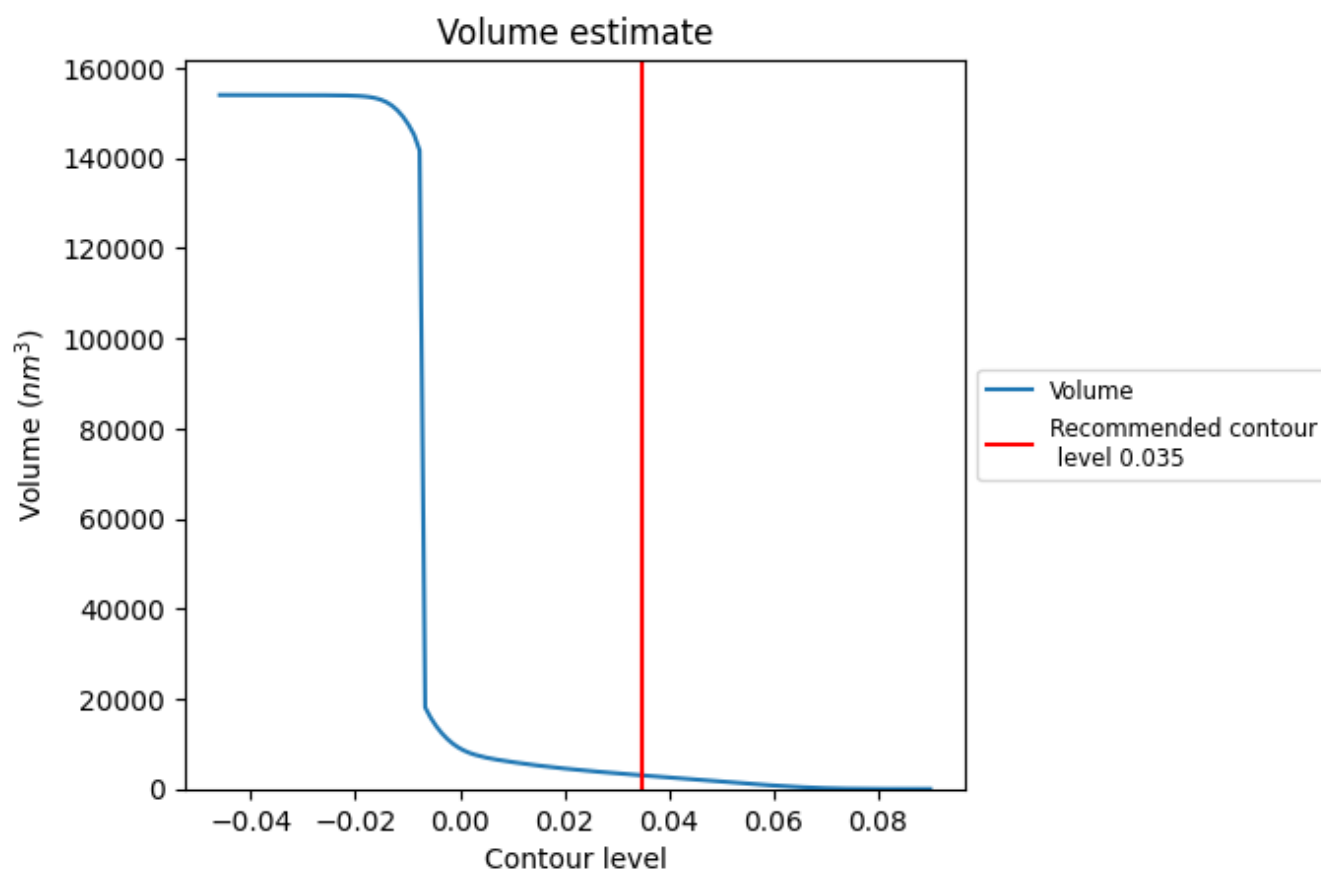
This section contains the results of statistical analysis of the map.

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.

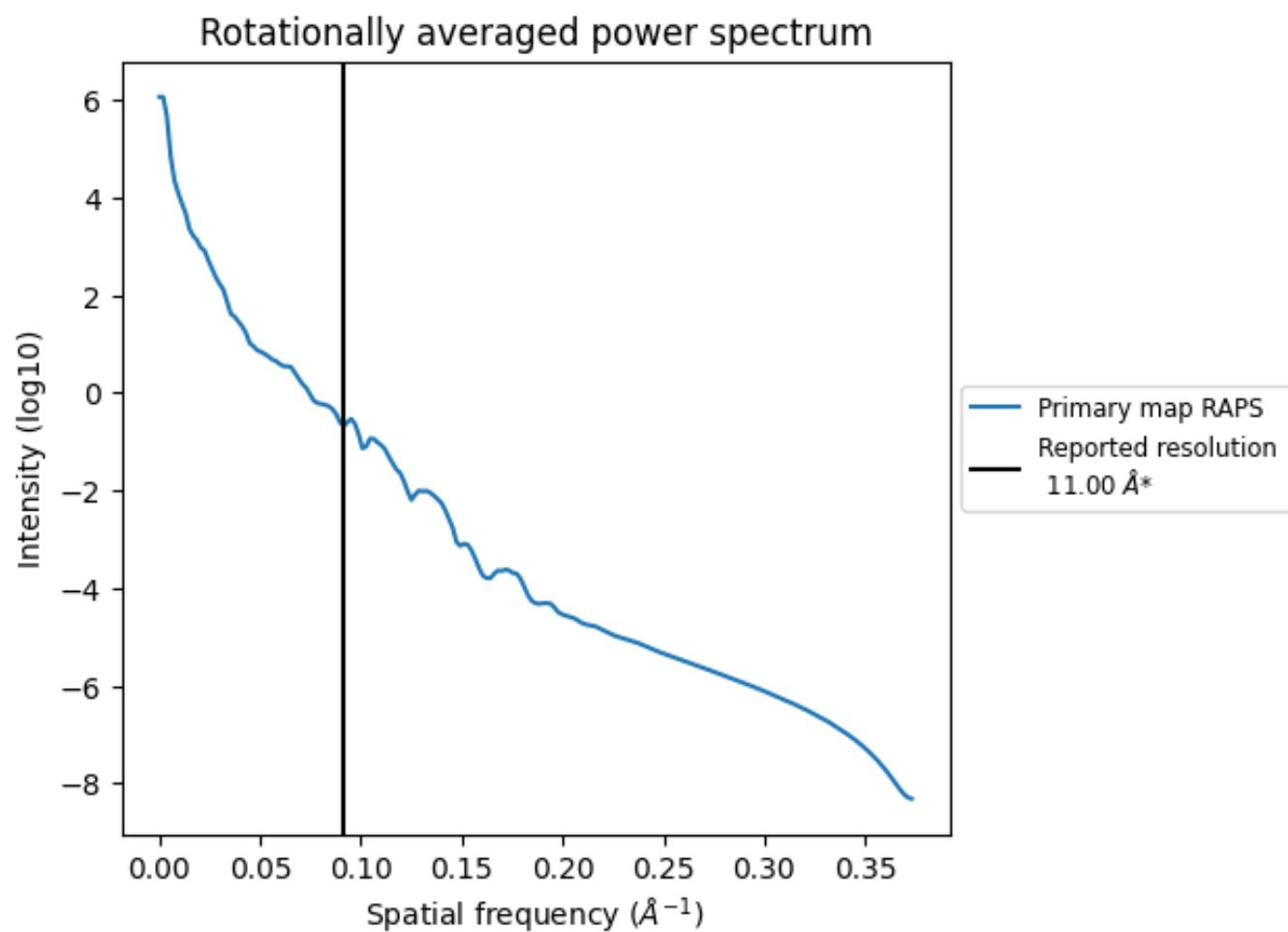
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3008 nm³; this corresponds to an approximate mass of 2718 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.091 Å⁻¹

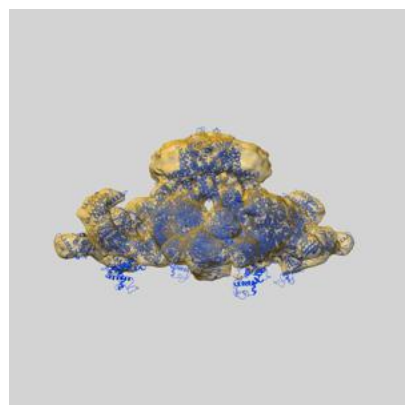
8 Fourier-Shell correlation

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

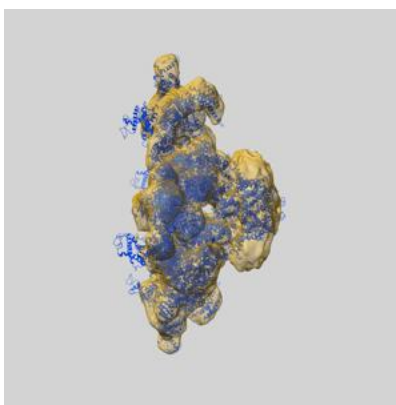
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8303 and PDB model 5L1D. Per-residue inclusion information can be found in section [3](#) on page [10](#).

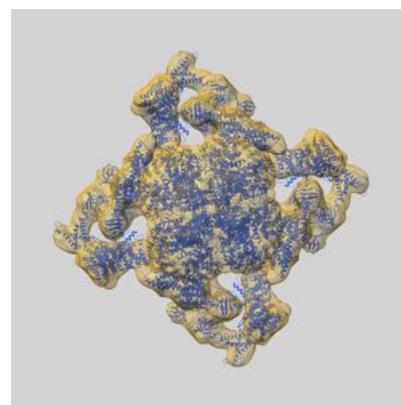
9.1 Map-model overlay [i](#)



X



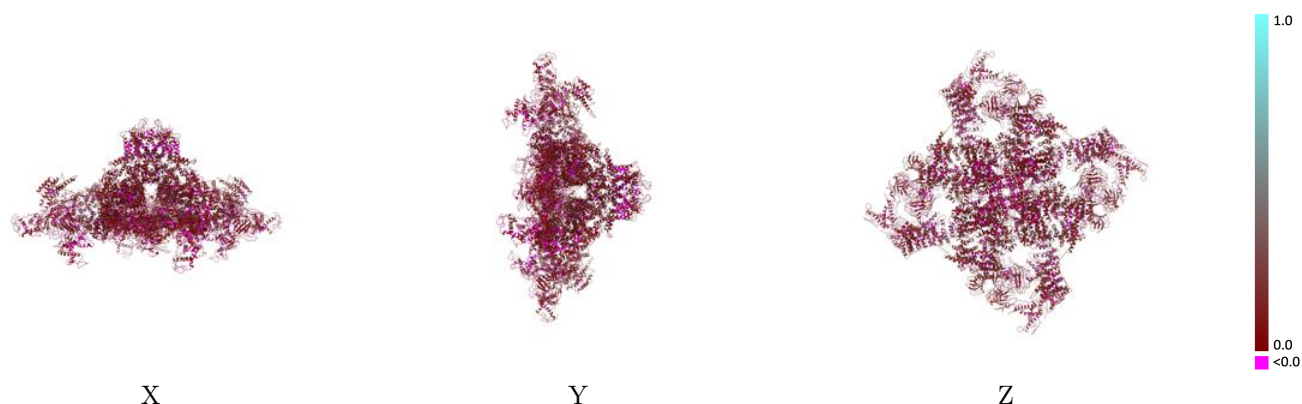
Y



Z

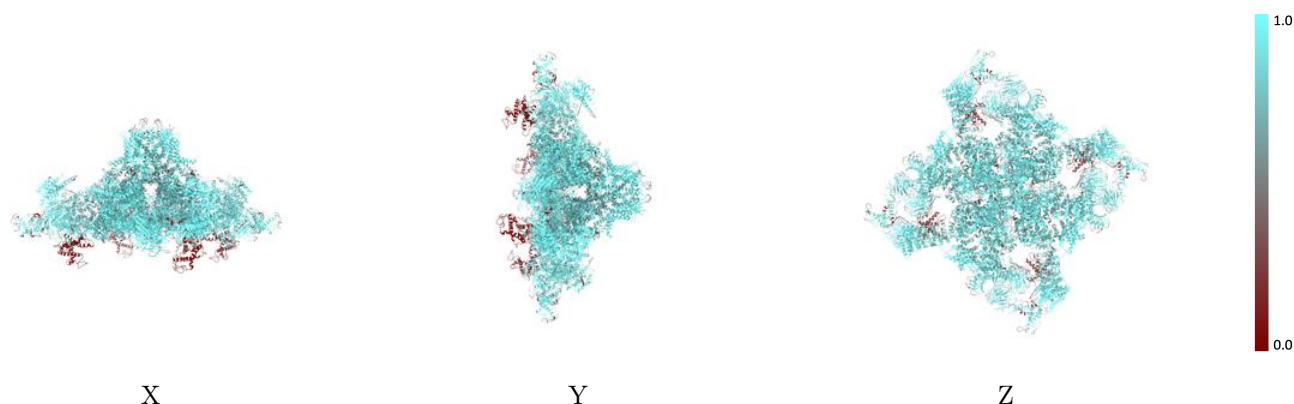
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



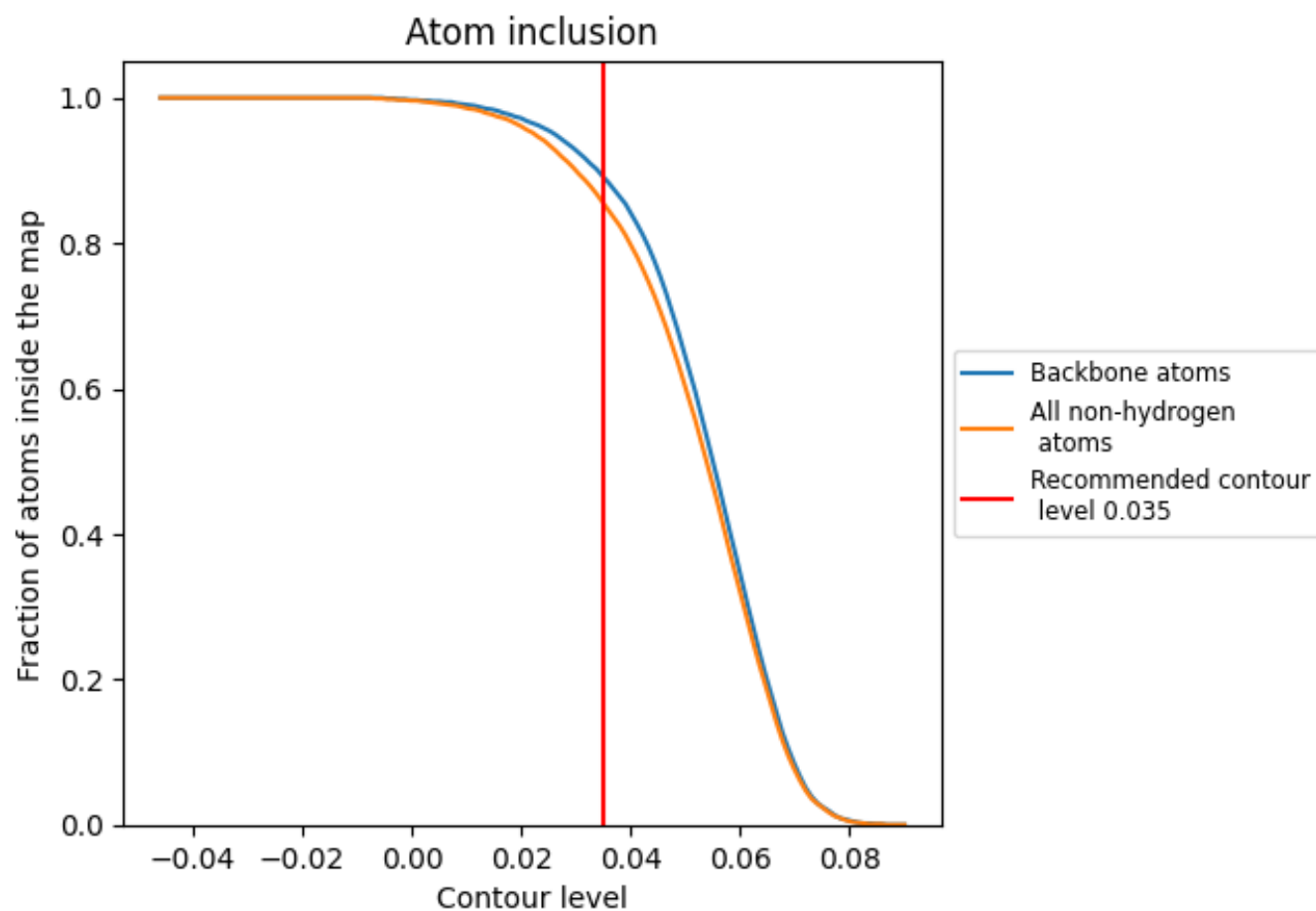
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 86% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8550	0.0820
A	0.8560	0.0820
B	0.8470	0.0660
C	0.8560	0.0820
D	0.8460	0.0720
E	0.8550	0.0820
F	0.8440	0.0750
G	0.8560	0.0830
H	0.8380	0.0700

1.0

0.0

<0.0