



## Full wwPDB EM Validation Report ⓘ

Jan 16, 2025 – 07:59 am GMT

PDB ID : 8CQ0  
EMDB ID : EMD-16792  
Title : Photorhabdus luminescens TcdA1 prepore-to-pore intermediate, K567W K2008W mutant  
Authors : Nganga, P.N.; Roderer, D.; Belyy, A.; Prumbaum, D.; Raunser, S.  
Deposited on : 2023-03-03  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

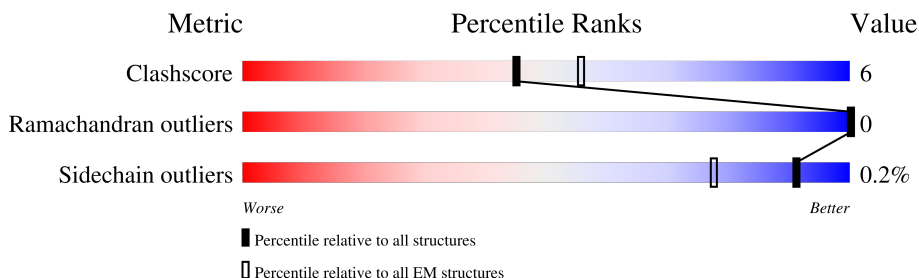
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	2535	
1	B	2535	
1	C	2535	
1	D	2535	
1	E	2535	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 84445 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 TcdA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2122	Total	C	N	O	S	0	0
			16889	10704	2868	3262	55		
1	B	2122	Total	C	N	O	S	0	0
			16889	10704	2868	3262	55		
1	C	2122	Total	C	N	O	S	0	0
			16889	10704	2868	3262	55		
1	D	2122	Total	C	N	O	S	0	0
			16889	10704	2868	3262	55		
1	E	2122	Total	C	N	O	S	0	0
			16889	10704	2868	3262	55		

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP Q9RN43
A	-17	ALA	-	expression tag	UNP Q9RN43
A	-16	HIS	-	expression tag	UNP Q9RN43
A	-15	HIS	-	expression tag	UNP Q9RN43
A	-14	HIS	-	expression tag	UNP Q9RN43
A	-13	HIS	-	expression tag	UNP Q9RN43
A	-12	HIS	-	expression tag	UNP Q9RN43
A	-11	HIS	-	expression tag	UNP Q9RN43
A	-10	SER	-	expression tag	UNP Q9RN43
A	-9	SER	-	expression tag	UNP Q9RN43
A	-8	GLY	-	expression tag	UNP Q9RN43
A	-7	LEU	-	expression tag	UNP Q9RN43
A	-6	GLU	-	expression tag	UNP Q9RN43
A	-5	VAL	-	expression tag	UNP Q9RN43
A	-4	LEU	-	expression tag	UNP Q9RN43
A	-3	PHE	-	expression tag	UNP Q9RN43
A	-2	GLN	-	expression tag	UNP Q9RN43
A	-1	GLY	-	expression tag	UNP Q9RN43
A	0	PRO	-	expression tag	UNP Q9RN43
A	567	TRP	LYS	engineered mutation	UNP Q9RN43

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2008	TRP	LYS	engineered mutation	UNP Q9RN43
B	-18	MET	-	initiating methionine	UNP Q9RN43
B	-17	ALA	-	expression tag	UNP Q9RN43
B	-16	HIS	-	expression tag	UNP Q9RN43
B	-15	HIS	-	expression tag	UNP Q9RN43
B	-14	HIS	-	expression tag	UNP Q9RN43
B	-13	HIS	-	expression tag	UNP Q9RN43
B	-12	HIS	-	expression tag	UNP Q9RN43
B	-11	HIS	-	expression tag	UNP Q9RN43
B	-10	SER	-	expression tag	UNP Q9RN43
B	-9	SER	-	expression tag	UNP Q9RN43
B	-8	GLY	-	expression tag	UNP Q9RN43
B	-7	LEU	-	expression tag	UNP Q9RN43
B	-6	GLU	-	expression tag	UNP Q9RN43
B	-5	VAL	-	expression tag	UNP Q9RN43
B	-4	LEU	-	expression tag	UNP Q9RN43
B	-3	PHE	-	expression tag	UNP Q9RN43
B	-2	GLN	-	expression tag	UNP Q9RN43
B	-1	GLY	-	expression tag	UNP Q9RN43
B	0	PRO	-	expression tag	UNP Q9RN43
B	567	TRP	LYS	engineered mutation	UNP Q9RN43
B	2008	TRP	LYS	engineered mutation	UNP Q9RN43
C	-18	MET	-	initiating methionine	UNP Q9RN43
C	-17	ALA	-	expression tag	UNP Q9RN43
C	-16	HIS	-	expression tag	UNP Q9RN43
C	-15	HIS	-	expression tag	UNP Q9RN43
C	-14	HIS	-	expression tag	UNP Q9RN43
C	-13	HIS	-	expression tag	UNP Q9RN43
C	-12	HIS	-	expression tag	UNP Q9RN43
C	-11	HIS	-	expression tag	UNP Q9RN43
C	-10	SER	-	expression tag	UNP Q9RN43
C	-9	SER	-	expression tag	UNP Q9RN43
C	-8	GLY	-	expression tag	UNP Q9RN43
C	-7	LEU	-	expression tag	UNP Q9RN43
C	-6	GLU	-	expression tag	UNP Q9RN43
C	-5	VAL	-	expression tag	UNP Q9RN43
C	-4	LEU	-	expression tag	UNP Q9RN43
C	-3	PHE	-	expression tag	UNP Q9RN43
C	-2	GLN	-	expression tag	UNP Q9RN43
C	-1	GLY	-	expression tag	UNP Q9RN43
C	0	PRO	-	expression tag	UNP Q9RN43
C	567	TRP	LYS	engineered mutation	UNP Q9RN43

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2008	TRP	LYS	engineered mutation	UNP Q9RN43
D	-18	MET	-	initiating methionine	UNP Q9RN43
D	-17	ALA	-	expression tag	UNP Q9RN43
D	-16	HIS	-	expression tag	UNP Q9RN43
D	-15	HIS	-	expression tag	UNP Q9RN43
D	-14	HIS	-	expression tag	UNP Q9RN43
D	-13	HIS	-	expression tag	UNP Q9RN43
D	-12	HIS	-	expression tag	UNP Q9RN43
D	-11	HIS	-	expression tag	UNP Q9RN43
D	-10	SER	-	expression tag	UNP Q9RN43
D	-9	SER	-	expression tag	UNP Q9RN43
D	-8	GLY	-	expression tag	UNP Q9RN43
D	-7	LEU	-	expression tag	UNP Q9RN43
D	-6	GLU	-	expression tag	UNP Q9RN43
D	-5	VAL	-	expression tag	UNP Q9RN43
D	-4	LEU	-	expression tag	UNP Q9RN43
D	-3	PHE	-	expression tag	UNP Q9RN43
D	-2	GLN	-	expression tag	UNP Q9RN43
D	-1	GLY	-	expression tag	UNP Q9RN43
D	0	PRO	-	expression tag	UNP Q9RN43
D	567	TRP	LYS	engineered mutation	UNP Q9RN43
D	2008	TRP	LYS	engineered mutation	UNP Q9RN43
E	-18	MET	-	initiating methionine	UNP Q9RN43
E	-17	ALA	-	expression tag	UNP Q9RN43
E	-16	HIS	-	expression tag	UNP Q9RN43
E	-15	HIS	-	expression tag	UNP Q9RN43
E	-14	HIS	-	expression tag	UNP Q9RN43
E	-13	HIS	-	expression tag	UNP Q9RN43
E	-12	HIS	-	expression tag	UNP Q9RN43
E	-11	HIS	-	expression tag	UNP Q9RN43
E	-10	SER	-	expression tag	UNP Q9RN43
E	-9	SER	-	expression tag	UNP Q9RN43
E	-8	GLY	-	expression tag	UNP Q9RN43
E	-7	LEU	-	expression tag	UNP Q9RN43
E	-6	GLU	-	expression tag	UNP Q9RN43
E	-5	VAL	-	expression tag	UNP Q9RN43
E	-4	LEU	-	expression tag	UNP Q9RN43
E	-3	PHE	-	expression tag	UNP Q9RN43
E	-2	GLN	-	expression tag	UNP Q9RN43
E	-1	GLY	-	expression tag	UNP Q9RN43
E	0	PRO	-	expression tag	UNP Q9RN43
E	567	TRP	LYS	engineered mutation	UNP Q9RN43

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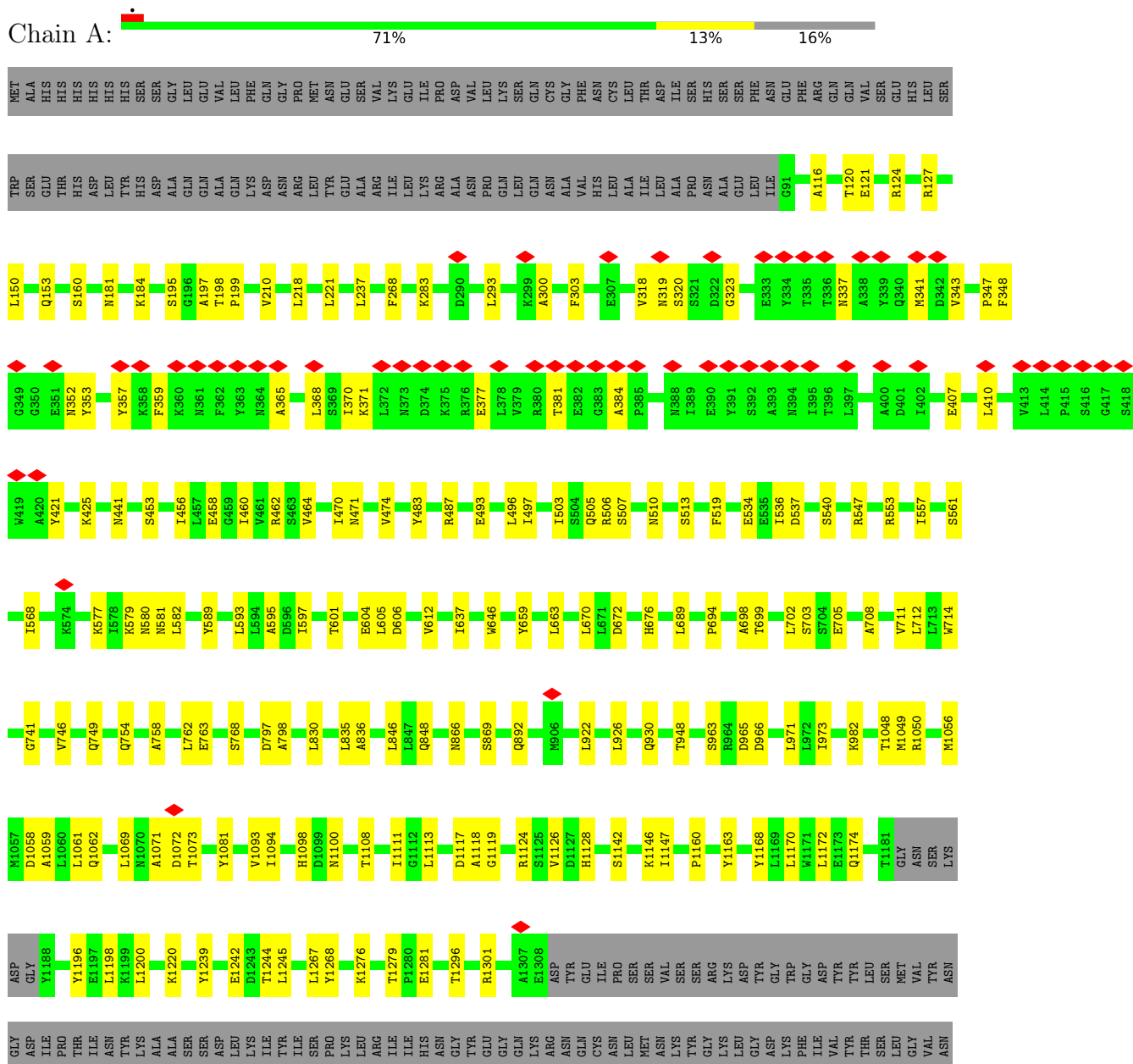
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Chain	Residue	Modelled	Actual	Comment	Reference
E	2008	TRP	LYS	engineered mutation	UNP Q9RN43

### 3 Residue-property plots

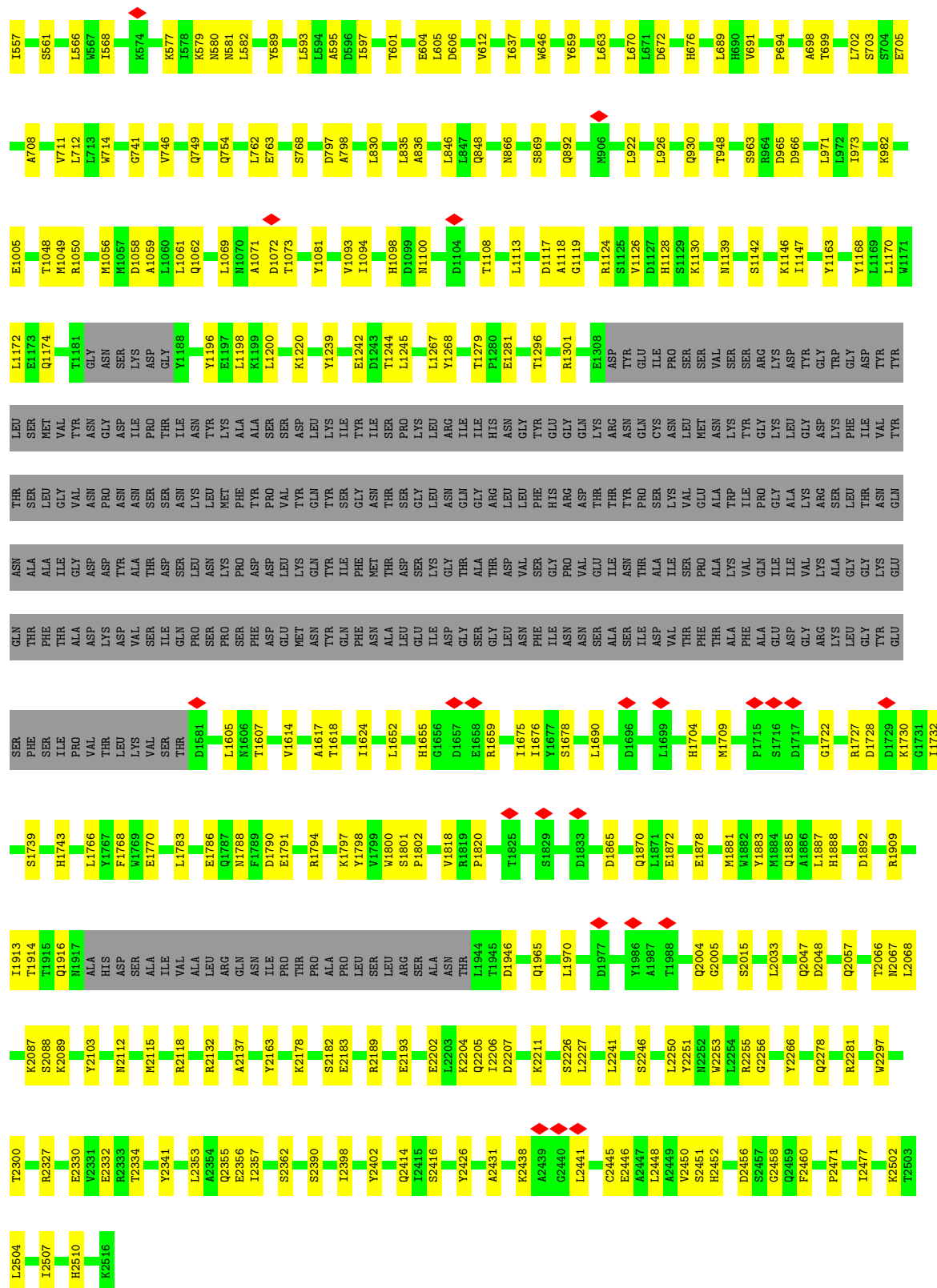
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: TcdA1

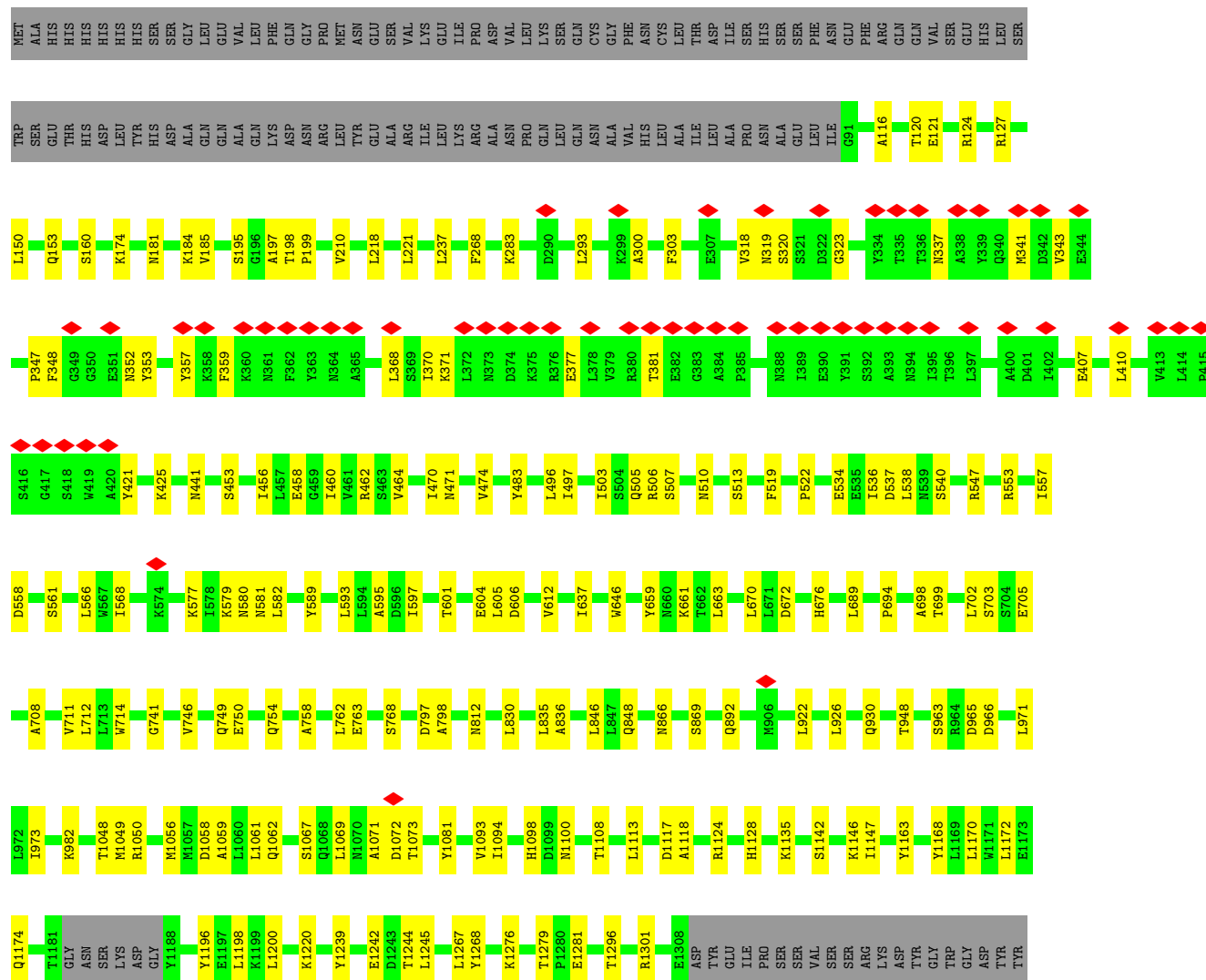








[illegible]





P2471	W2297	Q2057	I1913	H1743	SER	ALA	LEU	Q1174	T1048	L713	K574	M441
F2472	T2300	T2066	T1914	L1766	ILE	GLY	VAL	T1181	M1049	W714	K577	S453
E2473	T2300	N2067	T1915	Y1767	PRO	ASN	ASN	ASP	R1050	A724	I578	I456
I2477	H2321	L2068	Q1916	F1768	THR	ASP	PRO	LYS	ASN	K729	K579	I457
K2502	D2325	K2087	A1917	H1768	LEU	THR	ASN	SER	M1056	G741	N580	E458
T2503	K2326	S2086	ALA	E1770	LYS	THR	ASN	ASP	D1058	V746	N581	G459
L2504	R2327	K2089	HIS	Y1774	VAL	THR	SER	GLY	A1059	L762	I460	V461
I2507	Y2103	Y2103	ALA	Y1774	THR	THR	ASN	ILE	L1060	E763	R462	S463
H2510	E2330	Y2103	ILE	L1783	D1581	PRO	LEU	LYS	L1061	S768	R463	V464
K2516	V2331	N2112	VAL	E1786	L1605	SER	LYS	Y1196	Q1062	E750	L593	I470
	E2332	M2115	ALA	Q1787	N1606	PHE	PHE	E1197	S1067	Q754	L594	N471
	R2333	W2118	LEU	Y1788	T1607	ASP	THR	L1198	Q1068	L762	A595	W474
	T2334	R2118	ARG	F1789	V1644	GLU	VAL	K1199	L1069	E763	I597	Y483
	Y2341	D1790	GLN	E1791	V1644	LEU	GLN	L1200	N1070	L762	T601	E493
	L2353	E1791	ASN	E1791	A1617	THR	THR	K1220	A1071	S768	E604	L496
	T2357	R1794	PRO	R1794	T1618	GLN	THR	Y1239	D1072	D797	L605	I497
	S2362	K1797	THR	K1797	I1624	PHE	ASN	E1242	T1073	A798	D606	R457
	S2390	Y1798	ALA	Y1798	L1652	ALA	THR	T1244	Y1081	L830	W646	E503
	T2398	W1800	SER	W1800	H1655	GLU	SER	L1245	H1093	L835	Y659	S564
	Q2414	S1801	LEU	P1802	G1656	ILE	LEU	L1267	H1098	A836	N660	Q505
	T2415	GLY	ARG	P1802	D1657	GLY	GLN	Y1268	N1099	L846	K661	R506
	S2416	ALA	SER	P1802	E1658	THR	ALA	T1279	M1100	Q848	T662	S507
	Y2426	R1813	ASN	P1820	R1659	LEU	THR	E1281	T1108	P860	L663	N510
	A2431	P1820	THR	P1820	I1675	ASN	VAL	T1296	L1113	L866	L670	S513
	K2438	P1820	THR	P1820	Y1677	PHE	GLY	R1301	D1117	N869	L671	F519
	A2439	T1825	ALA	T1825	S1678	ASN	THR	E1308	A1118	Q892	H676	E534
	G2440	S1829	ILE	S1829	L1690	VAL	GLU	ASP	R1124	H906	L689	E535
	L2441	D1833	SER	D1833	D1696	GLU	THR	ASP	V1125	L922	H690	I536
	C2445	Y1848	SER	Y1848	L1699	ILE	THR	TRP	S1126	L926	D537	L538
	E2446	D1865	ASP	D1865	H1704	VAL	LYS	ILE	D1127	Q930	V691	N539
	A2447	Q1870	THR	Q1870	M1709	ALA	VAL	SER	H1128	T948	P694	S540
	L2448	E1872	THR	E1872	P1715	THR	THR	VAL	K1146	A698	T699	R547
	L2250	E1878	PHE	E1878	S1716	ALA	GLY	ASP	I1147	L702	L702	R553
	Y2251	M1881	ALA	M1881	D1722	GLY	LYS	TRP	Y1163	S963	I557	I557
	W2252	W1882	ASP	W1882	R1727	VAL	LYS	GLY	L1167	R964	S704	S661
	W2253	Y1883	ARG	Y1883	D1728	ALA	GLY	ASP	Y1168	D965	E705	L566
	L2254	Q1885	LEU	Q1885	D1729	LEU	THR	ILE	L1170	D966	A708	W567
	R2255	H1888	THR	H1888	K1730	ASN	GLN	THR	W1171	L971	V711	I568
	G2256	D1892	GLU	D1892	I1732	THR	ALA	SER	L1172	L972	L712	
	Y2266	R1909	PHE	R1909	S1739	THR	ALA		E1173			
	Q2278											
	R2281											
	L2470											

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	13356	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	57	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	492.8, 492.8, 492.8	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.26	0/17254	0.51	0/23440
1	B	0.26	0/17254	0.51	0/23440
1	C	0.26	0/17254	0.51	0/23440
1	D	0.26	0/17254	0.51	0/23440
1	E	0.26	0/17254	0.51	0/23440
All	All	0.26	0/86270	0.51	0/117200

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	16889	0	16504	227	0
1	B	16889	0	16504	221	0
1	C	16889	0	16504	232	0
1	D	16889	0	16504	223	0
1	E	16889	0	16504	225	0
All	All	84445	0	82520	1013	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 6.

All (1013) 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:C:1108:THR:HG1	1:C:1128:HIS:HE2	1.23	0.83
1:B:1108:THR:HG1	1:B:1128:HIS:HE2	1.26	0.80
1:C:1797:LYS:HG3	1:C:1801:SER:HB2	1.64	0.80
1:E:1108:THR:HG1	1:E:1128:HIS:HE2	1.29	0.79
1:A:1797:LYS:HG3	1:A:1801:SER:HB2	1.65	0.79
1:D:1797:LYS:HG3	1:D:1801:SER:HB2	1.65	0.79
1:B:1797:LYS:HG3	1:B:1801:SER:HB2	1.65	0.78
1:E:1797:LYS:HG3	1:E:1801:SER:HB2	1.64	0.78
1:B:689:LEU:HD11	1:B:712:LEU:HB3	1.67	0.78
1:A:689:LEU:HD11	1:A:712:LEU:HB3	1.66	0.77
1:C:689:LEU:HD11	1:C:712:LEU:HB3	1.66	0.77
1:D:689:LEU:HD11	1:D:712:LEU:HB3	1.66	0.76
1:E:689:LEU:HD11	1:E:712:LEU:HB3	1.66	0.75
1:D:460:ILE:HG12	1:D:496:LEU:HD21	1.71	0.73
1:C:2089:LYS:HB2	1:C:2206:ILE:HG21	1.70	0.73
1:E:2089:LYS:HB2	1:E:2206:ILE:HG21	1.71	0.73
1:D:2089:LYS:HB2	1:D:2206:ILE:HG21	1.70	0.72
1:B:460:ILE:HG12	1:B:496:LEU:HD21	1.70	0.72
1:E:460:ILE:HG12	1:E:496:LEU:HD21	1.72	0.72
1:C:1093:VAL:HG21	1:C:1605:LEU:HD23	1.72	0.72
1:B:2089:LYS:HB2	1:B:2206:ILE:HG21	1.70	0.72
1:C:460:ILE:HG12	1:C:496:LEU:HD21	1.71	0.71
1:C:2204:LYS:O	1:D:2087:LYS:NZ	2.24	0.71
1:A:2089:LYS:HB2	1:A:2206:ILE:HG21	1.72	0.71
1:A:2204:LYS:O	1:B:2087:LYS:NZ	2.24	0.71
1:D:2204:LYS:O	1:E:2087:LYS:NZ	2.24	0.71
1:A:1059:ALA:HA	1:A:1062:GLN:HE21	1.56	0.70
1:D:1093:VAL:HG21	1:D:1605:LEU:HD23	1.73	0.70
1:A:460:ILE:HG12	1:A:496:LEU:HD21	1.71	0.70
1:E:1059:ALA:HA	1:E:1062:GLN:HE21	1.56	0.70
1:A:1093:VAL:HG21	1:A:1605:LEU:HD23	1.74	0.70
1:E:1093:VAL:HG21	1:E:1605:LEU:HD23	1.73	0.69
1:B:1093:VAL:HG21	1:B:1605:LEU:HD23	1.74	0.69
1:B:1059:ALA:HA	1:B:1062:GLN:HE21	1.57	0.69
1:A:2087:LYS:NZ	1:E:2204:LYS:O	2.24	0.69
1:D:1146:LYS:NZ	1:D:1147:ILE:O	2.26	0.69
1:D:1059:ALA:HA	1:D:1062:GLN:HE21	1.57	0.69
1:A:1146:LYS:NZ	1:A:1147:ILE:O	2.26	0.68
1:E:1916:GLN:NE2	1:E:1946:ASP:OD2	2.26	0.68
1:C:612:VAL:HG22	1:C:637:ILE:HD12	1.76	0.68
1:C:1059:ALA:HA	1:C:1062:GLN:HE21	1.57	0.68
1:E:237:LEU:HD11	1:E:483:TYR:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:LEU:HD11	1:B:483:TYR:HB2	1.75	0.68
1:A:237:LEU:HD11	1:A:483:TYR:HB2	1.76	0.67
1:C:237:LEU:HD11	1:C:483:TYR:HB2	1.76	0.67
1:E:1146:LYS:NZ	1:E:1147:ILE:O	2.25	0.67
1:D:237:LEU:HD11	1:D:483:TYR:HB2	1.77	0.67
1:C:1916:GLN:NE2	1:C:1946:ASP:OD2	2.28	0.67
1:A:2047:GLN:HB3	1:A:2251:TYR:HB3	1.77	0.67
1:A:2087:LYS:HD3	1:E:2204:LYS:HG2	1.77	0.67
1:A:2426:TYR:HB3	1:B:2334:THR:HG21	1.75	0.67
1:D:2426:TYR:HB3	1:E:2334:THR:HG21	1.77	0.67
1:A:300:ALA:HA	1:A:303:PHE:CD2	2.30	0.67
1:B:2047:GLN:HB3	1:B:2251:TYR:HB3	1.77	0.67
1:C:1146:LYS:NZ	1:C:1147:ILE:O	2.26	0.67
1:B:1916:GLN:NE2	1:B:1946:ASP:OD2	2.27	0.67
1:C:300:ALA:HA	1:C:303:PHE:CD2	2.30	0.67
1:A:612:VAL:HG22	1:A:637:ILE:HD12	1.76	0.66
1:D:300:ALA:HA	1:D:303:PHE:CD2	2.30	0.66
1:C:2204:LYS:HG2	1:D:2087:LYS:HD3	1.78	0.66
1:E:612:VAL:HG22	1:E:637:ILE:HD12	1.76	0.66
1:B:1146:LYS:NZ	1:B:1147:ILE:O	2.26	0.66
1:D:2204:LYS:HG2	1:E:2087:LYS:HD3	1.77	0.66
1:A:2205:GLN:OE1	1:B:2088:SER:OG	2.13	0.66
1:D:2205:GLN:OE1	1:E:2088:SER:OG	2.13	0.66
1:B:612:VAL:HG22	1:B:637:ILE:HD12	1.77	0.66
1:E:300:ALA:HA	1:E:303:PHE:CD2	2.31	0.66
1:E:2047:GLN:HB3	1:E:2251:TYR:HB3	1.77	0.66
1:A:2204:LYS:HG2	1:B:2087:LYS:HD3	1.77	0.66
1:B:121:GLU:HG2	1:B:124:ARG:HH21	1.60	0.66
1:D:1916:GLN:NE2	1:D:1946:ASP:OD2	2.28	0.66
1:C:830:LEU:HD21	1:C:835:LEU:HD12	1.78	0.65
1:C:963:SER:OG	1:C:965:ASP:OD1	2.14	0.65
1:B:300:ALA:HA	1:B:303:PHE:CD2	2.31	0.65
1:E:2438:LYS:HG3	1:E:2446:GLU:HG3	1.78	0.65
1:D:612:VAL:HG22	1:D:637:ILE:HD12	1.77	0.65
1:A:1916:GLN:NE2	1:A:1946:ASP:OD2	2.28	0.65
1:B:2204:LYS:O	1:C:2087:LYS:NZ	2.23	0.65
1:C:2047:GLN:HB3	1:C:2251:TYR:HB3	1.77	0.65
1:A:2334:THR:HG21	1:E:2426:TYR:HB3	1.79	0.65
1:D:963:SER:OG	1:D:965:ASP:OD1	2.15	0.65
1:D:2047:GLN:HB3	1:D:2251:TYR:HB3	1.77	0.65
1:A:121:GLU:HG2	1:A:124:ARG:HH21	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:830:LEU:HD21	1:B:835:LEU:HD12	1.79	0.64
1:E:963:SER:OG	1:E:965:ASP:OD1	2.14	0.64
1:C:1069:LEU:HD23	1:C:1786:GLU:HG3	1.80	0.64
1:A:963:SER:OG	1:A:965:ASP:OD1	2.14	0.64
1:B:2204:LYS:HG2	1:C:2087:LYS:HD3	1.77	0.64
1:A:368:LEU:N	1:A:381:THR:O	2.28	0.64
1:C:2205:GLN:OE1	1:D:2088:SER:OG	2.12	0.64
1:B:1069:LEU:HD23	1:B:1786:GLU:HG3	1.80	0.64
1:C:2182:SER:OG	1:E:1067:SER:OG	2.12	0.64
1:C:2451:SER:HB3	1:D:2332:GLU:HG2	1.80	0.64
1:D:830:LEU:HD21	1:D:835:LEU:HD12	1.79	0.64
1:B:963:SER:OG	1:B:965:ASP:OD1	2.15	0.64
1:D:121:GLU:HG2	1:D:124:ARG:HH21	1.63	0.64
1:A:210:VAL:HG11	1:A:922:LEU:HB3	1.81	0.63
1:A:2438:LYS:HG3	1:A:2446:GLU:HG3	1.78	0.63
1:D:1069:LEU:HD23	1:D:1786:GLU:HG3	1.80	0.63
1:C:121:GLU:HG2	1:C:124:ARG:HH21	1.61	0.63
1:E:121:GLU:HG2	1:E:124:ARG:HH21	1.63	0.63
1:E:1069:LEU:HD23	1:E:1786:GLU:HG3	1.80	0.63
1:A:1069:LEU:HD23	1:A:1786:GLU:HG3	1.80	0.63
1:B:2438:LYS:HG3	1:B:2446:GLU:HG3	1.81	0.63
1:D:210:VAL:HG11	1:D:922:LEU:HB3	1.79	0.63
1:E:830:LEU:HD21	1:E:835:LEU:HD12	1.79	0.63
1:C:210:VAL:HG11	1:C:922:LEU:HB3	1.81	0.63
1:D:2438:LYS:HG3	1:D:2446:GLU:HG3	1.79	0.63
1:A:2255:ARG:NH2	1:E:703:SER:O	2.25	0.62
1:E:210:VAL:HG11	1:E:922:LEU:HB3	1.80	0.62
1:A:830:LEU:HD21	1:A:835:LEU:HD12	1.80	0.62
1:B:2451:SER:HB3	1:C:2332:GLU:HG2	1.79	0.62
1:B:2205:GLN:OE1	1:C:2088:SER:OG	2.12	0.62
1:B:337:ASN:ND2	1:B:421:TYR:O	2.25	0.62
1:D:2451:SER:HB3	1:E:2332:GLU:HG2	1.81	0.62
1:B:659:TYR:HB2	1:B:754:GLN:HG2	1.82	0.62
1:E:368:LEU:N	1:E:381:THR:O	2.28	0.62
1:C:659:TYR:HB2	1:C:754:GLN:HG2	1.83	0.61
1:C:1239:TYR:CD2	1:C:1242:GLU:HB3	2.36	0.61
1:B:2460:PHE:CE1	1:C:2330:GLU:HB3	2.36	0.61
1:C:2438:LYS:HG3	1:C:2446:GLU:HG3	1.82	0.61
1:A:2332:GLU:HG2	1:E:2451:SER:HB3	1.81	0.61
1:A:2451:SER:HB3	1:B:2332:GLU:HG2	1.81	0.61
1:B:210:VAL:HG11	1:B:922:LEU:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:LEU:N	1:C:381:THR:O	2.28	0.61
1:B:1239:TYR:CD2	1:B:1242:GLU:HB3	2.36	0.61
1:C:2460:PHE:CE1	1:D:2330:GLU:HB3	2.35	0.61
1:D:659:TYR:HB2	1:D:754:GLN:HG2	1.83	0.61
1:D:1239:TYR:CD2	1:D:1242:GLU:HB3	2.36	0.61
1:A:2088:SER:OG	1:E:2205:GLN:OE1	2.13	0.61
1:D:2460:PHE:CE1	1:E:2330:GLU:HB3	2.36	0.61
1:E:1220:LYS:HE2	1:E:1267:LEU:HB3	1.83	0.60
1:D:1220:LYS:HE2	1:D:1267:LEU:HB3	1.84	0.60
1:A:337:ASN:ND2	1:A:421:TYR:O	2.25	0.60
1:A:540:SER:HB2	1:B:848:GLN:HE22	1.67	0.60
1:A:703:SER:O	1:B:2255:ARG:NH2	2.25	0.60
1:A:2460:PHE:CE1	1:B:2330:GLU:HB3	2.36	0.60
1:A:848:GLN:HE22	1:E:540:SER:HB2	1.67	0.60
1:D:124:ARG:HD3	1:D:1914:THR:HB	1.84	0.60
1:E:1239:TYR:CD2	1:E:1242:GLU:HB3	2.36	0.60
1:B:540:SER:HB2	1:C:848:GLN:HE22	1.67	0.60
1:A:659:TYR:HB2	1:A:754:GLN:HG2	1.83	0.60
1:A:2137:ALA:HB2	1:C:1118:ALA:HB2	1.82	0.59
1:A:2330:GLU:HB3	1:E:2460:PHE:CE1	2.36	0.59
1:C:337:ASN:ND2	1:C:421:TYR:O	2.25	0.59
1:A:1239:TYR:CD2	1:A:1242:GLU:HB3	2.36	0.59
1:B:2426:TYR:HB3	1:C:2334:THR:HG21	1.84	0.59
1:D:368:LEU:N	1:D:381:THR:O	2.29	0.59
1:D:540:SER:HB2	1:E:848:GLN:HE22	1.67	0.59
1:E:337:ASN:ND2	1:E:421:TYR:O	2.25	0.59
1:D:746:VAL:HB	1:D:749:GLN:HB2	1.85	0.59
1:A:1220:LYS:HE2	1:A:1267:LEU:HB3	1.85	0.59
1:B:1296:THR:HG23	1:B:1301:ARG:HH12	1.68	0.59
1:C:2137:ALA:HB2	1:E:1118:ALA:HB2	1.83	0.59
1:E:659:TYR:HB2	1:E:754:GLN:HG2	1.84	0.59
1:B:1220:LYS:HE2	1:B:1267:LEU:HB3	1.84	0.59
1:D:703:SER:O	1:E:2255:ARG:NH2	2.24	0.59
1:D:2103:TYR:CE1	1:D:2189:ARG:HG2	2.38	0.59
1:A:797:ASP:OD1	1:A:798:ALA:N	2.36	0.58
1:B:746:VAL:HB	1:B:749:GLN:HB2	1.85	0.58
1:C:746:VAL:HB	1:C:749:GLN:HB2	1.84	0.58
1:B:124:ARG:HD3	1:B:1914:THR:HB	1.85	0.58
1:D:2504:LEU:HD21	1:D:2507:ILE:HD11	1.86	0.58
1:E:124:ARG:HD3	1:E:1914:THR:HB	1.85	0.58
1:C:1774:TYR:OH	1:C:1848:TYR:OH	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1296:THR:HG23	1:D:1301:ARG:HH12	1.68	0.58
1:E:1296:THR:HG23	1:E:1301:ARG:HH12	1.67	0.58
1:A:124:ARG:HD3	1:A:1914:THR:HB	1.85	0.58
1:A:1296:THR:HG23	1:A:1301:ARG:HH12	1.68	0.58
1:D:2103:TYR:CE1	1:D:2193:GLU:HG2	2.38	0.58
1:A:2327:ARG:NH1	1:E:2445:CYS:SG	2.76	0.58
1:B:458:GLU:OE2	1:B:506:ARG:NH1	2.33	0.58
1:B:2103:TYR:CE1	1:B:2193:GLU:HG2	2.39	0.58
1:B:797:ASP:OD1	1:B:798:ALA:N	2.37	0.58
1:B:2137:ALA:HB2	1:D:1118:ALA:HB2	1.84	0.58
1:C:1296:THR:HG23	1:C:1301:ARG:HH12	1.69	0.58
1:E:2103:TYR:CE1	1:E:2189:ARG:HG2	2.39	0.58
1:D:337:ASN:ND2	1:D:421:TYR:O	2.25	0.58
1:E:2103:TYR:CE1	1:E:2193:GLU:HG2	2.38	0.58
1:A:2103:TYR:CE1	1:A:2193:GLU:HG2	2.39	0.58
1:C:1220:LYS:HE2	1:C:1267:LEU:HB3	1.86	0.58
1:D:797:ASP:OD1	1:D:798:ALA:N	2.37	0.58
1:B:703:SER:O	1:C:2255:ARG:NH2	2.25	0.57
1:C:124:ARG:HD3	1:C:1914:THR:HB	1.86	0.57
1:C:2103:TYR:CE1	1:C:2189:ARG:HG2	2.40	0.57
1:D:510:ASN:OD1	1:E:153:GLN:NE2	2.37	0.57
1:D:1865:ASP:OD1	1:D:1883:TYR:OH	2.21	0.57
1:E:746:VAL:HB	1:E:749:GLN:HB2	1.84	0.57
1:A:153:GLN:NE2	1:E:510:ASN:OD1	2.38	0.57
1:A:1865:ASP:OD1	1:A:1883:TYR:OH	2.20	0.57
1:B:519:PHE:O	1:B:553:ARG:NH2	2.38	0.57
1:A:519:PHE:O	1:A:553:ARG:NH2	2.38	0.57
1:A:1783:LEU:HD12	1:A:1788:ASN:HB3	1.87	0.57
1:B:2103:TYR:CE1	1:B:2189:ARG:HG2	2.39	0.57
1:C:2504:LEU:HD21	1:C:2507:ILE:HD11	1.86	0.57
1:E:797:ASP:OD1	1:E:798:ALA:N	2.37	0.57
1:A:746:VAL:HB	1:A:749:GLN:HB2	1.85	0.57
1:C:703:SER:O	1:D:2255:ARG:NH2	2.24	0.57
1:C:1774:TYR:HH	1:C:1848:TYR:HH	1.49	0.57
1:C:540:SER:HB2	1:D:848:GLN:HE22	1.68	0.57
1:C:2103:TYR:CE1	1:C:2193:GLU:HG2	2.39	0.57
1:C:2426:TYR:HB3	1:D:2334:THR:HG21	1.86	0.57
1:E:519:PHE:O	1:E:553:ARG:NH2	2.38	0.57
1:A:2445:CYS:SG	1:B:2327:ARG:NH1	2.78	0.57
1:B:2057:GLN:HG3	1:B:2241:LEU:HD12	1.85	0.57
1:E:2504:LEU:HD21	1:E:2507:ILE:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1072:ASP:OD1	1:E:1073:THR:N	2.38	0.57
1:B:1072:ASP:OD1	1:B:1073:THR:N	2.38	0.56
1:C:1783:LEU:HD12	1:C:1788:ASN:HB3	1.87	0.56
1:B:1655:HIS:NE2	1:B:1659:ARG:HA	2.20	0.56
1:C:797:ASP:OD1	1:C:798:ALA:N	2.37	0.56
1:A:1072:ASP:OD1	1:A:1073:THR:N	2.38	0.56
1:A:1655:HIS:NE2	1:A:1659:ARG:HA	2.20	0.56
1:B:510:ASN:OD1	1:C:153:GLN:NE2	2.38	0.56
1:C:510:ASN:OD1	1:D:153:GLN:NE2	2.38	0.56
1:E:1865:ASP:OD1	1:E:1883:TYR:OH	2.20	0.56
1:C:519:PHE:O	1:C:553:ARG:NH2	2.37	0.56
1:A:1722:GLY:O	1:A:1739:SER:HB2	2.06	0.56
1:A:2103:TYR:CE1	1:A:2189:ARG:HG2	2.40	0.56
1:C:458:GLU:OE2	1:C:506:ARG:NH1	2.35	0.56
1:C:1655:HIS:NE2	1:C:1659:ARG:HA	2.20	0.56
1:C:2057:GLN:HG3	1:C:2241:LEU:HD12	1.87	0.56
1:D:1655:HIS:NE2	1:D:1659:ARG:HA	2.20	0.56
1:E:1655:HIS:NE2	1:E:1659:ARG:HA	2.20	0.56
1:B:1783:LEU:HD12	1:B:1788:ASN:HB3	1.88	0.56
1:C:1072:ASP:OD1	1:C:1073:THR:N	2.38	0.56
1:A:2504:LEU:HD21	1:A:2507:ILE:HD11	1.87	0.56
1:D:519:PHE:O	1:D:553:ARG:NH2	2.38	0.56
1:D:1072:ASP:OD1	1:D:1073:THR:N	2.38	0.55
1:E:458:GLU:OE2	1:E:506:ARG:NH1	2.34	0.55
1:B:2504:LEU:HD21	1:B:2507:ILE:HD11	1.87	0.55
1:B:1722:GLY:O	1:B:1739:SER:HB2	2.06	0.55
1:C:1722:GLY:O	1:C:1739:SER:HB2	2.07	0.55
1:D:2057:GLN:HG3	1:D:2241:LEU:HD12	1.88	0.55
1:E:1722:GLY:O	1:E:1739:SER:HB2	2.06	0.55
1:E:1783:LEU:HD12	1:E:1788:ASN:HB3	1.87	0.55
1:E:368:LEU:HG	1:E:370:ILE:HD11	1.88	0.55
1:B:1885:GLN:HA	1:B:1888:HIS:CE1	2.42	0.55
1:C:503:ILE:HB	1:C:582:LEU:HD11	1.89	0.55
1:B:368:LEU:HG	1:B:370:ILE:HD11	1.88	0.55
1:C:1728:ASP:OD2	1:C:1730:LYS:NZ	2.40	0.55
1:A:1794:ARG:NH2	1:A:1798:TYR:OH	2.40	0.54
1:A:407:GLU:HA	1:A:425:LYS:HA	1.88	0.54
1:D:407:GLU:HA	1:D:425:LYS:HA	1.89	0.54
1:A:368:LEU:HG	1:A:370:ILE:HD11	1.88	0.54
1:A:1885:GLN:HA	1:A:1888:HIS:CE1	2.42	0.54
1:B:1865:ASP:OD1	1:B:1883:TYR:OH	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2182:SER:HG	1:E:1067:SER:HG	1.49	0.54
1:D:1722:GLY:O	1:D:1739:SER:HB2	2.07	0.54
1:B:503:ILE:HB	1:B:582:LEU:HD11	1.90	0.54
1:D:1783:LEU:HD12	1:D:1788:ASN:HB3	1.87	0.54
1:E:2033:LEU:HD11	1:E:2266:TYR:HA	1.90	0.54
1:E:2448:LEU:HD23	1:E:2471:PRO:HB2	1.90	0.54
1:A:503:ILE:HB	1:A:582:LEU:HD11	1.90	0.54
1:A:2448:LEU:HD23	1:A:2471:PRO:HB2	1.89	0.54
1:E:503:ILE:HB	1:E:582:LEU:HD11	1.90	0.54
1:D:1885:GLN:HA	1:D:1888:HIS:CE1	2.43	0.54
1:D:1728:ASP:OD2	1:D:1730:LYS:NZ	2.41	0.54
1:B:1794:ARG:NH2	1:B:1798:TYR:OH	2.41	0.54
1:D:368:LEU:HG	1:D:370:ILE:HD11	1.89	0.54
1:B:341:MET:HE1	1:B:359:PHE:CE1	2.43	0.54
1:C:407:GLU:HA	1:C:425:LYS:HA	1.89	0.54
1:C:1865:ASP:OD1	1:C:1883:TYR:OH	2.19	0.54
1:D:1790:ASP:OD1	1:D:1791:GLU:N	2.42	0.54
1:E:1790:ASP:OD1	1:E:1791:GLU:N	2.41	0.54
1:E:1885:GLN:HA	1:E:1888:HIS:CE1	2.42	0.54
1:A:2057:GLN:HG3	1:A:2241:LEU:HD12	1.90	0.53
1:C:368:LEU:HG	1:C:370:ILE:HD11	1.88	0.53
1:C:1885:GLN:HA	1:C:1888:HIS:CE1	2.43	0.53
1:E:866:ASN:HA	1:E:869:SER:HB3	1.91	0.53
1:A:510:ASN:OD1	1:B:153:GLN:NE2	2.39	0.53
1:E:2057:GLN:HG3	1:E:2241:LEU:HD12	1.89	0.53
1:A:2087:LYS:HZ2	1:E:2205:GLN:HA	1.73	0.53
1:B:407:GLU:HA	1:B:425:LYS:HA	1.89	0.53
1:C:341:MET:HE1	1:C:359:PHE:CE1	2.43	0.53
1:C:1790:ASP:OD1	1:C:1791:GLU:N	2.41	0.53
1:D:503:ILE:HB	1:D:582:LEU:HD11	1.90	0.53
1:D:2353:LEU:HD23	1:D:2357:ILE:HD11	1.90	0.53
1:D:458:GLU:OE2	1:D:506:ARG:NH1	2.34	0.53
1:A:341:MET:HE2	1:A:359:PHE:CE1	2.43	0.53
1:A:2353:LEU:HD23	1:A:2357:ILE:HD11	1.90	0.53
1:B:2205:GLN:HA	1:C:2087:LYS:HZ2	1.72	0.53
1:C:866:ASN:HA	1:C:869:SER:HB3	1.90	0.53
1:D:670:LEU:HA	1:D:699:THR:HG21	1.91	0.53
1:A:1790:ASP:OD1	1:A:1791:GLU:N	2.42	0.53
1:C:2353:LEU:HD23	1:C:2357:ILE:HD11	1.90	0.53
1:D:2033:LEU:HD11	1:D:2266:TYR:HA	1.91	0.53
1:E:1794:ARG:NH2	1:E:1798:TYR:OH	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:LEU:N	1:B:381:THR:O	2.28	0.53
1:B:2266:TYR:CZ	1:B:2297:TRP:HB2	2.43	0.53
1:B:2445:CYS:SG	1:C:2327:ARG:NH1	2.81	0.53
1:D:2448:LEU:HD23	1:D:2471:PRO:HB2	1.91	0.53
1:D:341:MET:HE1	1:D:359:PHE:CE1	2.43	0.53
1:E:341:MET:HE1	1:E:359:PHE:CE1	2.43	0.53
1:E:2266:TYR:CZ	1:E:2297:TRP:HB2	2.44	0.53
1:A:866:ASN:HA	1:A:869:SER:HB3	1.90	0.53
1:A:2266:TYR:CZ	1:A:2297:TRP:HB2	2.44	0.53
1:C:2266:TYR:CZ	1:C:2297:TRP:HB2	2.44	0.53
1:D:2341:TYR:OH	1:D:2390:SER:O	2.19	0.53
1:A:2033:LEU:HD11	1:A:2266:TYR:HA	1.90	0.52
1:B:2353:LEU:HD23	1:B:2357:ILE:HD11	1.90	0.52
1:D:866:ASN:HA	1:D:869:SER:HB3	1.91	0.52
1:E:407:GLU:HA	1:E:425:LYS:HA	1.90	0.52
1:A:497:ILE:HG21	1:A:589:TYR:HD2	1.74	0.52
1:A:1117:ASP:OD1	1:A:1118:ALA:N	2.40	0.52
1:B:1709:MET:HB3	1:B:1743:HIS:CE1	2.45	0.52
1:C:497:ILE:HG21	1:C:589:TYR:HD2	1.73	0.52
1:D:1794:ARG:NH2	1:D:1798:TYR:OH	2.43	0.52
1:B:497:ILE:HG21	1:B:589:TYR:HD2	1.74	0.52
1:D:698:ALA:HB1	1:E:2253:TRP:HA	1.90	0.52
1:D:2266:TYR:CZ	1:D:2297:TRP:HB2	2.44	0.52
1:E:1728:ASP:OD2	1:E:1730:LYS:NZ	2.41	0.52
1:A:670:LEU:HA	1:A:699:THR:HG21	1.92	0.52
1:A:1709:MET:HB3	1:A:1743:HIS:CE1	2.45	0.52
1:A:2253:TRP:HA	1:E:698:ALA:HB1	1.91	0.52
1:B:1118:ALA:HB2	1:E:2137:ALA:HB2	1.92	0.52
1:A:2068:LEU:HD22	1:A:2227:LEU:HG	1.92	0.52
1:C:1709:MET:HB3	1:C:1743:HIS:CE1	2.45	0.52
1:C:2033:LEU:HD11	1:C:2266:TYR:HA	1.91	0.52
1:D:540:SER:HB2	1:E:848:GLN:NE2	2.25	0.52
1:E:1709:MET:HB3	1:E:1743:HIS:CE1	2.44	0.52
1:A:1239:TYR:HD2	1:A:1242:GLU:HB3	1.75	0.52
1:A:1728:ASP:OD2	1:A:1730:LYS:NZ	2.41	0.52
1:B:670:LEU:HA	1:B:699:THR:HG21	1.92	0.52
1:C:1794:ARG:NH2	1:C:1798:TYR:OH	2.43	0.52
1:D:1117:ASP:OD1	1:D:1118:ALA:N	2.40	0.52
1:C:698:ALA:HB1	1:D:2253:TRP:HA	1.91	0.52
1:A:698:ALA:HB1	1:B:2253:TRP:HA	1.91	0.51
1:A:2205:GLN:HA	1:B:2087:LYS:HZ2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:ILE:HD11	1:B:606:ASP:HB2	1.92	0.51
1:B:1790:ASP:OD1	1:B:1791:GLU:N	2.41	0.51
1:B:2033:LEU:HD11	1:B:2266:TYR:HA	1.91	0.51
1:E:1117:ASP:OD1	1:E:1118:ALA:N	2.40	0.51
1:E:1239:TYR:HD2	1:E:1242:GLU:HB3	1.75	0.51
1:A:343:VAL:HG23	1:A:357:TYR:HB3	1.92	0.51
1:A:848:GLN:NE2	1:E:540:SER:HB2	2.26	0.51
1:C:300:ALA:HA	1:C:303:PHE:HD2	1.76	0.51
1:C:343:VAL:HG23	1:C:357:TYR:HB3	1.93	0.51
1:D:1709:MET:HB3	1:D:1743:HIS:CE1	2.45	0.51
1:E:497:ILE:HG21	1:E:589:TYR:HD2	1.74	0.51
1:E:2353:LEU:HD23	1:E:2357:ILE:HD11	1.91	0.51
1:B:698:ALA:HB1	1:C:2253:TRP:HA	1.91	0.51
1:B:866:ASN:HA	1:B:869:SER:HB3	1.91	0.51
1:E:471:ASN:H	1:E:474:VAL:HG12	1.76	0.51
1:A:540:SER:HB2	1:B:848:GLN:NE2	2.25	0.51
1:A:2087:LYS:NZ	1:E:2205:GLN:HA	2.26	0.51
1:B:2205:GLN:HA	1:C:2087:LYS:NZ	2.26	0.51
1:B:2341:TYR:OH	1:B:2390:SER:O	2.19	0.51
1:C:2068:LEU:HD22	1:C:2227:LEU:HG	1.93	0.51
1:D:2068:LEU:HD22	1:D:2227:LEU:HG	1.92	0.51
1:C:1239:TYR:HD2	1:C:1242:GLU:HB3	1.75	0.51
1:A:1118:ALA:HB2	1:D:2137:ALA:HB2	1.93	0.51
1:E:670:LEU:HA	1:E:699:THR:HG21	1.92	0.51
1:E:470:ILE:HA	1:E:474:VAL:HG11	1.93	0.51
1:B:557:ILE:HB	1:B:561:SER:OG	2.11	0.51
1:C:471:ASN:H	1:C:474:VAL:HG12	1.76	0.51
1:C:2448:LEU:HD23	1:C:2471:PRO:HB2	1.92	0.51
1:D:497:ILE:HG21	1:D:589:TYR:HD2	1.75	0.51
1:E:343:VAL:HG23	1:E:357:TYR:HB3	1.92	0.51
1:B:540:SER:HB2	1:C:848:GLN:NE2	2.26	0.51
1:B:2068:LEU:HD22	1:B:2227:LEU:HG	1.93	0.51
1:A:568:ILE:HD11	1:A:606:ASP:HB2	1.93	0.50
1:C:670:LEU:HA	1:C:699:THR:HG21	1.92	0.50
1:C:1614:VAL:O	1:C:1618:THR:HG23	2.11	0.50
1:D:1108:THR:OG1	1:D:1128:HIS:NE2	2.36	0.50
1:D:1239:TYR:HD2	1:D:1242:GLU:HB3	1.75	0.50
1:B:120:THR:O	1:B:124:ARG:HG3	2.11	0.50
1:B:343:VAL:HG23	1:B:357:TYR:HB3	1.93	0.50
1:D:343:VAL:HG23	1:D:357:TYR:HB3	1.93	0.50
1:E:2341:TYR:OH	1:E:2390:SER:O	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2205:GLN:HA	1:B:2087:LYS:NZ	2.26	0.50
1:B:1117:ASP:OD1	1:B:1118:ALA:N	2.40	0.50
1:C:540:SER:HB2	1:D:848:GLN:NE2	2.25	0.50
1:C:2047:GLN:NE2	1:C:2048:ASP:OD1	2.44	0.50
1:D:471:ASN:H	1:D:474:VAL:HG12	1.76	0.50
1:D:2205:GLN:HA	1:E:2087:LYS:NZ	2.26	0.50
1:E:2068:LEU:HD22	1:E:2227:LEU:HG	1.92	0.50
1:B:471:ASN:H	1:B:474:VAL:HG12	1.76	0.50
1:D:2205:GLN:HA	1:E:2087:LYS:HZ2	1.75	0.50
1:C:462:ARG:HH11	1:C:506:ARG:HH11	1.60	0.50
1:E:120:THR:O	1:E:124:ARG:HG3	2.12	0.50
1:A:300:ALA:HA	1:A:303:PHE:HD2	1.75	0.50
1:A:471:ASN:H	1:A:474:VAL:HG12	1.76	0.50
1:C:120:THR:O	1:C:124:ARG:HG3	2.11	0.50
1:C:2341:TYR:OH	1:C:2390:SER:O	2.19	0.50
1:D:120:THR:O	1:D:124:ARG:HG3	2.12	0.50
1:D:470:ILE:HA	1:D:474:VAL:HG11	1.94	0.50
1:B:1168:TYR:HB3	1:B:1200:LEU:HD11	1.93	0.50
1:B:2047:GLN:NE2	1:B:2048:ASP:OD1	2.45	0.50
1:C:507:SER:HB3	1:C:513:SER:HB2	1.93	0.50
1:D:1614:VAL:O	1:D:1618:THR:HG23	2.11	0.50
1:E:1614:VAL:O	1:E:1618:THR:HG23	2.11	0.50
1:A:557:ILE:HB	1:A:561:SER:OG	2.11	0.50
1:A:1883:TYR:HD2	1:A:1970:LEU:HD11	1.77	0.50
1:B:1239:TYR:HD2	1:B:1242:GLU:HB3	1.76	0.50
1:C:2204:LYS:C	1:D:2087:LYS:HZ3	2.13	0.50
1:E:1774:TYR:OH	1:E:1848:TYR:OH	2.21	0.50
1:C:836:ALA:HB2	1:C:846:LEU:HD12	1.94	0.49
1:D:300:ALA:HA	1:D:303:PHE:HD2	1.76	0.49
1:E:300:ALA:HA	1:E:303:PHE:HD2	1.76	0.49
1:A:120:THR:O	1:A:124:ARG:HG3	2.12	0.49
1:B:698:ALA:HB2	1:C:2256:GLY:HA3	1.94	0.49
1:C:1168:TYR:HB3	1:C:1200:LEU:HD11	1.93	0.49
1:E:1883:TYR:HD2	1:E:1970:LEU:HD11	1.77	0.49
1:A:1614:VAL:O	1:A:1618:THR:HG23	2.11	0.49
1:A:2005:GLY:HA2	1:D:741:GLY:HA2	1.94	0.49
1:A:2047:GLN:NE2	1:A:2048:ASP:OD1	2.45	0.49
1:B:300:ALA:HA	1:B:303:PHE:HD2	1.76	0.49
1:B:1617:ALA:HA	1:B:1624:ILE:HD11	1.93	0.49
1:B:2448:LEU:HD23	1:B:2471:PRO:HB2	1.92	0.49
1:C:568:ILE:HD11	1:C:606:ASP:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:836:ALA:HB2	1:D:846:LEU:HD12	1.94	0.49
1:B:1614:VAL:O	1:B:1618:THR:HG23	2.11	0.49
1:B:1728:ASP:OD2	1:B:1730:LYS:NZ	2.41	0.49
1:B:2246:SER:HA	1:B:2250:LEU:HD23	1.94	0.49
1:C:557:ILE:HB	1:C:561:SER:OG	2.12	0.49
1:C:2004:GLN:H	1:C:2300:THR:HG22	1.76	0.49
1:C:2205:GLN:HA	1:D:2087:LYS:NZ	2.26	0.49
1:D:1617:ALA:HA	1:D:1624:ILE:HD11	1.94	0.49
1:E:1168:TYR:HB3	1:E:1200:LEU:HD11	1.93	0.49
1:A:197:ALA:N	1:A:948:THR:HG21	2.28	0.49
1:B:197:ALA:N	1:B:948:THR:HG21	2.27	0.49
1:D:2047:GLN:NE2	1:D:2048:ASP:OD1	2.45	0.49
1:E:2047:GLN:NE2	1:E:2048:ASP:OD1	2.46	0.49
1:A:1878:GLU:HA	1:A:1881:MET:HG3	1.94	0.49
1:A:2057:GLN:HG3	1:A:2241:LEU:CD1	2.42	0.49
1:E:347:PRO:HA	1:E:353:TYR:HA	1.95	0.49
1:A:348:PHE:CE1	1:A:352:ASN:HB3	2.48	0.49
1:B:507:SER:HB3	1:B:513:SER:HB2	1.94	0.49
1:C:1878:GLU:HA	1:C:1881:MET:HG3	1.94	0.49
1:E:348:PHE:CE1	1:E:352:ASN:HB3	2.48	0.49
1:A:470:ILE:HA	1:A:474:VAL:HG11	1.94	0.49
1:A:507:SER:HB3	1:A:513:SER:HB2	1.94	0.49
1:A:836:ALA:HB2	1:A:846:LEU:HD12	1.93	0.49
1:A:1617:ALA:HA	1:A:1624:ILE:HD11	1.94	0.49
1:A:2246:SER:HA	1:A:2250:LEU:HD23	1.94	0.49
1:D:1168:TYR:HB3	1:D:1200:LEU:HD11	1.94	0.49
1:E:568:ILE:HD11	1:E:606:ASP:HB2	1.93	0.49
1:B:348:PHE:CE1	1:B:352:ASN:HB3	2.48	0.49
1:B:836:ALA:HB2	1:B:846:LEU:HD12	1.94	0.49
1:C:197:ALA:N	1:C:948:THR:HG21	2.28	0.49
1:C:1617:ALA:HA	1:C:1624:ILE:HD11	1.94	0.49
1:D:2246:SER:HA	1:D:2250:LEU:HD23	1.94	0.49
1:E:557:ILE:HB	1:E:561:SER:OG	2.11	0.49
1:E:2057:GLN:HG3	1:E:2241:LEU:CD1	2.43	0.49
1:E:2246:SER:HA	1:E:2250:LEU:HD23	1.94	0.49
1:B:470:ILE:HA	1:B:474:VAL:HG11	1.94	0.49
1:E:197:ALA:N	1:E:948:THR:HG21	2.28	0.49
1:E:672:ASP:O	1:E:676:HIS:ND1	2.46	0.49
1:C:198:THR:HB	1:C:199:PRO:HA	1.95	0.48
1:C:371:LYS:HG2	1:C:377:GLU:HA	1.95	0.48
1:D:557:ILE:HB	1:D:561:SER:OG	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2118:ARG:HG2	1:E:2178:LYS:HB2	1.94	0.48
1:B:1870:GLN:HB3	1:B:1872:GLU:OE1	2.14	0.48
1:C:348:PHE:CE1	1:C:352:ASN:HB3	2.48	0.48
1:C:1124:ARG:NE	1:C:1142:SER:O	2.47	0.48
1:A:195:SER:HB3	1:A:198:THR:OG1	2.13	0.48
1:B:2118:ARG:HG2	1:B:2178:LYS:HB2	1.95	0.48
1:C:470:ILE:HA	1:C:474:VAL:HG11	1.93	0.48
1:C:2057:GLN:HG3	1:C:2241:LEU:CD1	2.43	0.48
1:D:348:PHE:CE1	1:D:352:ASN:HB3	2.48	0.48
1:B:347:PRO:HA	1:B:353:TYR:HA	1.95	0.48
1:B:1878:GLU:HA	1:B:1881:MET:HG3	1.95	0.48
1:C:2118:ARG:HG2	1:C:2178:LYS:HB2	1.96	0.48
1:D:198:THR:HB	1:D:199:PRO:HA	1.95	0.48
1:D:1878:GLU:HA	1:D:1881:MET:HG3	1.95	0.48
1:B:195:SER:HB3	1:B:198:THR:OG1	2.14	0.48
1:D:2057:GLN:HG3	1:D:2241:LEU:CD1	2.43	0.48
1:E:507:SER:HB3	1:E:513:SER:HB2	1.95	0.48
1:E:1172:LEU:HD11	1:E:1196:TYR:HB3	1.95	0.48
1:A:458:GLU:OE2	1:A:506:ARG:NH1	2.35	0.48
1:A:462:ARG:HH11	1:A:506:ARG:HH11	1.61	0.48
1:A:1870:GLN:HB3	1:A:1872:GLU:OE1	2.13	0.48
1:D:672:ASP:O	1:D:676:HIS:ND1	2.46	0.48
1:D:1909:ARG:HH11	1:D:1913:ILE:HD12	1.79	0.48
1:D:2204:LYS:C	1:E:2087:LYS:HZ3	2.14	0.48
1:A:1058:ASP:O	1:A:1062:GLN:HG3	2.14	0.48
1:B:462:ARG:HH11	1:B:506:ARG:HH11	1.62	0.48
1:C:1870:GLN:HB3	1:C:1872:GLU:OE1	2.14	0.48
1:D:197:ALA:N	1:D:948:THR:HG21	2.28	0.48
1:D:347:PRO:HA	1:D:353:TYR:HA	1.96	0.48
1:A:318:VAL:HG23	1:A:319:ASN:H	1.79	0.48
1:A:2182:SER:HG	1:C:1067:SER:HG	1.53	0.48
1:B:2067:ASN:HB3	1:B:2227:LEU:HD21	1.95	0.48
1:D:195:SER:HB3	1:D:198:THR:OG1	2.14	0.48
1:D:568:ILE:HD11	1:D:606:ASP:HB2	1.94	0.48
1:B:741:GLY:HA2	1:D:2005:GLY:HA2	1.95	0.48
1:D:371:LYS:HG2	1:D:377:GLU:HA	1.96	0.48
1:A:347:PRO:HA	1:A:353:TYR:HA	1.96	0.48
1:C:694:PRO:HA	1:C:705:GLU:OE1	2.14	0.48
1:C:741:GLY:HA2	1:E:2005:GLY:HA2	1.96	0.48
1:C:2246:SER:HA	1:C:2250:LEU:HD23	1.94	0.48
1:D:1124:ARG:NE	1:D:1142:SER:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1870:GLN:HB3	1:D:1872:GLU:OE1	2.14	0.48
1:D:2445:CYS:SG	1:E:2327:ARG:NH1	2.87	0.48
1:E:283:LYS:HB2	1:E:293:LEU:HD22	1.96	0.48
1:E:1617:ALA:HA	1:E:1624:ILE:HD11	1.94	0.48
1:A:2341:TYR:OH	1:A:2390:SER:O	2.19	0.47
1:C:181:ASN:HD21	1:C:184:LYS:HG2	1.79	0.47
1:E:198:THR:HB	1:E:199:PRO:HA	1.95	0.47
1:A:198:THR:HB	1:A:199:PRO:HA	1.96	0.47
1:A:2256:GLY:HA3	1:E:698:ALA:HB2	1.96	0.47
1:B:198:THR:HB	1:B:199:PRO:HA	1.95	0.47
1:B:2004:GLN:H	1:B:2300:THR:HG22	1.78	0.47
1:C:672:ASP:O	1:C:676:HIS:ND1	2.46	0.47
1:E:836:ALA:HB2	1:E:846:LEU:HD12	1.94	0.47
1:E:1730:LYS:HZ3	1:E:1732:ILE:HD12	1.78	0.47
1:A:1108:THR:OG1	1:A:1128:HIS:NE2	2.38	0.47
1:A:1168:TYR:HB3	1:A:1200:LEU:HD11	1.95	0.47
1:C:283:LYS:HB2	1:C:293:LEU:HD22	1.96	0.47
1:C:1909:ARG:HH11	1:C:1913:ILE:HD12	1.79	0.47
1:C:2018:ARG:NH1	1:C:2466:ASP:O	2.46	0.47
1:D:2004:GLN:H	1:D:2300:THR:HG22	1.77	0.47
1:E:195:SER:HB3	1:E:198:THR:OG1	2.14	0.47
1:E:1058:ASP:O	1:E:1062:GLN:HG3	2.15	0.47
1:E:1124:ARG:NE	1:E:1142:SER:O	2.46	0.47
1:A:371:LYS:HG2	1:A:377:GLU:HA	1.95	0.47
1:A:2004:GLN:H	1:A:2300:THR:HG22	1.79	0.47
1:B:1730:LYS:HZ3	1:B:1732:ILE:HD12	1.78	0.47
1:D:181:ASN:HD21	1:D:184:LYS:HG2	1.79	0.47
1:D:507:SER:HB3	1:D:513:SER:HB2	1.95	0.47
1:E:646:TRP:CZ2	1:E:768:SER:HB3	2.50	0.47
1:E:1878:GLU:HA	1:E:1881:MET:HG3	1.95	0.47
1:A:694:PRO:HA	1:A:705:GLU:OE1	2.15	0.47
1:A:741:GLY:HA2	1:C:2005:GLY:HA2	1.95	0.47
1:A:1730:LYS:HZ3	1:A:1732:ILE:HD12	1.79	0.47
1:B:1124:ARG:NE	1:B:1142:SER:O	2.47	0.47
1:B:1909:ARG:HH11	1:B:1913:ILE:HD12	1.79	0.47
1:C:318:VAL:HG23	1:C:319:ASN:H	1.79	0.47
1:D:462:ARG:HH11	1:D:506:ARG:HH11	1.62	0.47
1:D:698:ALA:HB2	1:E:2256:GLY:HA3	1.97	0.47
1:E:2004:GLN:H	1:E:2300:THR:HG22	1.79	0.47
1:B:672:ASP:O	1:B:676:HIS:ND1	2.47	0.47
1:B:702:LEU:HD22	1:B:708:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2204:LYS:C	1:C:2087:LYS:HZ3	2.15	0.47
1:C:195:SER:HB3	1:C:198:THR:OG1	2.14	0.47
1:C:2067:ASN:HB3	1:C:2227:LEU:HD21	1.97	0.47
1:A:672:ASP:O	1:A:676:HIS:ND1	2.47	0.47
1:B:505:GLN:HE22	1:B:582:LEU:HD13	1.79	0.47
1:C:646:TRP:CZ2	1:C:768:SER:HB3	2.50	0.47
1:C:702:LEU:HD22	1:C:708:ALA:HB2	1.96	0.47
1:C:1117:ASP:OD1	1:C:1118:ALA:N	2.40	0.47
1:C:1883:TYR:HD2	1:C:1970:LEU:HD11	1.80	0.47
1:D:646:TRP:CZ2	1:D:768:SER:HB3	2.50	0.47
1:D:1058:ASP:O	1:D:1062:GLN:HG3	2.15	0.47
1:D:1883:TYR:HD2	1:D:1970:LEU:HD11	1.79	0.47
1:E:462:ARG:HH11	1:E:506:ARG:HH11	1.63	0.47
1:E:1909:ARG:HH11	1:E:1913:ILE:HD12	1.80	0.47
1:A:698:ALA:HB2	1:B:2256:GLY:HA3	1.96	0.47
1:A:1909:ARG:HH11	1:A:1913:ILE:HD12	1.79	0.47
1:A:2118:ARG:HG2	1:A:2178:LYS:HB2	1.95	0.47
1:B:2005:GLY:HA2	1:E:741:GLY:HA2	1.97	0.47
1:A:536:ILE:HD13	1:A:547:ARG:HB2	1.96	0.47
1:C:347:PRO:HA	1:C:353:TYR:HA	1.96	0.47
1:D:702:LEU:HD22	1:D:708:ALA:HB2	1.96	0.47
1:D:1168:TYR:HD2	1:D:1200:LEU:HD11	1.80	0.47
1:E:1870:GLN:HB3	1:E:1872:GLU:OE1	2.14	0.47
1:A:127:ARG:HG3	1:A:127:ARG:HH11	1.80	0.47
1:A:1098:HIS:HE1	1:A:1100:ASN:HB3	1.81	0.47
1:B:181:ASN:HD21	1:B:184:LYS:HG2	1.79	0.47
1:B:318:VAL:HG23	1:B:319:ASN:H	1.79	0.47
1:B:1883:TYR:HD2	1:B:1970:LEU:HD11	1.80	0.47
1:D:127:ARG:HG3	1:D:127:ARG:HH11	1.80	0.47
1:D:505:GLN:HE22	1:D:582:LEU:HD13	1.79	0.47
1:E:505:GLN:HE22	1:E:582:LEU:HD13	1.80	0.47
1:A:1172:LEU:HD11	1:A:1196:TYR:HB3	1.96	0.46
1:B:694:PRO:HA	1:B:705:GLU:OE1	2.15	0.46
1:B:1058:ASP:O	1:B:1062:GLN:HG3	2.15	0.46
1:C:127:ARG:HG3	1:C:127:ARG:HH11	1.80	0.46
1:C:1058:ASP:O	1:C:1062:GLN:HG3	2.15	0.46
1:E:127:ARG:HG3	1:E:127:ARG:HH11	1.80	0.46
1:A:702:LEU:HD22	1:A:708:ALA:HB2	1.96	0.46
1:B:283:LYS:HB2	1:B:293:LEU:HD22	1.96	0.46
1:B:2183:GLU:OE1	1:C:2108:ASN:ND2	2.42	0.46
1:C:505:GLN:HE22	1:C:582:LEU:HD13	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:VAL:HG23	1:D:319:ASN:H	1.79	0.46
1:E:694:PRO:HA	1:E:705:GLU:OE1	2.15	0.46
1:A:646:TRP:CZ2	1:A:768:SER:HB3	2.51	0.46
1:D:2018:ARG:NH1	1:D:2466:ASP:O	2.47	0.46
1:D:2067:ASN:HB3	1:D:2227:LEU:HD21	1.97	0.46
1:A:1124:ARG:NE	1:A:1142:SER:O	2.47	0.46
1:B:1098:HIS:HE1	1:B:1100:ASN:HB3	1.80	0.46
1:D:283:LYS:HB2	1:D:293:LEU:HD22	1.96	0.46
1:E:318:VAL:HG23	1:E:319:ASN:H	1.79	0.46
1:E:318:VAL:HG23	1:E:319:ASN:N	2.30	0.46
1:A:1892:ASP:OD1	1:A:1892:ASP:N	2.49	0.46
1:B:127:ARG:HG3	1:B:127:ARG:HH11	1.81	0.46
1:D:1892:ASP:OD1	1:D:1892:ASP:N	2.49	0.46
1:E:1892:ASP:OD1	1:E:1892:ASP:N	2.49	0.46
1:A:2067:ASN:HB3	1:A:2227:LEU:HD21	1.96	0.46
1:B:537:ASP:HA	1:B:577:LYS:HA	1.98	0.46
1:C:1172:LEU:HD11	1:C:1196:TYR:HB3	1.96	0.46
1:D:694:PRO:HA	1:D:705:GLU:OE1	2.15	0.46
1:E:702:LEU:HD22	1:E:708:ALA:HB2	1.96	0.46
1:A:318:VAL:HG23	1:A:319:ASN:N	2.31	0.46
1:A:505:GLN:HE22	1:A:582:LEU:HD13	1.80	0.46
1:B:371:LYS:HG2	1:B:377:GLU:HA	1.96	0.46
1:D:1172:LEU:HD11	1:D:1196:TYR:HB3	1.97	0.46
1:A:711:VAL:HG11	1:A:763:GLU:OE2	2.16	0.46
1:B:646:TRP:CZ2	1:B:768:SER:HB3	2.50	0.46
1:B:2362:SER:OG	1:B:2502:LYS:NZ	2.47	0.46
1:D:536:ILE:HD13	1:D:547:ARG:HB2	1.97	0.46
1:E:371:LYS:HG2	1:E:377:GLU:HA	1.96	0.46
1:B:341:MET:HE3	1:B:410:LEU:HD22	1.98	0.46
1:B:2057:GLN:HG3	1:B:2241:LEU:CD1	2.44	0.46
1:C:370:ILE:HG13	1:C:410:LEU:HG	1.98	0.46
1:C:698:ALA:HB2	1:D:2256:GLY:HA3	1.98	0.46
1:D:318:VAL:HG23	1:D:319:ASN:N	2.31	0.46
1:D:1730:LYS:HZ3	1:D:1732:ILE:HD12	1.80	0.46
1:D:341:MET:CE	1:D:410:LEU:HD22	2.46	0.46
1:A:1168:TYR:HD2	1:A:1200:LEU:HD11	1.80	0.45
1:B:536:ILE:HD13	1:B:547:ARG:HB2	1.97	0.45
1:D:1676:ILE:HD12	1:D:1690:LEU:HD13	1.98	0.45
1:E:181:ASN:HD21	1:E:184:LYS:HG2	1.80	0.45
1:B:370:ILE:HG13	1:B:410:LEU:HG	1.98	0.45
1:B:711:VAL:HG11	1:B:763:GLU:OE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:505:GLN:NE2	1:D:582:LEU:HD13	2.32	0.45
1:D:711:VAL:HG11	1:D:763:GLU:OE2	2.16	0.45
1:D:1071:ALA:HB2	1:D:1791:GLU:OE2	2.17	0.45
1:D:2118:ARG:HG2	1:D:2178:LYS:HB2	1.97	0.45
1:E:341:MET:CE	1:E:410:LEU:HD22	2.46	0.45
1:A:197:ALA:H	1:A:948:THR:HG21	1.82	0.45
1:A:2278:GLN:OE1	1:A:2281:ARG:NH2	2.50	0.45
1:C:505:GLN:NE2	1:C:582:LEU:HD13	2.31	0.45
1:D:370:ILE:HG13	1:D:410:LEU:HG	1.98	0.45
1:E:536:ILE:HD13	1:E:547:ARG:HB2	1.97	0.45
1:E:1098:HIS:HE1	1:E:1100:ASN:HB3	1.81	0.45
1:E:2018:ARG:NH1	1:E:2466:ASP:O	2.49	0.45
1:A:181:ASN:HD21	1:A:184:LYS:HG2	1.80	0.45
1:A:2018:ARG:NH1	1:A:2466:ASP:O	2.46	0.45
1:A:2204:LYS:C	1:B:2087:LYS:HZ3	2.14	0.45
1:B:318:VAL:HG23	1:B:319:ASN:N	2.31	0.45
1:B:1168:TYR:HD2	1:B:1200:LEU:HD11	1.81	0.45
1:C:2205:GLN:HA	1:D:2087:LYS:HZ2	1.82	0.45
1:A:341:MET:CE	1:A:410:LEU:HD22	2.46	0.45
1:A:534:GLU:OE2	1:A:580:ASN:ND2	2.49	0.45
1:C:197:ALA:H	1:C:948:THR:HG21	1.82	0.45
1:C:318:VAL:HG23	1:C:319:ASN:N	2.31	0.45
1:C:1098:HIS:HE1	1:C:1100:ASN:HB3	1.81	0.45
1:A:1056:MET:HG3	1:A:1081:TYR:HE1	1.82	0.45
1:B:1056:MET:HG3	1:B:1081:TYR:HE1	1.82	0.45
1:E:370:ILE:HG13	1:E:410:LEU:HG	1.99	0.45
1:A:283:LYS:HB2	1:A:293:LEU:HD22	1.98	0.45
1:A:505:GLN:NE2	1:A:582:LEU:HD13	2.32	0.45
1:A:1676:ILE:HD12	1:A:1690:LEU:HD13	1.98	0.45
1:B:341:MET:CE	1:B:410:LEU:HD22	2.47	0.45
1:B:1172:LEU:HD11	1:B:1196:TYR:HB3	1.97	0.45
1:C:341:MET:CE	1:C:410:LEU:HD22	2.46	0.45
1:D:1098:HIS:HE1	1:D:1100:ASN:HB3	1.81	0.45
1:D:2132:ARG:HH11	1:D:2163:TYR:HB3	1.82	0.45
1:E:210:VAL:HG22	1:E:926:LEU:HD11	1.99	0.45
1:E:1163:TYR:CD1	1:E:1245:LEU:HD22	2.52	0.45
1:E:1168:TYR:HD2	1:E:1200:LEU:HD11	1.81	0.45
1:B:197:ALA:H	1:B:948:THR:HG21	1.81	0.45
1:D:2362:SER:OG	1:D:2502:LYS:NZ	2.47	0.45
1:E:464:VAL:HG21	1:E:474:VAL:HA	1.98	0.45
1:E:505:GLN:NE2	1:E:582:LEU:HD13	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:971:LEU:O	1:A:973:ILE:HG12	2.17	0.45
1:B:505:GLN:NE2	1:B:582:LEU:HD13	2.32	0.45
1:C:1163:TYR:CD1	1:C:1245:LEU:HD22	2.52	0.45
1:C:1268:TYR:N	1:C:1276:LYS:O	2.48	0.45
1:C:2132:ARG:HH11	1:C:2163:TYR:HB3	1.81	0.45
1:B:1676:ILE:HD12	1:B:1690:LEU:HD13	1.98	0.45
1:C:1168:TYR:HD2	1:C:1200:LEU:HD11	1.81	0.45
1:C:2445:CYS:SG	1:D:2327:ARG:NH1	2.90	0.45
1:D:601:THR:HG22	1:D:604:GLU:OE1	2.17	0.45
1:D:971:LEU:O	1:D:973:ILE:HG12	2.17	0.45
1:E:2067:ASN:HB3	1:E:2227:LEU:HD21	1.98	0.45
1:A:370:ILE:HG13	1:A:410:LEU:HG	1.99	0.44
1:A:1071:ALA:HB2	1:A:1791:GLU:OE2	2.17	0.44
1:B:1892:ASP:OD1	1:B:1892:ASP:N	2.49	0.44
1:C:711:VAL:HG11	1:C:763:GLU:OE2	2.16	0.44
1:D:2416:SER:HB2	1:D:2510:HIS:HB2	1.99	0.44
1:E:197:ALA:H	1:E:948:THR:HG21	1.82	0.44
1:E:534:GLU:OE2	1:E:580:ASN:ND2	2.50	0.44
1:E:1071:ALA:HB2	1:E:1791:GLU:OE2	2.16	0.44
1:E:1676:ILE:HD12	1:E:1690:LEU:HD13	1.99	0.44
1:E:2398:ILE:HB	1:E:2477:ILE:HG21	1.99	0.44
1:A:2087:LYS:HZ3	1:E:2204:LYS:C	2.15	0.44
1:C:2398:ILE:HB	1:C:2477:ILE:HG21	1.99	0.44
1:D:341:MET:HE3	1:D:410:LEU:HD22	1.98	0.44
1:D:453:SER:HB3	1:D:456:ILE:HG12	1.99	0.44
1:E:663:LEU:HD22	1:E:749:GLN:NE2	2.33	0.44
1:E:1056:MET:HG3	1:E:1081:TYR:HE1	1.82	0.44
1:A:487:ARG:O	1:A:487:ARG:NH1	2.46	0.44
1:B:971:LEU:O	1:B:973:ILE:HG12	2.17	0.44
1:B:1071:ALA:HB2	1:B:1791:GLU:OE2	2.17	0.44
1:E:711:VAL:HG11	1:E:763:GLU:OE2	2.16	0.44
1:A:1887:LEU:HD12	1:A:1887:LEU:HA	1.88	0.44
1:A:2398:ILE:HB	1:A:2477:ILE:HG21	2.00	0.44
1:C:536:ILE:HD13	1:C:547:ARG:HB2	1.98	0.44
1:D:464:VAL:HG21	1:D:474:VAL:HA	2.00	0.44
1:D:1163:TYR:CD1	1:D:1245:LEU:HD22	2.52	0.44
1:E:1094:ILE:HD11	1:E:1113:LEU:HB2	2.00	0.44
1:C:462:ARG:NH1	1:C:506:ARG:HH11	2.16	0.44
1:C:534:GLU:OE2	1:C:580:ASN:ND2	2.50	0.44
1:C:724:ALA:O	1:C:729:LYS:NZ	2.35	0.44
1:D:197:ALA:H	1:D:948:THR:HG21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1056:MET:HG3	1:D:1081:TYR:CE1	2.53	0.44
1:E:971:LEU:O	1:E:973:ILE:HG12	2.18	0.44
1:A:1163:TYR:CD1	1:A:1245:LEU:HD22	2.52	0.44
1:B:464:VAL:HG21	1:B:474:VAL:HA	2.00	0.44
1:B:534:GLU:OE2	1:B:580:ASN:ND2	2.50	0.44
1:C:971:LEU:O	1:C:973:ILE:HG12	2.17	0.44
1:D:1056:MET:HG3	1:D:1081:TYR:HE1	1.82	0.44
1:A:1094:ILE:HD11	1:A:1113:LEU:HB2	2.00	0.44
1:B:1094:ILE:HD11	1:B:1113:LEU:HB2	2.00	0.44
1:C:1071:ALA:HB2	1:C:1791:GLU:OE2	2.17	0.44
1:C:2362:SER:OG	1:C:2502:LYS:NZ	2.50	0.44
1:D:210:VAL:HG22	1:D:926:LEU:HD11	2.00	0.44
1:D:1094:ILE:HD11	1:D:1113:LEU:HB2	2.00	0.44
1:E:2278:GLN:OE1	1:E:2281:ARG:NH2	2.50	0.44
1:A:1050:ARG:NH2	1:A:1770:GLU:OE1	2.51	0.44
1:B:1163:TYR:CD1	1:B:1245:LEU:HD22	2.52	0.44
1:E:1056:MET:HG3	1:E:1081:TYR:CE1	2.53	0.44
1:E:1675:ILE:HD11	1:E:1678:SER:HB2	2.00	0.44
1:A:210:VAL:HG22	1:A:926:LEU:HD11	1.99	0.44
1:A:464:VAL:HG21	1:A:474:VAL:HA	1.99	0.44
1:A:1048:THR:HG23	1:A:1061:LEU:HD11	2.00	0.44
1:A:663:LEU:HD22	1:A:749:GLN:NE2	2.33	0.43
1:A:2066:THR:HG21	1:E:2226:SER:HB2	1.99	0.43
1:B:453:SER:HB3	1:B:456:ILE:HG12	2.00	0.43
1:B:1048:THR:HG23	1:B:1061:LEU:HD11	2.00	0.43
1:C:595:ALA:HB2	1:C:605:LEU:HD22	1.99	0.43
1:C:1676:ILE:HD12	1:C:1690:LEU:HD13	1.99	0.43
1:D:1135:LYS:HA	1:D:1135:LYS:HD3	1.82	0.43
1:E:2132:ARG:HH11	1:E:2163:TYR:HB3	1.83	0.43
1:B:1056:MET:HG3	1:B:1081:TYR:CE1	2.53	0.43
1:C:210:VAL:HG22	1:C:926:LEU:HD11	2.00	0.43
1:C:2458:GLY:O	1:D:2330:GLU:HB2	2.19	0.43
1:A:1056:MET:HG3	1:A:1081:TYR:CE1	2.53	0.43
1:B:2458:GLY:O	1:C:2330:GLU:HB2	2.18	0.43
1:C:601:THR:HG22	1:C:604:GLU:OE1	2.18	0.43
1:D:1652:LEU:HA	1:D:1655:HIS:HB3	2.00	0.43
1:A:601:THR:HG22	1:A:604:GLU:OE1	2.18	0.43
1:A:1268:TYR:N	1:A:1276:LYS:O	2.48	0.43
1:A:1963:LEU:HD23	1:A:1963:LEU:HA	1.93	0.43
1:B:579:LYS:HG3	1:B:581:ASN:H	1.84	0.43
1:C:453:SER:HB3	1:C:456:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:VAL:HG21	1:C:474:VAL:HA	2.01	0.43
1:C:1730:LYS:HZ3	1:C:1732:ILE:HD12	1.84	0.43
1:E:601:THR:HG22	1:E:604:GLU:OE1	2.18	0.43
1:E:1048:THR:HG23	1:E:1061:LEU:HD11	2.00	0.43
1:B:1652:LEU:HA	1:B:1655:HIS:HB3	2.01	0.43
1:C:320:SER:HB2	1:C:323:GLY:HA2	2.01	0.43
1:E:462:ARG:NH1	1:E:506:ARG:HH11	2.17	0.43
1:A:1652:LEU:HA	1:A:1655:HIS:HB3	2.00	0.43
1:B:210:VAL:HG22	1:B:926:LEU:HD11	2.00	0.43
1:C:579:LYS:HG3	1:C:581:ASN:H	1.84	0.43
1:D:534:GLU:OE2	1:D:580:ASN:ND2	2.51	0.43
1:D:595:ALA:HB2	1:D:605:LEU:HD22	2.00	0.43
1:D:1050:ARG:NH2	1:D:1770:GLU:OE1	2.51	0.43
1:A:341:MET:HE1	1:A:410:LEU:HD22	2.01	0.43
1:A:2458:GLY:O	1:B:2330:GLU:HB2	2.19	0.43
1:B:320:SER:HB2	1:B:323:GLY:HA2	2.01	0.43
1:B:2112:ASN:HA	1:B:2115:MET:HG2	2.01	0.43
1:C:537:ASP:HA	1:C:577:LYS:HA	2.00	0.43
1:C:965:ASP:OD1	1:C:966:ASP:N	2.52	0.43
1:C:1056:MET:HG3	1:C:1081:TYR:CE1	2.54	0.43
1:C:1094:ILE:HD11	1:C:1113:LEU:HB2	2.01	0.43
1:D:558:ASP:OD1	1:D:558:ASP:N	2.48	0.43
1:D:2398:ILE:HB	1:D:2477:ILE:HG21	2.00	0.43
1:A:714:TRP:CZ3	1:A:762:LEU:HD22	2.54	0.43
1:B:601:THR:HG22	1:B:604:GLU:OE1	2.19	0.43
1:B:965:ASP:OD1	1:B:966:ASP:N	2.52	0.43
1:C:116:ALA:HB1	1:C:150:LEU:HD22	2.01	0.43
1:C:848:GLN:OE1	1:C:892:GLN:NE2	2.52	0.43
1:C:1048:THR:HG23	1:C:1061:LEU:HD11	2.00	0.43
1:D:320:SER:HB2	1:D:323:GLY:HA2	2.01	0.43
1:E:2416:SER:HB2	1:E:2510:HIS:HB2	2.01	0.43
1:E:2452:HIS:CE1	1:E:2456:ASP:HB2	2.54	0.43
1:A:462:ARG:NH1	1:A:506:ARG:HH11	2.16	0.43
1:B:595:ALA:HB2	1:B:605:LEU:HD22	2.00	0.43
1:B:663:LEU:HD22	1:B:749:GLN:NE2	2.34	0.43
1:B:1766:LEU:O	1:B:1770:GLU:HB2	2.19	0.43
1:C:714:TRP:CZ3	1:C:762:LEU:HD22	2.54	0.43
1:C:1607:THR:HG21	1:C:1768:PHE:HZ	1.83	0.43
1:C:1675:ILE:HD11	1:C:1678:SER:HB2	2.01	0.43
1:D:537:ASP:HA	1:D:577:LYS:HA	2.01	0.43
1:D:1048:THR:HG23	1:D:1061:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:453:SER:HB3	1:E:456:ILE:HG12	1.99	0.43
1:A:2416:SER:HB2	1:A:2510:HIS:HB2	2.00	0.43
1:B:2226:SER:HB2	1:C:2066:THR:HG21	2.01	0.43
1:C:1652:LEU:HA	1:C:1655:HIS:HB3	2.01	0.43
1:C:1892:ASP:OD1	1:C:1892:ASP:N	2.49	0.43
1:D:2226:SER:HB2	1:E:2066:THR:HG21	2.01	0.43
1:E:595:ALA:HB2	1:E:605:LEU:HD22	2.00	0.43
1:E:714:TRP:CZ3	1:E:762:LEU:HD22	2.54	0.43
1:E:1050:ARG:NH2	1:E:1770:GLU:OE1	2.52	0.43
1:A:2330:GLU:HB2	1:E:2458:GLY:O	2.18	0.42
1:B:1050:ARG:NH2	1:B:1770:GLU:OE1	2.52	0.42
1:B:1704:HIS:CE1	1:B:1727:ARG:H	2.37	0.42
1:D:462:ARG:NH1	1:D:506:ARG:HH11	2.17	0.42
1:D:663:LEU:HD22	1:D:749:GLN:NE2	2.34	0.42
1:D:1675:ILE:HD11	1:D:1678:SER:HB2	2.01	0.42
1:D:2452:HIS:CE1	1:D:2456:ASP:HB2	2.54	0.42
1:E:368:LEU:HG	1:E:370:ILE:CD1	2.50	0.42
1:A:1766:LEU:O	1:A:1770:GLU:HB2	2.20	0.42
1:B:2398:ILE:HB	1:B:2477:ILE:HG21	2.00	0.42
1:C:663:LEU:HD22	1:C:749:GLN:NE2	2.34	0.42
1:C:1056:MET:HG3	1:C:1081:TYR:HE1	1.83	0.42
1:C:1135:LYS:HA	1:C:1135:LYS:HD3	1.82	0.42
1:D:1268:TYR:N	1:D:1276:LYS:O	2.49	0.42
1:E:1652:LEU:HA	1:E:1655:HIS:HB3	2.00	0.42
1:A:368:LEU:HG	1:A:370:ILE:CD1	2.50	0.42
1:A:453:SER:HB3	1:A:456:ILE:HG12	2.00	0.42
1:A:497:ILE:HG21	1:A:589:TYR:CD2	2.54	0.42
1:A:1675:ILE:HD11	1:A:1678:SER:HB2	2.00	0.42
1:B:253:GLU:O	1:B:442:LYS:NZ	2.38	0.42
1:C:2112:ASN:HA	1:C:2115:MET:HG2	2.01	0.42
1:C:2226:SER:HB2	1:D:2066:THR:HG21	2.00	0.42
1:C:2278:GLN:OE1	1:C:2281:ARG:NH2	2.51	0.42
1:D:1170:LEU:HD22	1:D:1198:LEU:HD11	2.01	0.42
1:A:2132:ARG:HH11	1:A:2163:TYR:HB3	1.82	0.42
1:B:368:LEU:HG	1:B:370:ILE:CD1	2.49	0.42
1:B:2441:LEU:HG	1:B:2445:CYS:HB2	2.02	0.42
1:D:368:LEU:HG	1:D:370:ILE:CD1	2.50	0.42
1:D:1766:LEU:O	1:D:1770:GLU:HB2	2.19	0.42
1:A:595:ALA:HB2	1:A:605:LEU:HD22	2.01	0.42
1:A:1607:THR:HG21	1:A:1768:PHE:HZ	1.84	0.42
1:A:2226:SER:HB2	1:B:2066:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:848:GLN:OE1	1:B:892:GLN:NE2	2.53	0.42
1:C:341:MET:HE3	1:C:410:LEU:HD22	2.01	0.42
1:C:1050:ARG:NH2	1:C:1770:GLU:OE1	2.53	0.42
1:C:1766:LEU:O	1:C:1770:GLU:HB2	2.19	0.42
1:D:2458:GLY:O	1:E:2330:GLU:HB2	2.19	0.42
1:E:1170:LEU:HD22	1:E:1198:LEU:HD11	2.01	0.42
1:E:1704:HIS:CE1	1:E:1727:ARG:H	2.38	0.42
1:A:926:LEU:HD22	1:A:930:GLN:HB3	2.02	0.42
1:A:2431:ALA:O	1:A:2450:VAL:HG12	2.20	0.42
1:B:174:LYS:HG2	1:B:185:VAL:HG21	2.02	0.42
1:B:2202:GLU:O	1:B:2205:GLN:HG2	2.20	0.42
1:C:926:LEU:HD22	1:C:930:GLN:HB3	2.02	0.42
1:C:2416:SER:HB2	1:C:2510:HIS:HB2	2.01	0.42
1:D:593:LEU:O	1:D:597:ILE:HG12	2.20	0.42
1:D:812:ASN:HA	1:E:1998:ALA:HB2	2.02	0.42
1:D:1607:THR:HG21	1:D:1768:PHE:HZ	1.84	0.42
1:E:537:ASP:HA	1:E:577:LYS:HA	2.01	0.42
1:A:579:LYS:HG3	1:A:581:ASN:H	1.85	0.42
1:B:462:ARG:NH1	1:B:506:ARG:HH11	2.16	0.42
1:B:1607:THR:HG21	1:B:1768:PHE:HZ	1.85	0.42
1:B:2278:GLN:OE1	1:B:2281:ARG:NH2	2.51	0.42
1:B:1113:LEU:HD11	1:B:1119:GLY:HA3	2.01	0.42
1:C:218:LEU:HB3	1:C:221:LEU:HB2	2.02	0.42
1:D:2033:LEU:CD1	1:D:2266:TYR:HA	2.50	0.42
1:E:320:SER:HB2	1:E:323:GLY:HA2	2.00	0.42
1:E:860:PRO:HA	1:E:861:PRO:HD3	1.97	0.42
1:B:218:LEU:HB3	1:B:221:LEU:HB2	2.02	0.42
1:B:593:LEU:O	1:B:597:ILE:HG12	2.20	0.42
1:B:926:LEU:HD22	1:B:930:GLN:HB3	2.02	0.42
1:B:2452:HIS:CE1	1:B:2456:ASP:HB2	2.54	0.42
1:C:1036:GLN:O	1:C:1040:TYR:N	2.41	0.42
1:D:965:ASP:OD1	1:D:966:ASP:N	2.52	0.42
1:E:579:LYS:HG3	1:E:581:ASN:H	1.84	0.42
1:E:724:ALA:O	1:E:729:LYS:NZ	2.35	0.42
1:B:2033:LEU:CD1	1:B:2266:TYR:HA	2.50	0.42
1:C:2033:LEU:CD1	1:C:2266:TYR:HA	2.50	0.42
1:D:2207:ASP:O	1:D:2211:LYS:HG2	2.20	0.42
1:E:593:LEU:O	1:E:597:ILE:HG12	2.20	0.42
1:E:1818:VAL:HG12	1:E:1820:PRO:HD2	2.02	0.42
1:E:2441:LEU:HG	1:E:2445:CYS:HB2	2.02	0.42
1:A:537:ASP:HA	1:A:577:LYS:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1818:VAL:HG12	1:A:1820:PRO:HD2	2.02	0.41
1:B:371:LYS:HA	1:B:377:GLU:HA	2.02	0.41
1:C:2202:GLU:O	1:C:2205:GLN:HG2	2.20	0.41
1:C:2355:GLN:HG2	1:C:2356:GLU:OE1	2.20	0.41
1:D:1818:VAL:HG12	1:D:1820:PRO:HD2	2.02	0.41
1:A:2202:GLU:O	1:A:2205:GLN:HG2	2.20	0.41
1:A:2330:GLU:HB3	1:E:2460:PHE:CZ	2.55	0.41
1:B:1279:THR:HG22	1:B:1281:GLU:H	1.86	0.41
1:B:1675:ILE:HD11	1:B:1678:SER:HB2	2.01	0.41
1:B:1887:LEU:HD12	1:B:1887:LEU:HA	1.88	0.41
1:C:593:LEU:O	1:C:597:ILE:HG12	2.20	0.41
1:C:2441:LEU:HG	1:C:2445:CYS:HB2	2.02	0.41
1:C:2452:HIS:CE1	1:C:2456:ASP:HB2	2.55	0.41
1:C:2460:PHE:CZ	1:D:2330:GLU:HB3	2.55	0.41
1:D:160:SER:HA	1:D:982:LYS:HA	2.03	0.41
1:E:926:LEU:HD22	1:E:930:GLN:HB3	2.02	0.41
1:E:965:ASP:OD1	1:E:966:ASP:N	2.52	0.41
1:E:1135:LYS:HA	1:E:1135:LYS:HD3	1.82	0.41
1:A:848:GLN:OE1	1:A:892:GLN:NE2	2.53	0.41
1:A:2452:HIS:CE1	1:A:2456:ASP:HB2	2.54	0.41
1:A:2460:PHE:CZ	1:B:2330:GLU:HB3	2.56	0.41
1:C:1800:TRP:CZ2	1:C:1802:PRO:HG3	2.55	0.41
1:C:2431:ALA:O	1:C:2450:VAL:HG12	2.21	0.41
1:D:218:LEU:HB3	1:D:221:LEU:HB2	2.02	0.41
1:E:2112:ASN:HA	1:E:2115:MET:HG2	2.03	0.41
1:E:2431:ALA:O	1:E:2450:VAL:HG12	2.20	0.41
1:A:2112:ASN:HA	1:A:2115:MET:HG2	2.02	0.41
1:A:2207:ASP:O	1:A:2211:LYS:HG2	2.21	0.41
1:A:2470:LEU:N	1:A:2473:GLU:OE1	2.52	0.41
1:C:268:PHE:HZ	1:C:441:ASN:HB2	1.85	0.41
1:D:2441:LEU:HG	1:D:2445:CYS:HB2	2.02	0.41
1:E:661:LYS:HB2	1:E:750:GLU:HB2	2.03	0.41
1:E:2341:TYR:CD2	1:E:2353:LEU:HD11	2.55	0.41
1:A:320:SER:HB2	1:A:323:GLY:HA2	2.01	0.41
1:A:1111:ILE:HG13	1:A:1160:PRO:HD3	2.03	0.41
1:B:2416:SER:HB2	1:B:2510:HIS:HB2	2.02	0.41
1:C:538:LEU:HD12	1:C:566:LEU:HD22	2.02	0.41
1:A:218:LEU:HB3	1:A:221:LEU:HB2	2.02	0.41
1:B:2182:SER:OG	1:D:1067:SER:N	2.54	0.41
1:C:1244:THR:HG21	1:C:1268:TYR:CD1	2.55	0.41
1:C:2341:TYR:CD2	1:C:2353:LEU:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:LYS:HG2	1:D:185:VAL:HG21	2.03	0.41
1:D:926:LEU:HD22	1:D:930:GLN:HB3	2.02	0.41
1:D:1279:THR:HG22	1:D:1281:GLU:H	1.85	0.41
1:E:538:LEU:HD12	1:E:566:LEU:HD22	2.03	0.41
1:A:116:ALA:HB1	1:A:150:LEU:HD22	2.02	0.41
1:A:965:ASP:OD1	1:A:966:ASP:N	2.52	0.41
1:A:2182:SER:OG	1:C:1067:SER:N	2.54	0.41
1:A:2362:SER:OG	1:A:2502:LYS:NZ	2.49	0.41
1:B:691:VAL:O	1:B:694:PRO:HD2	2.21	0.41
1:B:2355:GLN:HG2	1:B:2356:GLU:OE1	2.21	0.41
1:C:2207:ASP:O	1:C:2211:LYS:HG2	2.21	0.41
1:D:2278:GLN:OE1	1:D:2281:ARG:NH2	2.52	0.41
1:D:2321:HIS:NE2	1:D:2325:ASP:OD2	2.53	0.41
1:E:218:LEU:HB3	1:E:221:LEU:HB2	2.02	0.41
1:E:2207:ASP:O	1:E:2211:LYS:HG2	2.20	0.41
1:A:268:PHE:HZ	1:A:441:ASN:HB2	1.86	0.41
1:A:365:ALA:HB3	1:A:384:ALA:HA	2.02	0.41
1:A:593:LEU:O	1:A:597:ILE:HG12	2.20	0.41
1:A:2033:LEU:CD1	1:A:2266:TYR:HA	2.50	0.41
1:B:714:TRP:CZ3	1:B:762:LEU:HD22	2.55	0.41
1:B:1108:THR:HB	1:B:1126:VAL:HG12	2.03	0.41
1:B:1170:LEU:HD22	1:B:1198:LEU:HD11	2.02	0.41
1:B:2207:ASP:O	1:B:2211:LYS:HG2	2.20	0.41
1:B:2460:PHE:CZ	1:C:2330:GLU:HB3	2.56	0.41
1:C:2087:LYS:HE3	1:C:2087:LYS:HB3	1.87	0.41
1:D:371:LYS:HA	1:D:377:GLU:HA	2.02	0.41
1:D:579:LYS:HG3	1:D:581:ASN:H	1.85	0.41
1:E:487:ARG:O	1:E:487:ARG:NH1	2.47	0.41
1:E:1244:THR:HG21	1:E:1268:TYR:CD1	2.56	0.41
1:A:659:TYR:CE2	1:A:758:ALA:HB2	2.56	0.41
1:A:1704:HIS:CE1	1:A:1727:ARG:H	2.39	0.41
1:A:1800:TRP:CZ2	1:A:1802:PRO:HG3	2.56	0.41
1:A:2355:GLN:HG2	1:A:2356:GLU:OE1	2.21	0.41
1:B:141:ARG:HH22	1:B:1005:GLU:CD	2.24	0.41
1:B:2132:ARG:HH11	1:B:2163:TYR:HB3	1.85	0.41
1:C:368:LEU:HG	1:C:370:ILE:CD1	2.50	0.41
1:C:2245:PHE:O	1:C:2246:SER:OG	2.39	0.41
1:D:522:PRO:O	1:D:553:ARG:NH1	2.53	0.41
1:D:1244:THR:HG21	1:D:1268:TYR:CD1	2.56	0.41
1:D:2112:ASN:HA	1:D:2115:MET:HG2	2.02	0.41
1:D:2202:GLU:O	1:D:2205:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:268:PHE:HZ	1:E:441:ASN:HB2	1.86	0.41
1:E:371:LYS:HA	1:E:377:GLU:HA	2.03	0.41
1:E:691:VAL:O	1:E:694:PRO:HD2	2.21	0.41
1:E:1607:THR:HG21	1:E:1768:PHE:HZ	1.85	0.41
1:E:1766:LEU:O	1:E:1770:GLU:HB2	2.20	0.41
1:E:2228:LYS:HE3	1:E:2228:LYS:HB2	1.82	0.41
1:A:160:SER:HA	1:A:982:LYS:HA	2.03	0.41
1:A:1244:THR:HG21	1:A:1268:TYR:CD1	2.56	0.41
1:B:538:LEU:HD12	1:B:566:LEU:HD22	2.03	0.41
1:B:1818:VAL:HG12	1:B:1820:PRO:HD2	2.02	0.41
1:B:2015:SER:HB2	1:C:2322:LEU:HD21	2.03	0.41
1:B:2431:ALA:O	1:B:2450:VAL:HG12	2.21	0.41
1:C:141:ARG:HH22	1:C:1005:GLU:CD	2.24	0.41
1:C:691:VAL:O	1:C:694:PRO:HD2	2.21	0.41
1:C:1164:LYS:HE2	1:D:1611:ARG:HG2	2.03	0.41
1:C:1170:LEU:HD22	1:C:1198:LEU:HD11	2.03	0.41
1:C:1818:VAL:HG12	1:C:1820:PRO:HD2	2.02	0.41
1:C:2321:HIS:NE2	1:C:2325:ASP:OD2	2.54	0.41
1:D:1704:HIS:CE1	1:D:1727:ARG:H	2.38	0.41
1:D:2431:ALA:O	1:D:2450:VAL:HG12	2.21	0.41
1:E:365:ALA:HB3	1:E:384:ALA:HA	2.03	0.41
1:E:2033:LEU:CD1	1:E:2266:TYR:HA	2.50	0.41
1:A:1279:THR:HG22	1:A:1281:GLU:H	1.86	0.40
1:A:2322:LEU:HD21	1:E:2015:SER:HB2	2.03	0.40
1:A:2432:ILE:HD11	1:B:2402:TYR:CE1	2.56	0.40
1:B:160:SER:HA	1:B:982:LYS:HA	2.02	0.40
1:B:1130:LYS:HZ3	1:B:1139:ASN:C	2.25	0.40
1:C:1704:HIS:CE1	1:C:1727:ARG:H	2.39	0.40
1:D:538:LEU:HD12	1:D:566:LEU:HD22	2.04	0.40
1:D:2355:GLN:HG2	1:D:2356:GLU:OE1	2.21	0.40
1:E:341:MET:HE3	1:E:410:LEU:HD22	2.03	0.40
1:E:1279:THR:HG22	1:E:1281:GLU:H	1.86	0.40
1:A:689:LEU:HD12	1:A:689:LEU:HA	1.91	0.40
1:A:1108:THR:HB	1:A:1126:VAL:HG12	2.03	0.40
1:A:2321:HIS:NE2	1:A:2325:ASP:OD2	2.54	0.40
1:A:2388:GLN:HA	1:A:2485:SER:HA	2.03	0.40
1:C:493:GLU:O	1:C:497:ILE:HG12	2.21	0.40
1:C:1108:THR:HB	1:C:1126:VAL:HG12	2.02	0.40
1:C:1111:ILE:HG13	1:C:1160:PRO:HD3	2.04	0.40
1:C:1279:THR:HG22	1:C:1281:GLU:H	1.85	0.40
1:C:1609:PHE:CZ	1:C:1613:LEU:HD13	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:538:LEU:HB2	1:D:566:LEU:HD22	2.03	0.40
1:D:661:LYS:HB2	1:D:750:GLU:HB2	2.04	0.40
1:E:1162:ILE:HD13	1:E:1167:LEU:HA	2.04	0.40
1:E:1800:TRP:CZ2	1:E:1802:PRO:HG3	2.57	0.40
1:E:2362:SER:OG	1:E:2502:LYS:NZ	2.51	0.40
1:B:268:PHE:HZ	1:B:441:ASN:HB2	1.85	0.40
1:B:1800:TRP:CZ2	1:B:1802:PRO:HG3	2.56	0.40
1:D:116:ALA:HB1	1:D:150:LEU:HD22	2.02	0.40
1:D:2328:ALA:HB2	1:D:2516:LYS:HB3	2.03	0.40
1:E:1108:THR:HB	1:E:1126:VAL:HG12	2.02	0.40
1:E:2202:GLU:O	1:E:2205:GLN:HG2	2.21	0.40
1:A:1113:LEU:HD11	1:A:1119:GLY:HA3	2.04	0.40
1:A:2341:TYR:CD2	1:A:2353:LEU:HD11	2.57	0.40
1:B:497:ILE:HG21	1:B:589:TYR:CD2	2.54	0.40
1:B:1244:THR:HG21	1:B:1268:TYR:CD1	2.56	0.40
1:C:659:TYR:CE2	1:C:758:ALA:HB2	2.56	0.40
1:D:268:PHE:HZ	1:D:441:ASN:HB2	1.87	0.40
1:D:714:TRP:CZ3	1:D:762:LEU:HD22	2.56	0.40
1:E:848:GLN:OE1	1:E:892:GLN:NE2	2.53	0.40
1:E:2470:LEU:N	1:E:2473:GLU:OE1	2.53	0.40
1:A:493:GLU:O	1:A:497:ILE:HG12	2.21	0.40
1:A:1170:LEU:HD22	1:A:1198:LEU:HD11	2.01	0.40
1:D:195:SER:OG	1:D:948:THR:HG22	2.22	0.40
1:D:659:TYR:CE2	1:D:758:ALA:HB2	2.57	0.40
1:D:689:LEU:HA	1:D:689:LEU:HD12	1.92	0.40
1:D:848:GLN:OE1	1:D:892:GLN:NE2	2.54	0.40
1:E:493:GLU:O	1:E:497:ILE:HG12	2.22	0.40
1:E:2321:HIS:NE2	1:E:2325:ASP:OD2	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2114/2535 (83%)	2069 (98%)	45 (2%)	0	100	100
1	B	2114/2535 (83%)	2071 (98%)	43 (2%)	0	100	100
1	C	2114/2535 (83%)	2072 (98%)	42 (2%)	0	100	100
1	D	2114/2535 (83%)	2070 (98%)	44 (2%)	0	100	100
1	E	2114/2535 (83%)	2071 (98%)	43 (2%)	0	100	100
All	All	10570/12675 (83%)	10353 (98%)	217 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	1816/2173 (84%)	1812 (100%)	4 (0%)	92	97
1	B	1816/2173 (84%)	1812 (100%)	4 (0%)	92	97
1	C	1816/2173 (84%)	1812 (100%)	4 (0%)	92	97
1	D	1816/2173 (84%)	1812 (100%)	4 (0%)	92	97
1	E	1816/2173 (84%)	1812 (100%)	4 (0%)	92	97
All	All	9080/10865 (84%)	9060 (100%)	20 (0%)	91	97

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1049	MET
1	A	1174	GLN
1	A	1965	GLN
1	A	2414	GLN
1	B	1049	MET
1	B	1174	GLN
1	B	1965	GLN
1	B	2414	GLN
1	C	1049	MET
1	C	1174	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	1965	GLN
1	C	2414	GLN
1	D	1049	MET
1	D	1174	GLN
1	D	1965	GLN
1	D	2414	GLN
1	E	1049	MET
1	E	1174	GLN
1	E	1965	GLN
1	E	2414	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	852	GLN
1	A	892	GLN
1	A	969	GLN
1	B	852	GLN
1	B	892	GLN
1	B	969	GLN
1	C	852	GLN
1	C	892	GLN
1	C	969	GLN
1	D	852	GLN
1	D	892	GLN
1	D	969	GLN
1	E	852	GLN
1	E	892	GLN
1	E	969	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no 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](#)

There are no chain breaks in this entry.

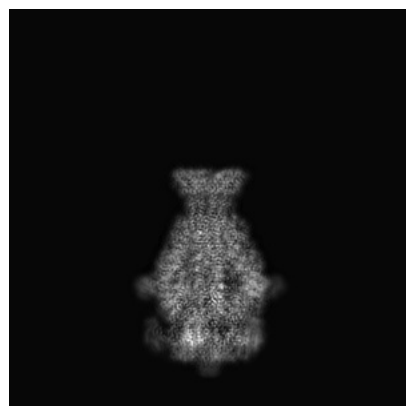
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16792. These allow visual inspection of the internal detail of the map and identification of artifacts.

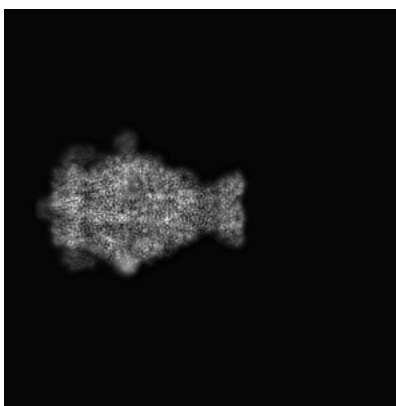
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

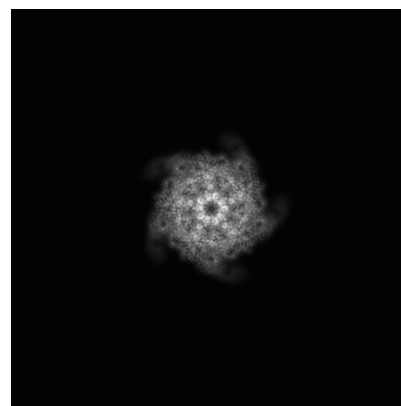
#### 6.1.1 Primary map



X

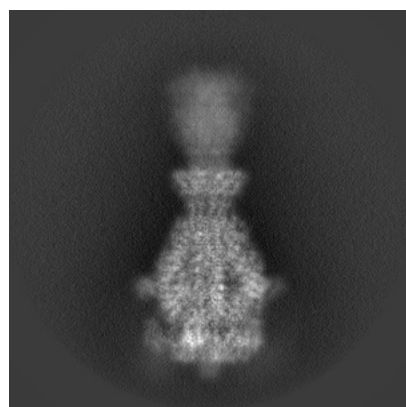


Y

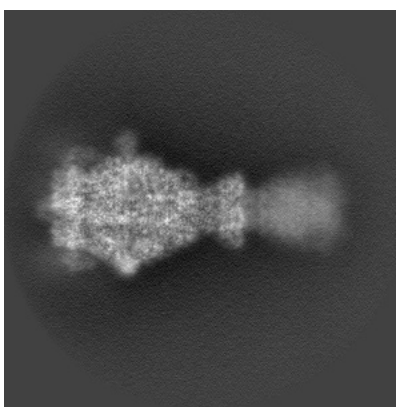


Z

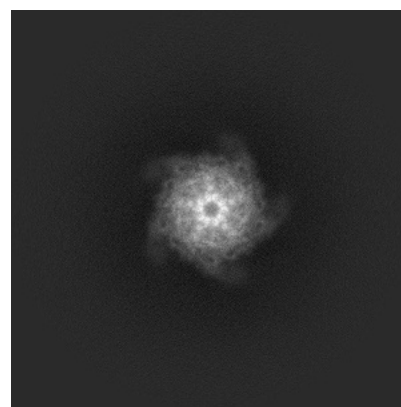
#### 6.1.2 Raw map



X



Y

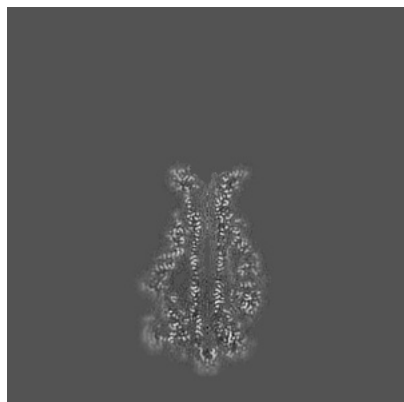


Z

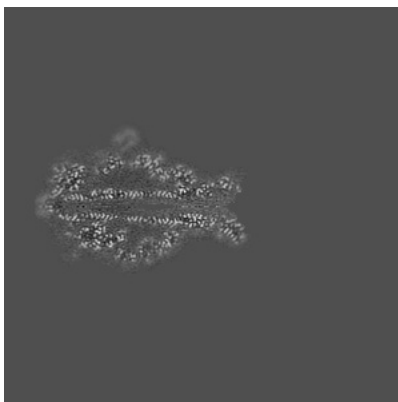
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

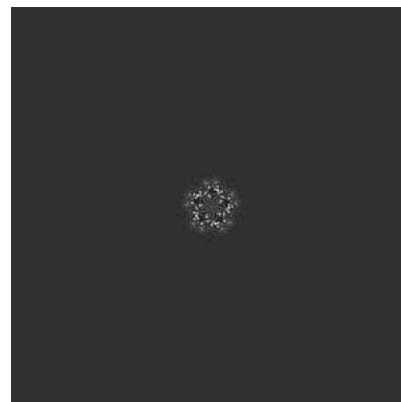
### 6.2.1 Primary map



X Index: 280

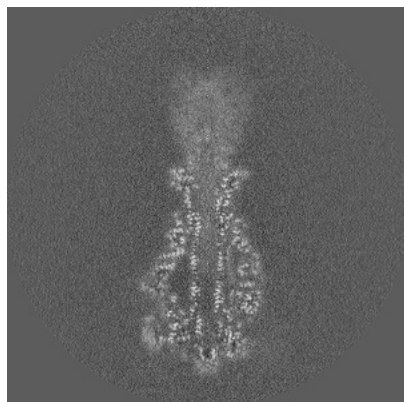


Y Index: 280

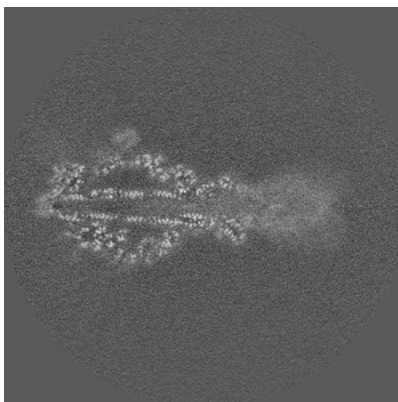


Z Index: 280

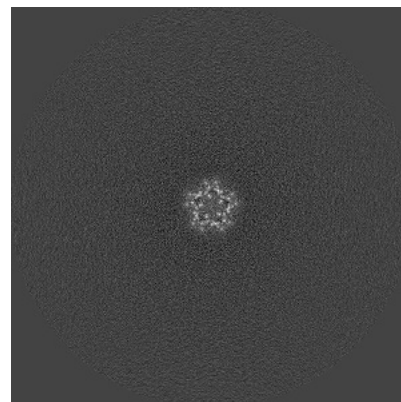
### 6.2.2 Raw map



X Index: 280



Y Index: 280

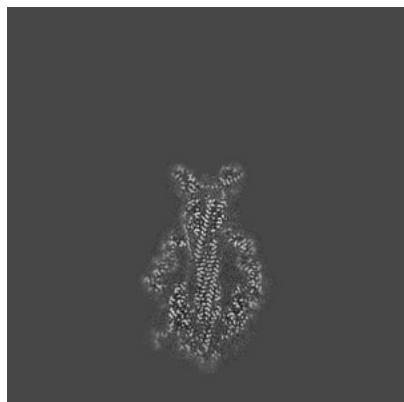


Z Index: 280

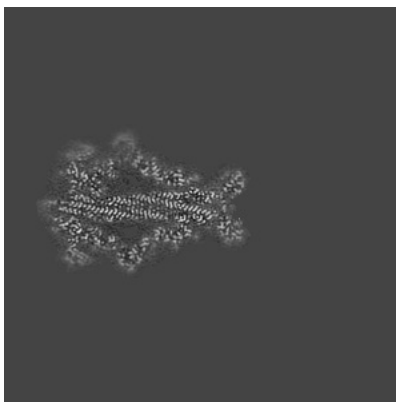
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

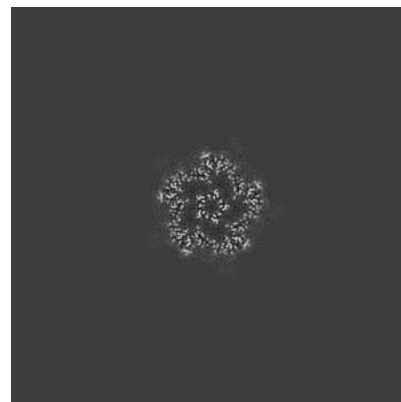
### 6.3.1 Primary map



X Index: 265

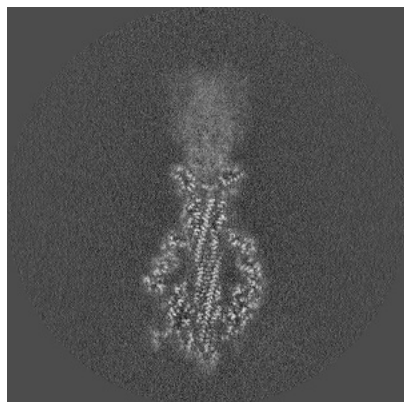


Y Index: 266

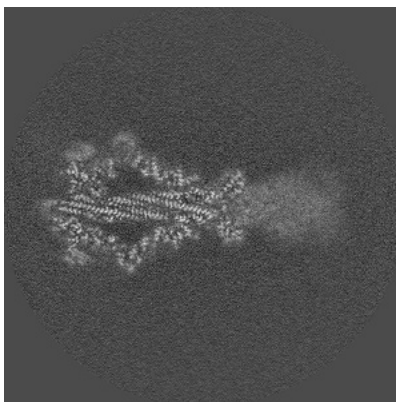


Z Index: 150

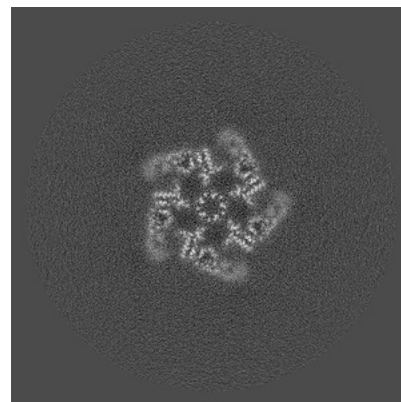
### 6.3.2 Raw map



X Index: 266



Y Index: 266

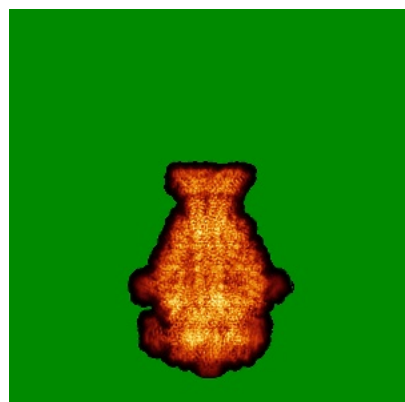


Z Index: 170

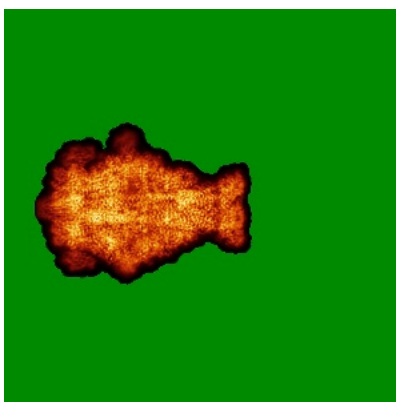
The images above show the largest variance slices of the map in three orthogonal directions.

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

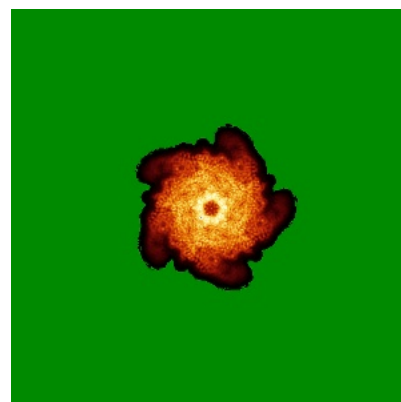
### 6.4.1 Primary map



X

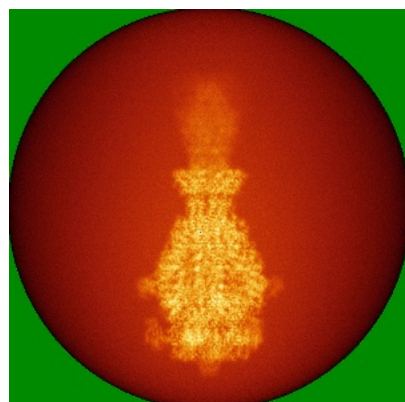


Y

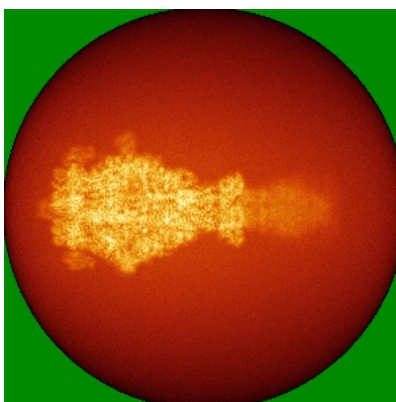


Z

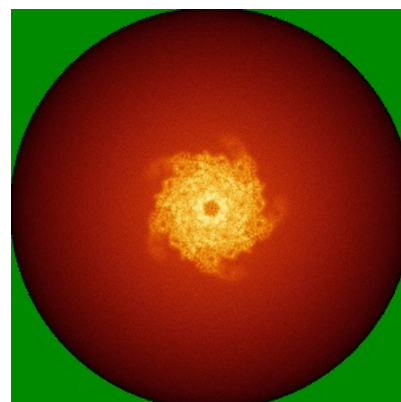
### 6.4.2 Raw map



X



Y



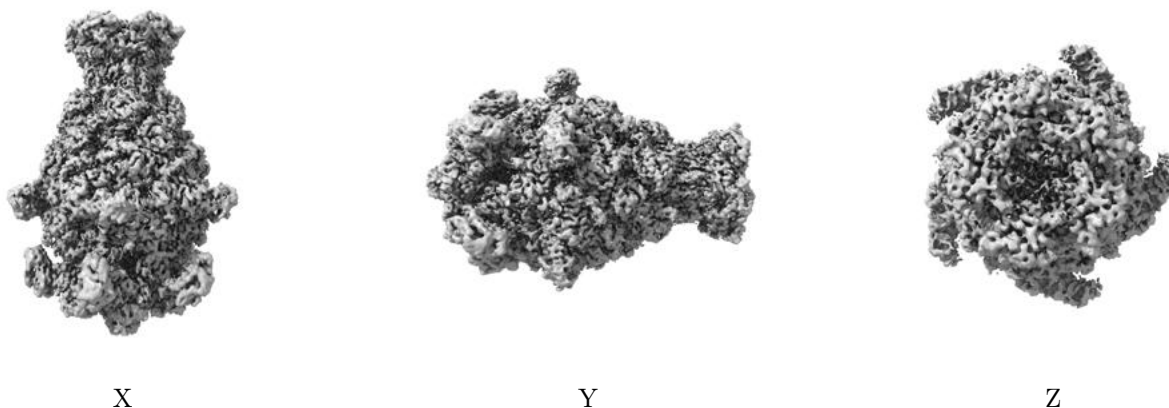
Z

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.



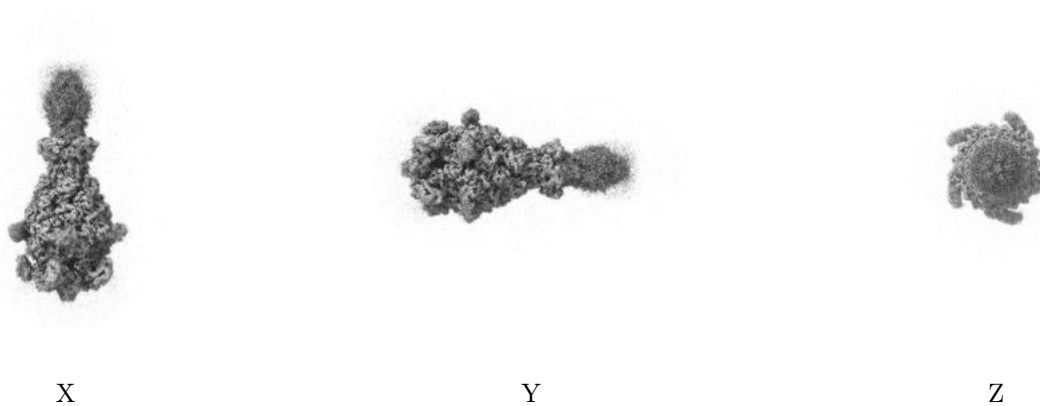
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.



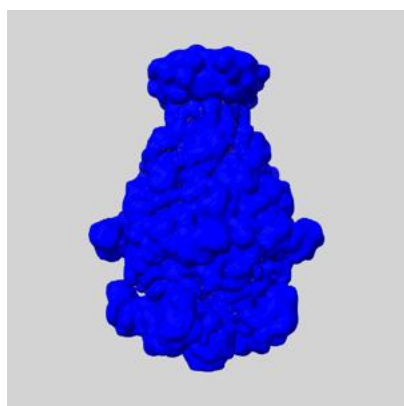
## 6.6 Mask visualisation [i](#)

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

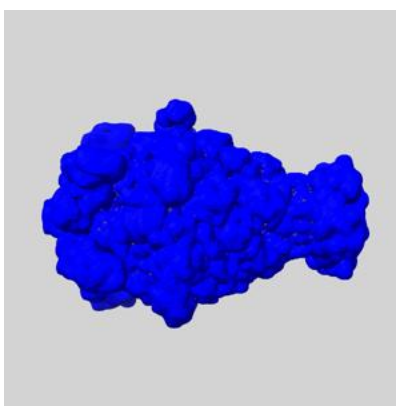
A mask typically either:

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

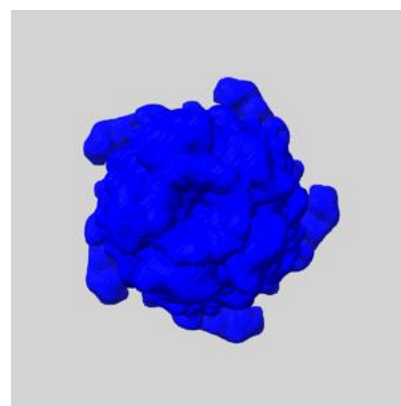
### 6.6.1 emd\_16792\_msk\_1.map [i](#)



X



Y

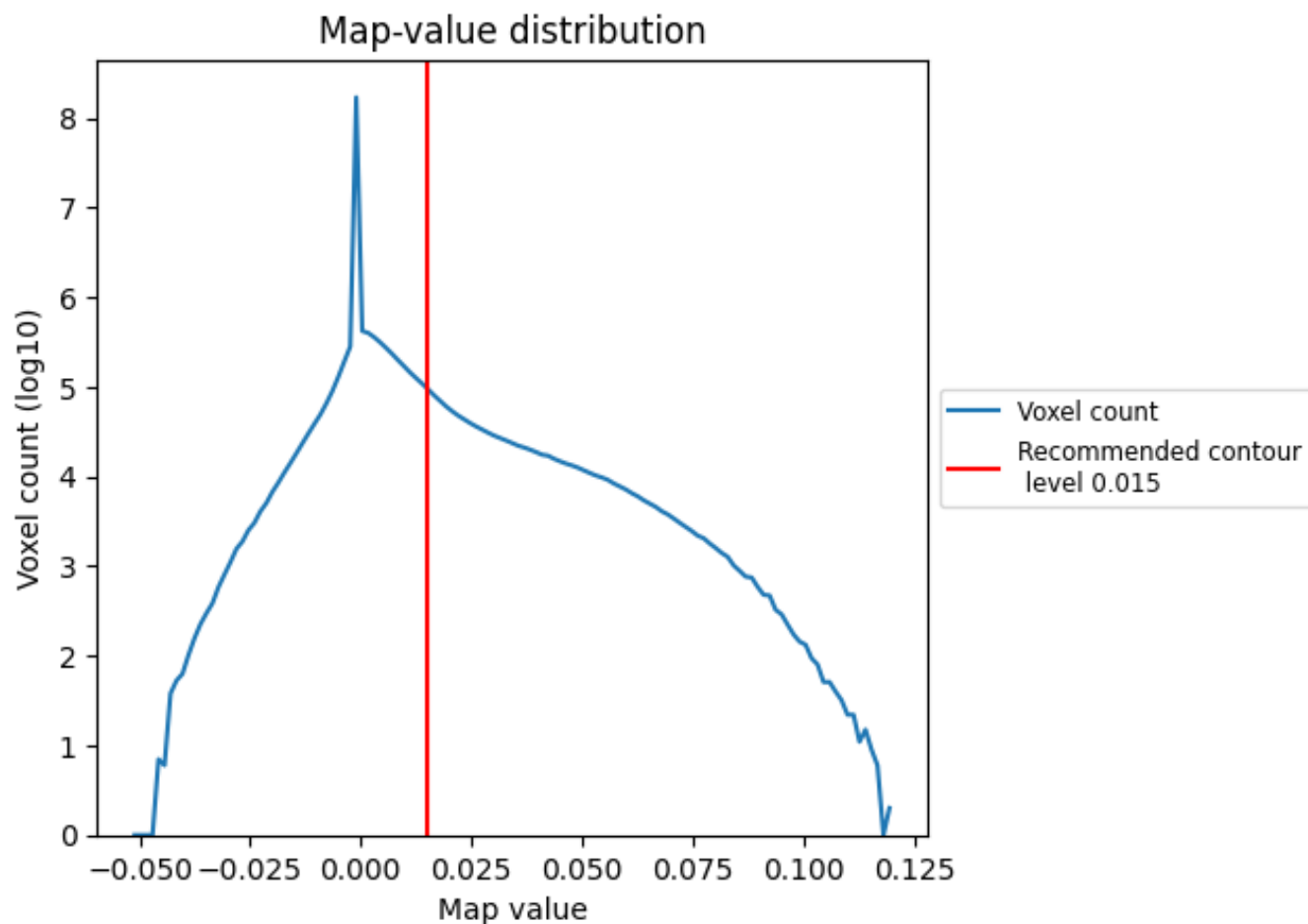


Z

## 7 Map analysis [i](#)

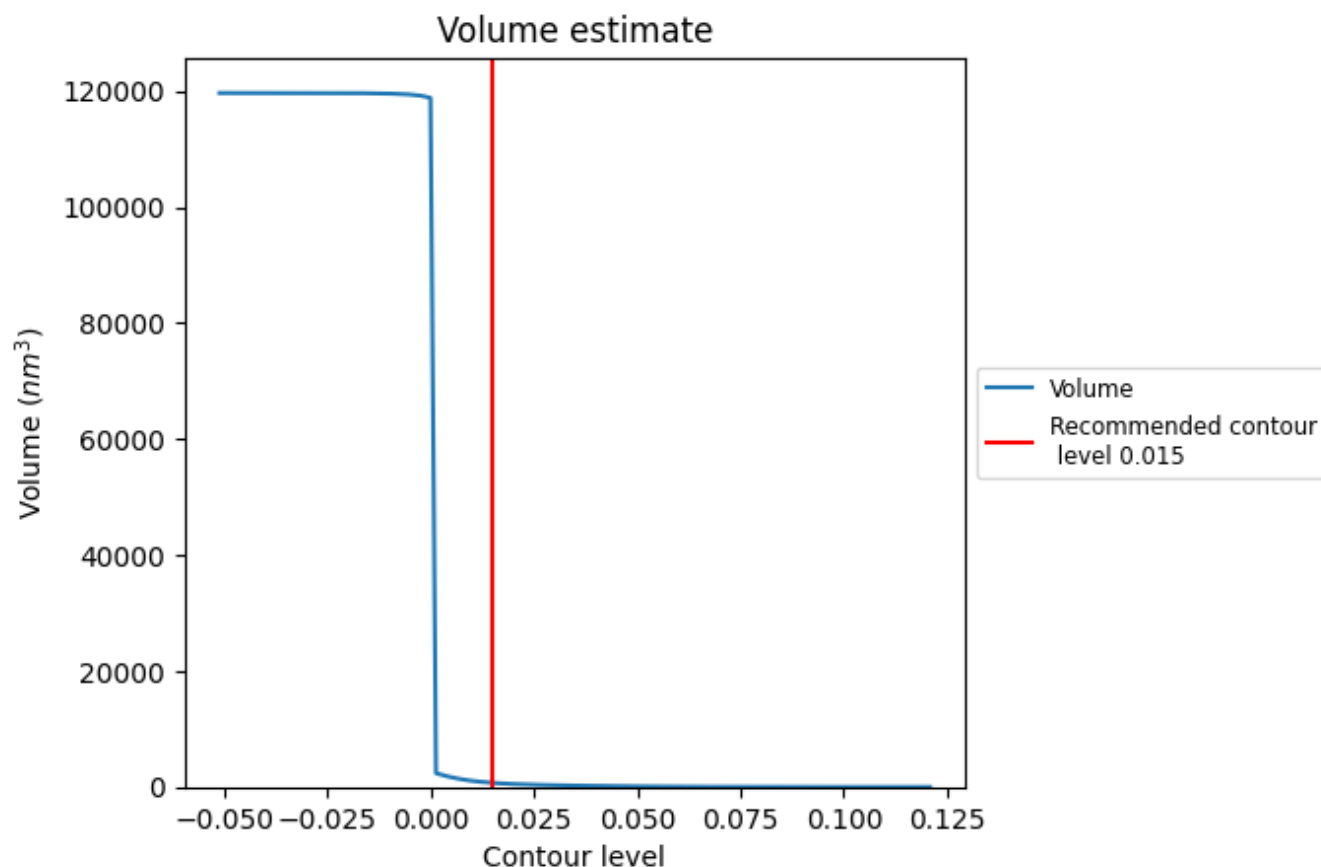
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

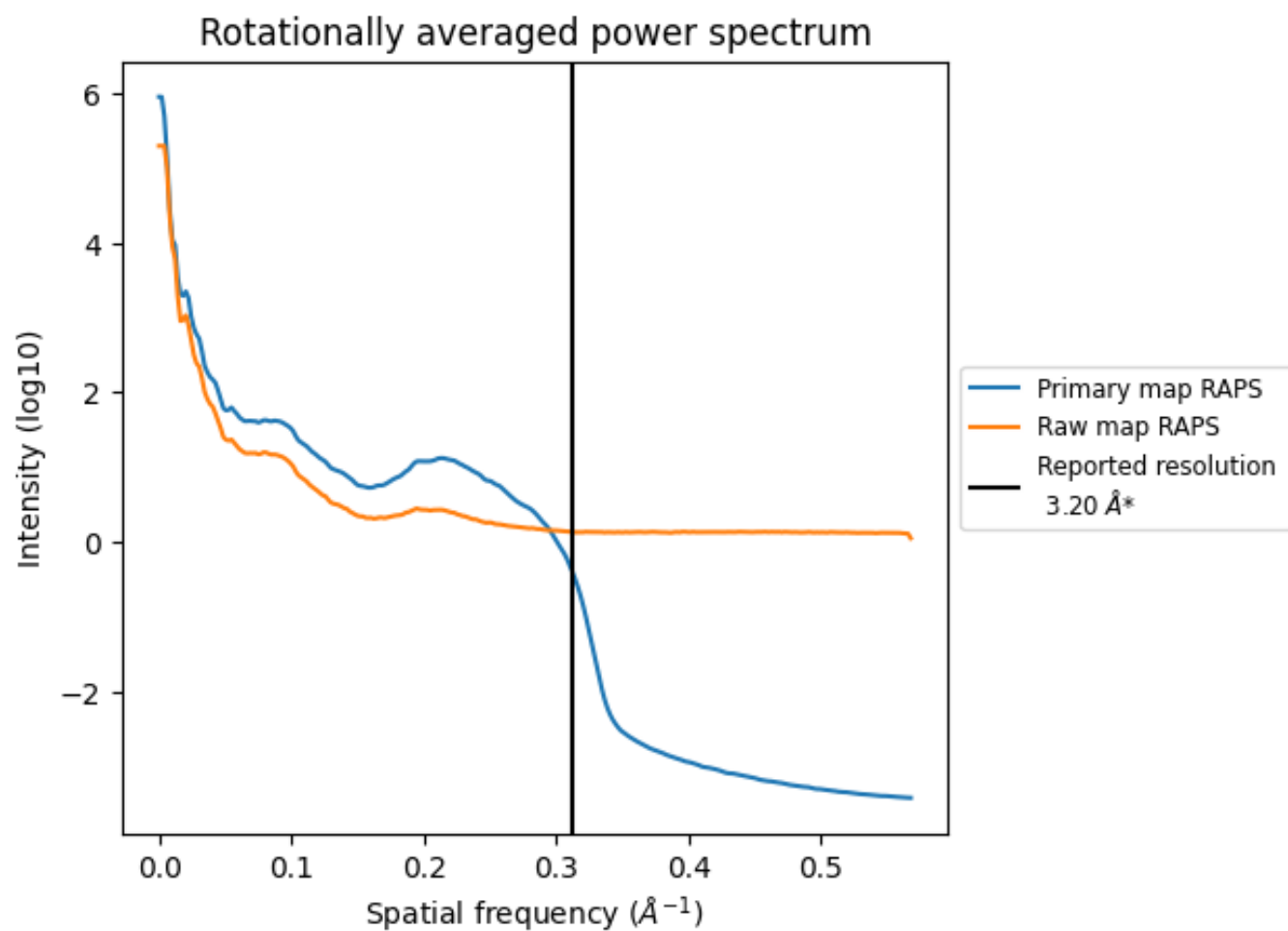
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 710 nm<sup>3</sup>; this corresponds to an approximate mass of 641 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

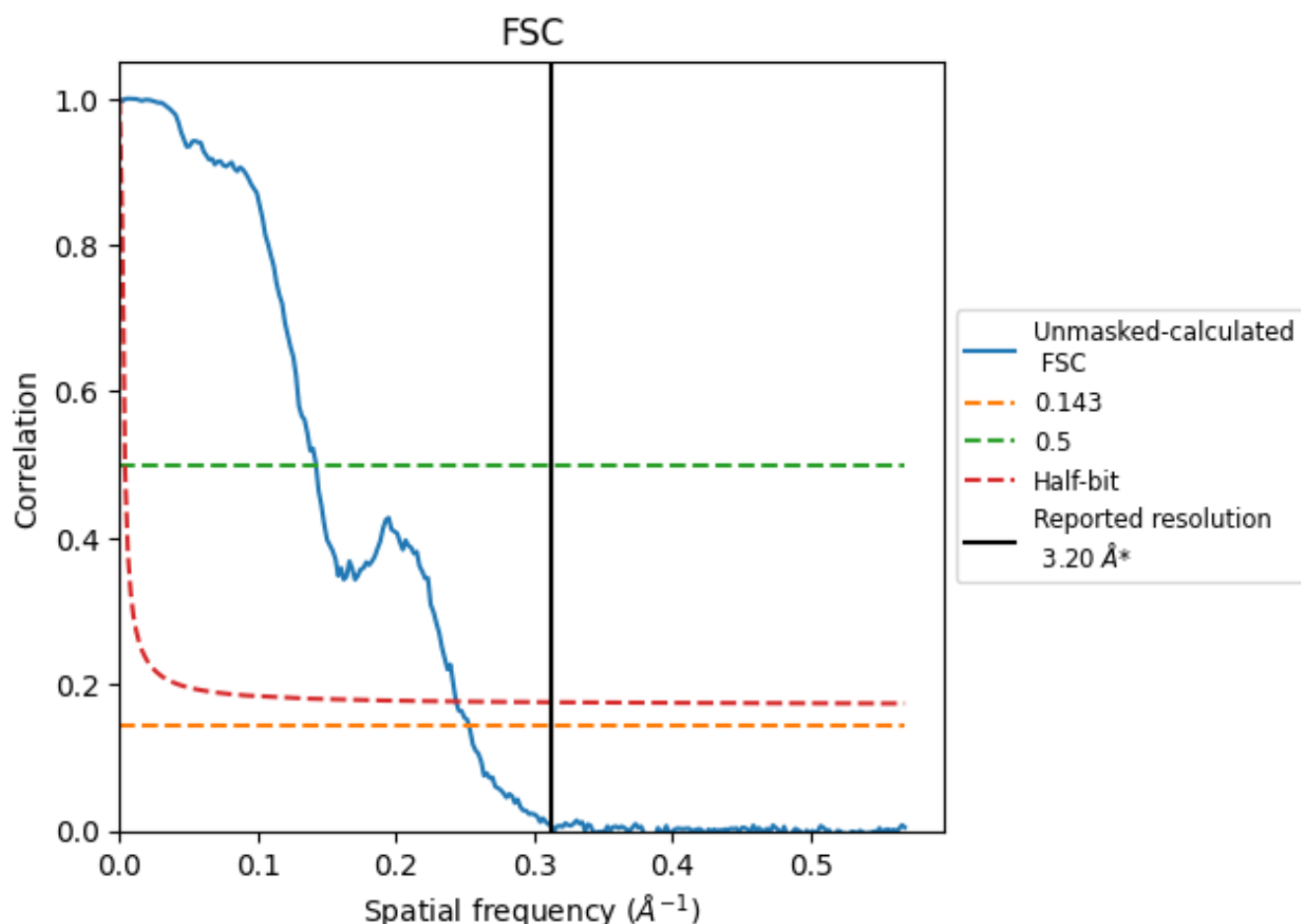


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.312  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

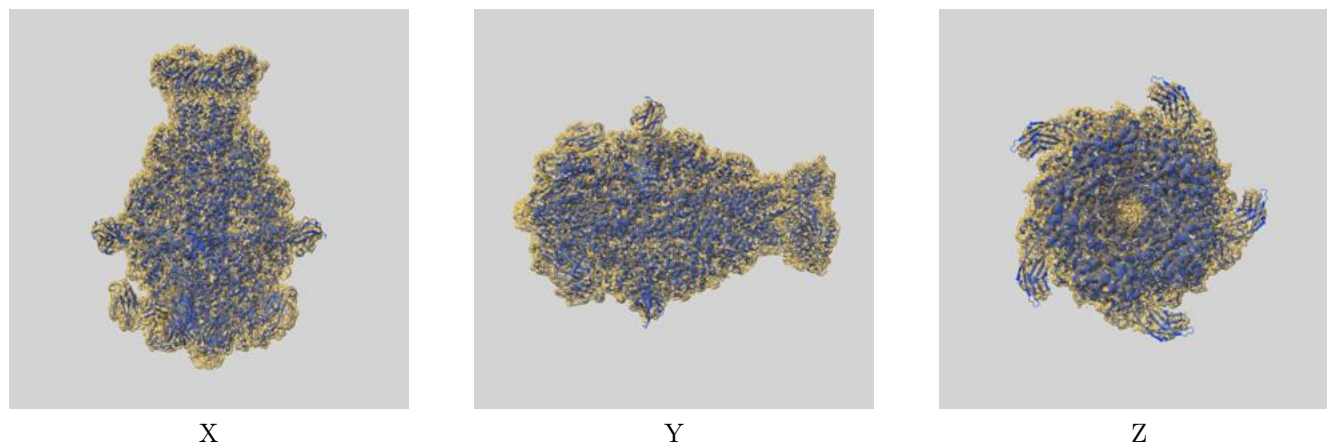
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.96	7.03	4.11

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.96 differs from the reported value 3.2 by more than 10 %

## 9 Map-model fit [i](#)

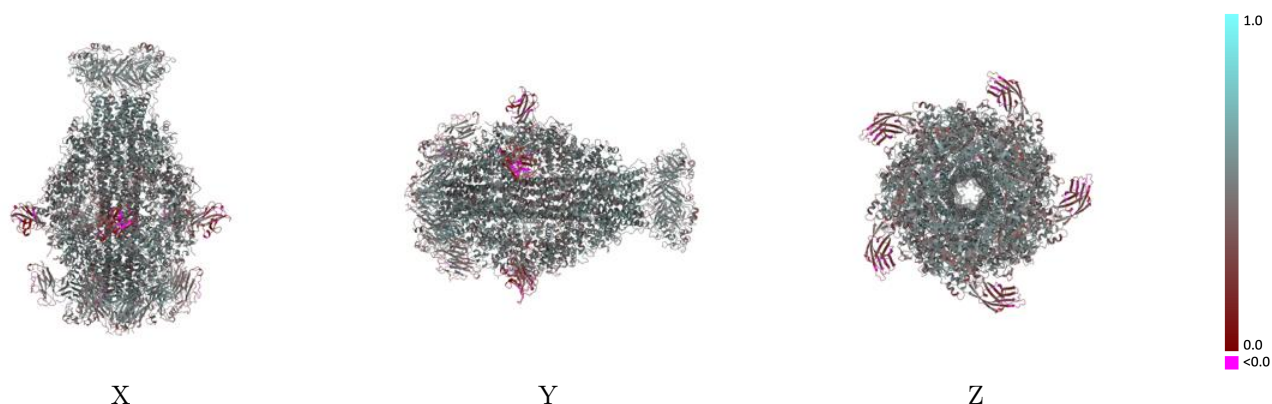
This section contains information regarding the fit between EMDB map EMD-16792 and PDB model 8CQ0. Per-residue inclusion information can be found in section [3](#) on page [7](#).

### 9.1 Map-model overlay [i](#)



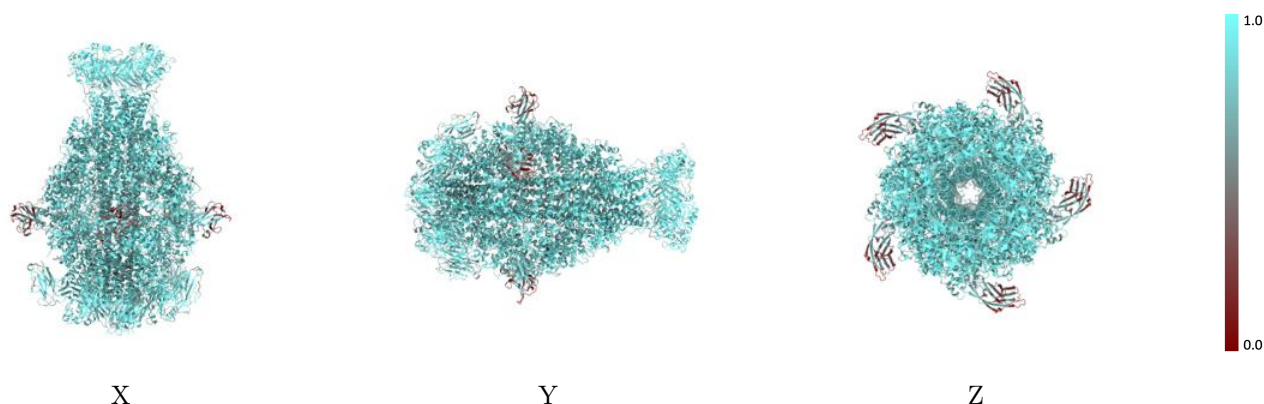
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

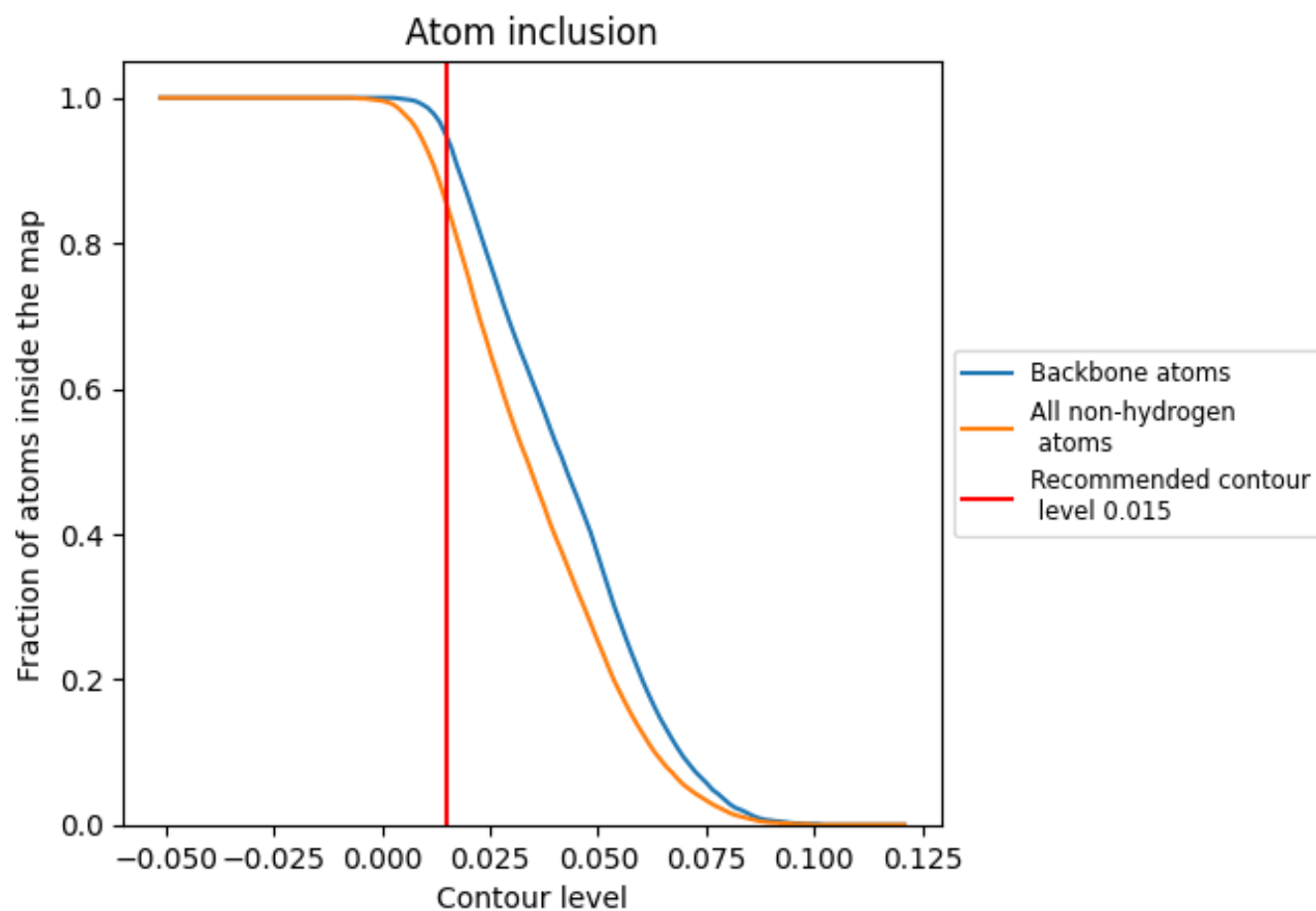
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.015).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 85% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8540	<div></div> 0.4660
A	<div></div> 0.8540	<div></div> 0.4660
B	<div></div> 0.8540	<div></div> 0.4660
C	<div></div> 0.8540	<div></div> 0.4670
D	<div></div> 0.8550	<div></div> 0.4670
E	<div></div> 0.8550	<div></div> 0.4650

