



Full wwPDB EM Validation Report ⓘ

Oct 14, 2025 – 06:21 PM JST

PDB ID : 9K4I / pdb_00009k4i
EMDB ID : EMD-62060
Title : Cryo-EM structure of the human TRPC1/C5 heteromer
Authors : Chen, Y.X.; Cheng, X.Y.; Zhang, J.
Deposited on : 2024-10-21
Resolution : 2.84 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.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

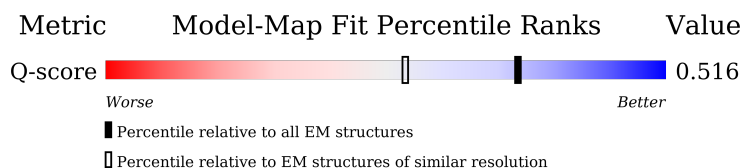
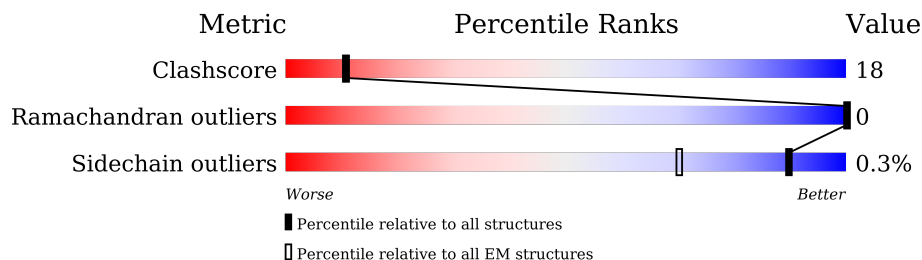
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.84 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	11884 (2.34 - 3.34)

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	1203	
1	C	1203	
1	D	1203	
2	B	1504	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22192 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 Maltose/maltodextrin-binding periplasmic protein,Short transient receptor potential channel 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	686	Total	C	N	O	S	0	0
			5563	3619	919	996	29		
1	C	686	Total	C	N	O	S	0	0
			5563	3619	919	996	29		
1	D	686	Total	C	N	O	S	0	0
			5563	3619	919	996	29		

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-437	MET	-	initiating methionine	UNP P0AEX9
A	-436	GLY	-	expression tag	UNP P0AEX9
A	-435	SER	-	expression tag	UNP P0AEX9
A	-434	ALA	-	expression tag	UNP P0AEX9
A	-433	GLY	-	expression tag	UNP P0AEX9
A	-432	ASP	-	expression tag	UNP P0AEX9
A	-431	TYR	-	expression tag	UNP P0AEX9
A	-430	LYS	-	expression tag	UNP P0AEX9
A	-429	ASP	-	expression tag	UNP P0AEX9
A	-428	HIS	-	expression tag	UNP P0AEX9
A	-427	ASP	-	expression tag	UNP P0AEX9
A	-426	GLY	-	expression tag	UNP P0AEX9
A	-425	ASP	-	expression tag	UNP P0AEX9
A	-424	TYR	-	expression tag	UNP P0AEX9
A	-423	LYS	-	expression tag	UNP P0AEX9
A	-422	ASP	-	expression tag	UNP P0AEX9
A	-421	HIS	-	expression tag	UNP P0AEX9
A	-420	ASP	-	expression tag	UNP P0AEX9
A	-419	ILE	-	expression tag	UNP P0AEX9
A	-418	ASP	-	expression tag	UNP P0AEX9
A	-417	TYR	-	expression tag	UNP P0AEX9
A	-416	LYS	-	expression tag	UNP P0AEX9
A	-415	ASP	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-414	ASP	-	expression tag	UNP P0AEX9
A	-413	ASP	-	expression tag	UNP P0AEX9
A	-412	ASP	-	expression tag	UNP P0AEX9
A	-411	LYS	-	expression tag	UNP P0AEX9
A	-410	GLY	-	expression tag	UNP P0AEX9
A	-409	SER	-	expression tag	UNP P0AEX9
A	-408	ALA	-	expression tag	UNP P0AEX9
A	-407	ALA	-	expression tag	UNP P0AEX9
A	-406	ALA	-	expression tag	UNP P0AEX9
A	-405	MET	-	expression tag	UNP P0AEX9
A	-404	GLY	-	expression tag	UNP P0AEX9
A	-403	SER	-	expression tag	UNP P0AEX9
A	-402	SER	-	expression tag	UNP P0AEX9
A	-401	HIS	-	expression tag	UNP P0AEX9
A	-400	HIS	-	expression tag	UNP P0AEX9
A	-399	HIS	-	expression tag	UNP P0AEX9
A	-398	HIS	-	expression tag	UNP P0AEX9
A	-397	HIS	-	expression tag	UNP P0AEX9
A	-396	HIS	-	expression tag	UNP P0AEX9
A	-395	GLY	-	expression tag	UNP P0AEX9
A	-394	SER	-	expression tag	UNP P0AEX9
A	-393	SER	-	expression tag	UNP P0AEX9
A	-392	MET	-	expression tag	UNP P0AEX9
A	-25	ASN	-	linker	UNP P0AEX9
A	-24	SER	-	linker	UNP P0AEX9
A	-23	SER	-	linker	UNP P0AEX9
A	-22	SER	-	linker	UNP P0AEX9
A	-21	ASN	-	linker	UNP P0AEX9
A	-20	ASN	-	linker	UNP P0AEX9
A	-19	ASN	-	linker	UNP P0AEX9
A	-18	ASN	-	linker	UNP P0AEX9
A	-17	ASN	-	linker	UNP P0AEX9
A	-16	ASN	-	linker	UNP P0AEX9
A	-15	ASN	-	linker	UNP P0AEX9
A	-14	ASN	-	linker	UNP P0AEX9
A	-13	ASN	-	linker	UNP P0AEX9
A	-12	ASN	-	linker	UNP P0AEX9
A	-11	LEU	-	linker	UNP P0AEX9
A	-10	GLY	-	linker	UNP P0AEX9
A	-9	ILE	-	linker	UNP P0AEX9
A	-8	GLU	-	linker	UNP P0AEX9
A	-7	LEU	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLU	-	linker	UNP P0AEX9
A	-5	VAL	-	linker	UNP P0AEX9
A	-4	LEU	-	linker	UNP P0AEX9
A	-3	PHE	-	linker	UNP P0AEX9
A	-2	GLN	-	linker	UNP P0AEX9
A	-1	GLY	-	linker	UNP P0AEX9
A	0	PRO	-	linker	UNP P0AEX9
C	-437	MET	-	initiating methionine	UNP P0AEX9
C	-436	GLY	-	expression tag	UNP P0AEX9
C	-435	SER	-	expression tag	UNP P0AEX9
C	-434	ALA	-	expression tag	UNP P0AEX9
C	-433	GLY	-	expression tag	UNP P0AEX9
C	-432	ASP	-	expression tag	UNP P0AEX9
C	-431	TYR	-	expression tag	UNP P0AEX9
C	-430	LYS	-	expression tag	UNP P0AEX9
C	-429	ASP	-	expression tag	UNP P0AEX9
C	-428	HIS	-	expression tag	UNP P0AEX9
C	-427	ASP	-	expression tag	UNP P0AEX9
C	-426	GLY	-	expression tag	UNP P0AEX9
C	-425	ASP	-	expression tag	UNP P0AEX9
C	-424	TYR	-	expression tag	UNP P0AEX9
C	-423	LYS	-	expression tag	UNP P0AEX9
C	-422	ASP	-	expression tag	UNP P0AEX9
C	-421	HIS	-	expression tag	UNP P0AEX9
C	-420	ASP	-	expression tag	UNP P0AEX9
C	-419	ILE	-	expression tag	UNP P0AEX9
C	-418	ASP	-	expression tag	UNP P0AEX9
C	-417	TYR	-	expression tag	UNP P0AEX9
C	-416	LYS	-	expression tag	UNP P0AEX9
C	-415	ASP	-	expression tag	UNP P0AEX9
C	-414	ASP	-	expression tag	UNP P0AEX9
C	-413	ASP	-	expression tag	UNP P0AEX9
C	-412	ASP	-	expression tag	UNP P0AEX9
C	-411	LYS	-	expression tag	UNP P0AEX9
C	-410	GLY	-	expression tag	UNP P0AEX9
C	-409	SER	-	expression tag	UNP P0AEX9
C	-408	ALA	-	expression tag	UNP P0AEX9
C	-407	ALA	-	expression tag	UNP P0AEX9
C	-406	ALA	-	expression tag	UNP P0AEX9
C	-405	MET	-	expression tag	UNP P0AEX9
C	-404	GLY	-	expression tag	UNP P0AEX9
C	-403	SER	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-402	SER	-	expression tag	UNP P0AEX9
C	-401	HIS	-	expression tag	UNP P0AEX9
C	-400	HIS	-	expression tag	UNP P0AEX9
C	-399	HIS	-	expression tag	UNP P0AEX9
C	-398	HIS	-	expression tag	UNP P0AEX9
C	-397	HIS	-	expression tag	UNP P0AEX9
C	-396	HIS	-	expression tag	UNP P0AEX9
C	-395	GLY	-	expression tag	UNP P0AEX9
C	-394	SER	-	expression tag	UNP P0AEX9
C	-393	SER	-	expression tag	UNP P0AEX9
C	-392	MET	-	expression tag	UNP P0AEX9
C	-25	ASN	-	linker	UNP P0AEX9
C	-24	SER	-	linker	UNP P0AEX9
C	-23	SER	-	linker	UNP P0AEX9
C	-22	SER	-	linker	UNP P0AEX9
C	-21	ASN	-	linker	UNP P0AEX9
C	-20	ASN	-	linker	UNP P0AEX9
C	-19	ASN	-	linker	UNP P0AEX9
C	-18	ASN	-	linker	UNP P0AEX9
C	-17	ASN	-	linker	UNP P0AEX9
C	-16	ASN	-	linker	UNP P0AEX9
C	-15	ASN	-	linker	UNP P0AEX9
C	-14	ASN	-	linker	UNP P0AEX9
C	-13	ASN	-	linker	UNP P0AEX9
C	-12	ASN	-	linker	UNP P0AEX9
C	-11	LEU	-	linker	UNP P0AEX9
C	-10	GLY	-	linker	UNP P0AEX9
C	-9	ILE	-	linker	UNP P0AEX9
C	-8	GLU	-	linker	UNP P0AEX9
C	-7	LEU	-	linker	UNP P0AEX9
C	-6	GLU	-	linker	UNP P0AEX9
C	-5	VAL	-	linker	UNP P0AEX9
C	-4	LEU	-	linker	UNP P0AEX9
C	-3	PHE	-	linker	UNP P0AEX9
C	-2	GLN	-	linker	UNP P0AEX9
C	-1	GLY	-	linker	UNP P0AEX9
C	0	PRO	-	linker	UNP P0AEX9
D	-437	MET	-	initiating methionine	UNP P0AEX9
D	-436	GLY	-	expression tag	UNP P0AEX9
D	-435	SER	-	expression tag	UNP P0AEX9
D	-434	ALA	-	expression tag	UNP P0AEX9
D	-433	GLY	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-432	ASP	-	expression tag	UNP P0AEX9
D	-431	TYR	-	expression tag	UNP P0AEX9
D	-430	LYS	-	expression tag	UNP P0AEX9
D	-429	ASP	-	expression tag	UNP P0AEX9
D	-428	HIS	-	expression tag	UNP P0AEX9
D	-427	ASP	-	expression tag	UNP P0AEX9
D	-426	GLY	-	expression tag	UNP P0AEX9
D	-425	ASP	-	expression tag	UNP P0AEX9
D	-424	TYR	-	expression tag	UNP P0AEX9
D	-423	LYS	-	expression tag	UNP P0AEX9
D	-422	ASP	-	expression tag	UNP P0AEX9
D	-421	HIS	-	expression tag	UNP P0AEX9
D	-420	ASP	-	expression tag	UNP P0AEX9
D	-419	ILE	-	expression tag	UNP P0AEX9
D	-418	ASP	-	expression tag	UNP P0AEX9
D	-417	TYR	-	expression tag	UNP P0AEX9
D	-416	LYS	-	expression tag	UNP P0AEX9
D	-415	ASP	-	expression tag	UNP P0AEX9
D	-414	ASP	-	expression tag	UNP P0AEX9
D	-413	ASP	-	expression tag	UNP P0AEX9
D	-412	ASP	-	expression tag	UNP P0AEX9
D	-411	LYS	-	expression tag	UNP P0AEX9
D	-410	GLY	-	expression tag	UNP P0AEX9
D	-409	SER	-	expression tag	UNP P0AEX9
D	-408	ALA	-	expression tag	UNP P0AEX9
D	-407	ALA	-	expression tag	UNP P0AEX9
D	-406	ALA	-	expression tag	UNP P0AEX9
D	-405	MET	-	expression tag	UNP P0AEX9
D	-404	GLY	-	expression tag	UNP P0AEX9
D	-403	SER	-	expression tag	UNP P0AEX9
D	-402	SER	-	expression tag	UNP P0AEX9
D	-401	HIS	-	expression tag	UNP P0AEX9
D	-400	HIS	-	expression tag	UNP P0AEX9
D	-399	HIS	-	expression tag	UNP P0AEX9
D	-398	HIS	-	expression tag	UNP P0AEX9
D	-397	HIS	-	expression tag	UNP P0AEX9
D	-396	HIS	-	expression tag	UNP P0AEX9
D	-395	GLY	-	expression tag	UNP P0AEX9
D	-394	SER	-	expression tag	UNP P0AEX9
D	-393	SER	-	expression tag	UNP P0AEX9
D	-392	MET	-	expression tag	UNP P0AEX9
D	-25	ASN	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-24	SER	-	linker	UNP P0AEX9
D	-23	SER	-	linker	UNP P0AEX9
D	-22	SER	-	linker	UNP P0AEX9
D	-21	ASN	-	linker	UNP P0AEX9
D	-20	ASN	-	linker	UNP P0AEX9
D	-19	ASN	-	linker	UNP P0AEX9
D	-18	ASN	-	linker	UNP P0AEX9
D	-17	ASN	-	linker	UNP P0AEX9
D	-16	ASN	-	linker	UNP P0AEX9
D	-15	ASN	-	linker	UNP P0AEX9
D	-14	ASN	-	linker	UNP P0AEX9
D	-13	ASN	-	linker	UNP P0AEX9
D	-12	ASN	-	linker	UNP P0AEX9
D	-11	LEU	-	linker	UNP P0AEX9
D	-10	GLY	-	linker	UNP P0AEX9
D	-9	ILE	-	linker	UNP P0AEX9
D	-8	GLU	-	linker	UNP P0AEX9
D	-7	LEU	-	linker	UNP P0AEX9
D	-6	GLU	-	linker	UNP P0AEX9
D	-5	VAL	-	linker	UNP P0AEX9
D	-4	LEU	-	linker	UNP P0AEX9
D	-3	PHE	-	linker	UNP P0AEX9
D	-2	GLN	-	linker	UNP P0AEX9
D	-1	GLY	-	linker	UNP P0AEX9
D	0	PRO	-	linker	UNP P0AEX9

- Molecule 2 is a protein called Maltose/maltodextrin-binding periplasmic protein,Short transient receptor potential channel 1,Extended tegument protein pp150.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	651	Total	C	N	O	S	0	0
			5239	3393	866	943	37		

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-409	ALA	-	expression tag	UNP P0AEX9
B	-408	THR	-	expression tag	UNP P0AEX9
B	-407	MET	-	expression tag	UNP P0AEX9
B	-406	GLY	-	expression tag	UNP P0AEX9
B	-405	MET	-	expression tag	UNP P0AEX9
B	-404	GLY	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-403	SER	-	expression tag	UNP P0AEX9
B	-402	SER	-	expression tag	UNP P0AEX9
B	-401	HIS	-	expression tag	UNP P0AEX9
B	-400	HIS	-	expression tag	UNP P0AEX9
B	-399	HIS	-	expression tag	UNP P0AEX9
B	-398	HIS	-	expression tag	UNP P0AEX9
B	-397	HIS	-	expression tag	UNP P0AEX9
B	-396	HIS	-	expression tag	UNP P0AEX9
B	-395	GLY	-	expression tag	UNP P0AEX9
B	-394	SER	-	expression tag	UNP P0AEX9
B	-393	SER	-	expression tag	UNP P0AEX9
B	-392	MET	-	expression tag	UNP P0AEX9
B	-25	ASN	-	linker	UNP P0AEX9
B	-24	SER	-	linker	UNP P0AEX9
B	-23	SER	-	linker	UNP P0AEX9
B	-22	SER	-	linker	UNP P0AEX9
B	-21	ASN	-	linker	UNP P0AEX9
B	-20	ASN	-	linker	UNP P0AEX9
B	-19	ASN	-	linker	UNP P0AEX9
B	-18	ASN	-	linker	UNP P0AEX9
B	-17	ASN	-	linker	UNP P0AEX9
B	-16	ASN	-	linker	UNP P0AEX9
B	-15	ASN	-	linker	UNP P0AEX9
B	-14	ASN	-	linker	UNP P0AEX9
B	-13	ASN	-	linker	UNP P0AEX9
B	-12	ASN	-	linker	UNP P0AEX9
B	-11	LEU	-	linker	UNP P0AEX9
B	-10	GLY	-	linker	UNP P0AEX9
B	-9	ILE	-	linker	UNP P0AEX9
B	-8	GLU	-	linker	UNP P0AEX9
B	-7	LEU	-	linker	UNP P0AEX9
B	-6	GLU	-	linker	UNP P0AEX9
B	-5	VAL	-	linker	UNP P0AEX9
B	-4	LEU	-	linker	UNP P0AEX9
B	-3	PHE	-	linker	UNP P0AEX9
B	-2	GLN	-	linker	UNP P0AEX9
B	-1	GLY	-	linker	UNP P0AEX9
B	0	PRO	-	linker	UNP P0AEX9
B	794	GLY	-	linker	UNP P48995
B	795	GLY	-	linker	UNP P48995
B	796	GLY	-	linker	UNP P48995
B	797	SER	-	linker	UNP P48995

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Chain	Residue	Modelled	Actual	Comment	Reference
B	798	GLY	-	linker	UNP P48995
B	799	GLY	-	linker	UNP P48995
B	800	GLY	-	linker	UNP P48995
B	801	SER	-	linker	UNP P48995
B	802	GLY	-	linker	UNP P48995
B	803	GLY	-	linker	UNP P48995
B	804	GLY	-	linker	UNP P48995
B	805	SER	-	linker	UNP P48995
B	806	GLU	-	linker	UNP P48995
B	807	ASN	-	linker	UNP P48995
B	808	LEU	-	linker	UNP P48995
B	809	TYR	-	linker	UNP P48995
B	810	PHE	-	linker	UNP P48995
B	811	GLN	-	linker	UNP P48995
B	812	GLY	-	linker	UNP P48995
B	1058	GLY	-	expression tag	UNP A0A076JQ90
B	1059	SER	-	expression tag	UNP A0A076JQ90
B	1060	ALA	-	expression tag	UNP A0A076JQ90
B	1061	GLY	-	expression tag	UNP A0A076JQ90
B	1062	SER	-	expression tag	UNP A0A076JQ90
B	1063	ALA	-	expression tag	UNP A0A076JQ90
B	1064	GLY	-	expression tag	UNP A0A076JQ90
B	1065	SER	-	expression tag	UNP A0A076JQ90
B	1066	ALA	-	expression tag	UNP A0A076JQ90
B	1067	TRP	-	expression tag	UNP A0A076JQ90
B	1068	SER	-	expression tag	UNP A0A076JQ90
B	1069	HIS	-	expression tag	UNP A0A076JQ90
B	1070	PRO	-	expression tag	UNP A0A076JQ90
B	1071	GLN	-	expression tag	UNP A0A076JQ90
B	1072	PHE	-	expression tag	UNP A0A076JQ90
B	1073	GLU	-	expression tag	UNP A0A076JQ90
B	1074	LYS	-	expression tag	UNP A0A076JQ90
B	1075	GLY	-	expression tag	UNP A0A076JQ90
B	1076	GLY	-	expression tag	UNP A0A076JQ90
B	1077	GLY	-	expression tag	UNP A0A076JQ90
B	1078	SER	-	expression tag	UNP A0A076JQ90
B	1079	GLY	-	expression tag	UNP A0A076JQ90
B	1080	GLY	-	expression tag	UNP A0A076JQ90
B	1081	GLY	-	expression tag	UNP A0A076JQ90
B	1082	SER	-	expression tag	UNP A0A076JQ90
B	1083	GLY	-	expression tag	UNP A0A076JQ90
B	1084	GLY	-	expression tag	UNP A0A076JQ90

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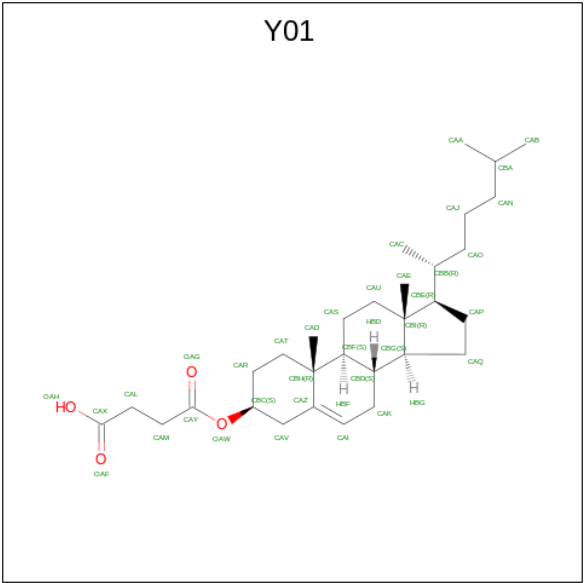
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Chain	Residue	Modelled	Actual	Comment	Reference
B	1085	GLY	-	expression tag	UNP A0A076JQ90
B	1086	SER	-	expression tag	UNP A0A076JQ90
B	1087	TRP	-	expression tag	UNP A0A076JQ90
B	1088	SER	-	expression tag	UNP A0A076JQ90
B	1089	HIS	-	expression tag	UNP A0A076JQ90
B	1090	PRO	-	expression tag	UNP A0A076JQ90
B	1091	GLN	-	expression tag	UNP A0A076JQ90
B	1092	PHE	-	expression tag	UNP A0A076JQ90
B	1093	GLU	-	expression tag	UNP A0A076JQ90
B	1094	LYS	-	expression tag	UNP A0A076JQ90

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

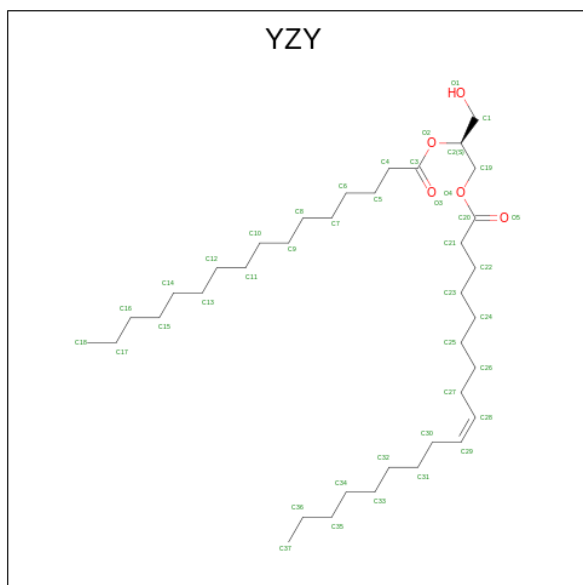
Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Ca 1 1	0
3	C	1	Total Ca 1 1	0
3	D	1	Total Ca 1 1	0

- Molecule 4 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄) (labeled as "Ligand of Interest" by depositor).

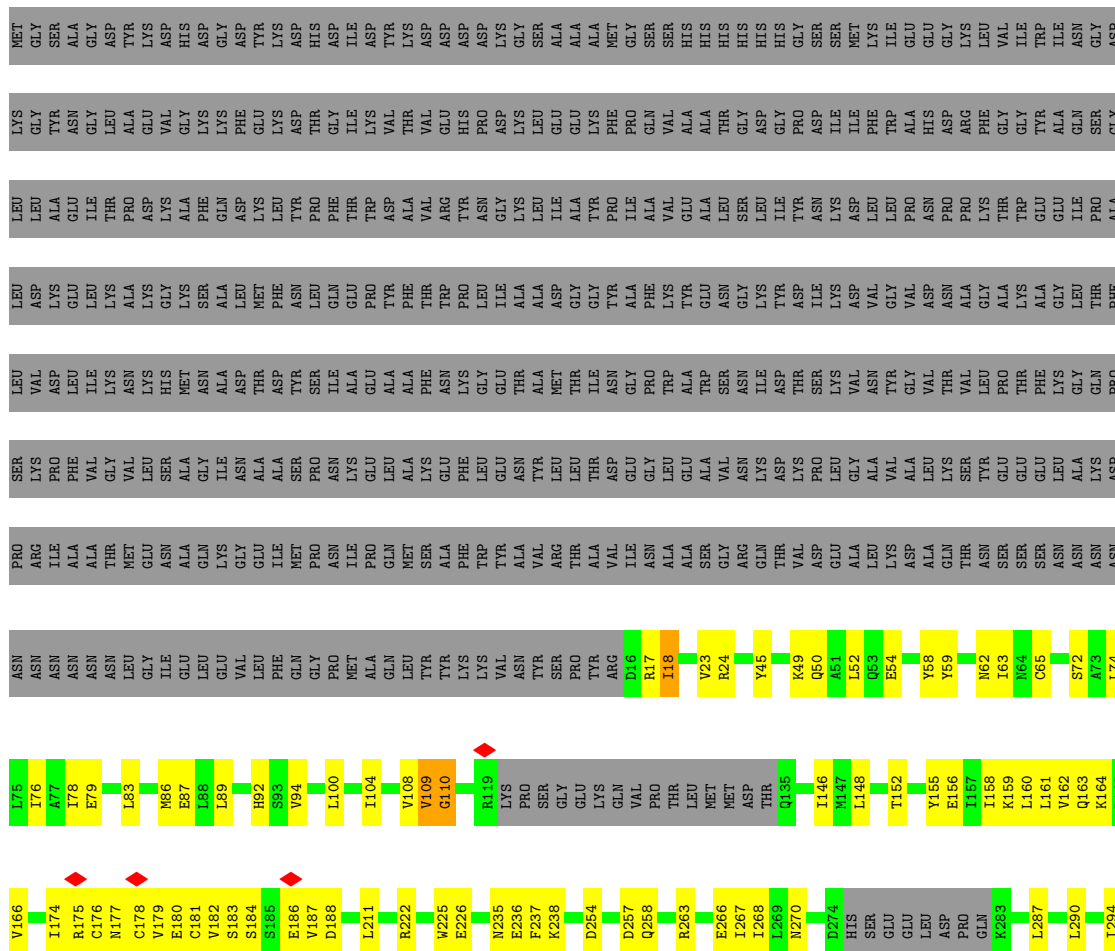


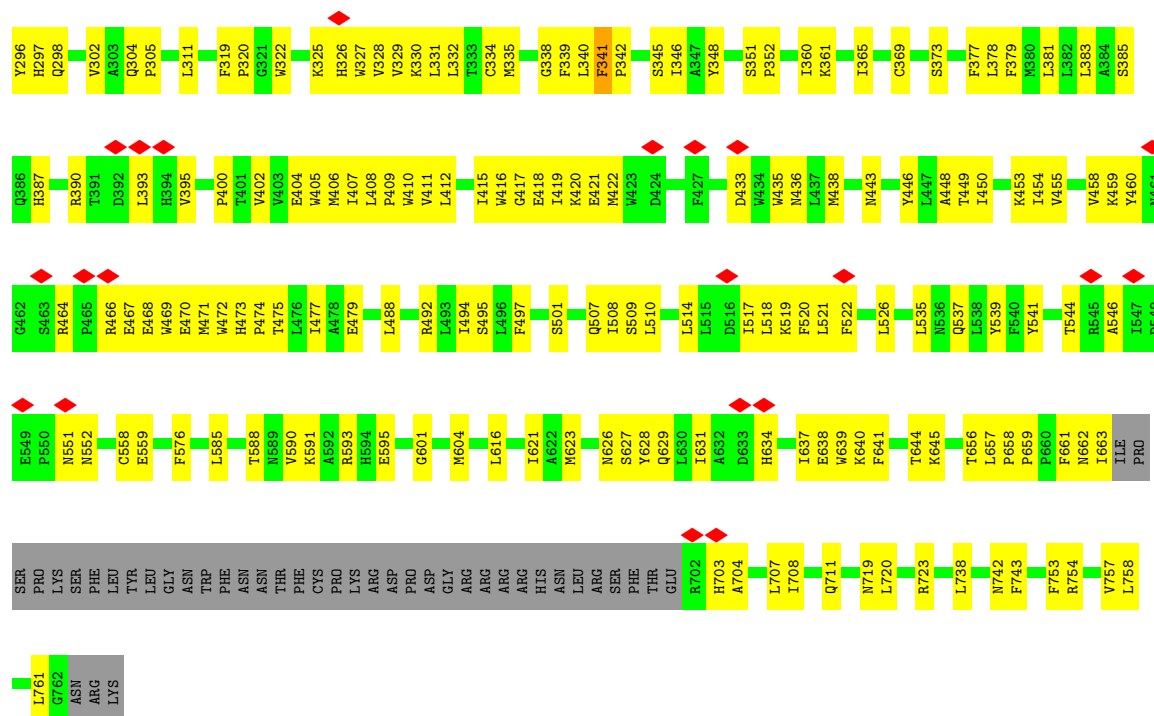
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			35	31	4	
4	C	1	Total	C	O	0
			35	31	4	
4	D	1	Total	C	O	0
			35	31	4	

- Molecule 5 is (2S)-2-(hexadecanoyloxy)-3-hydroxypropyl (9Z)-octadec-9-enoate (CCD ID: YZY) (formula: C₃₇H₇₀O₅) (labeled as "Ligand of Interest" by depositor).



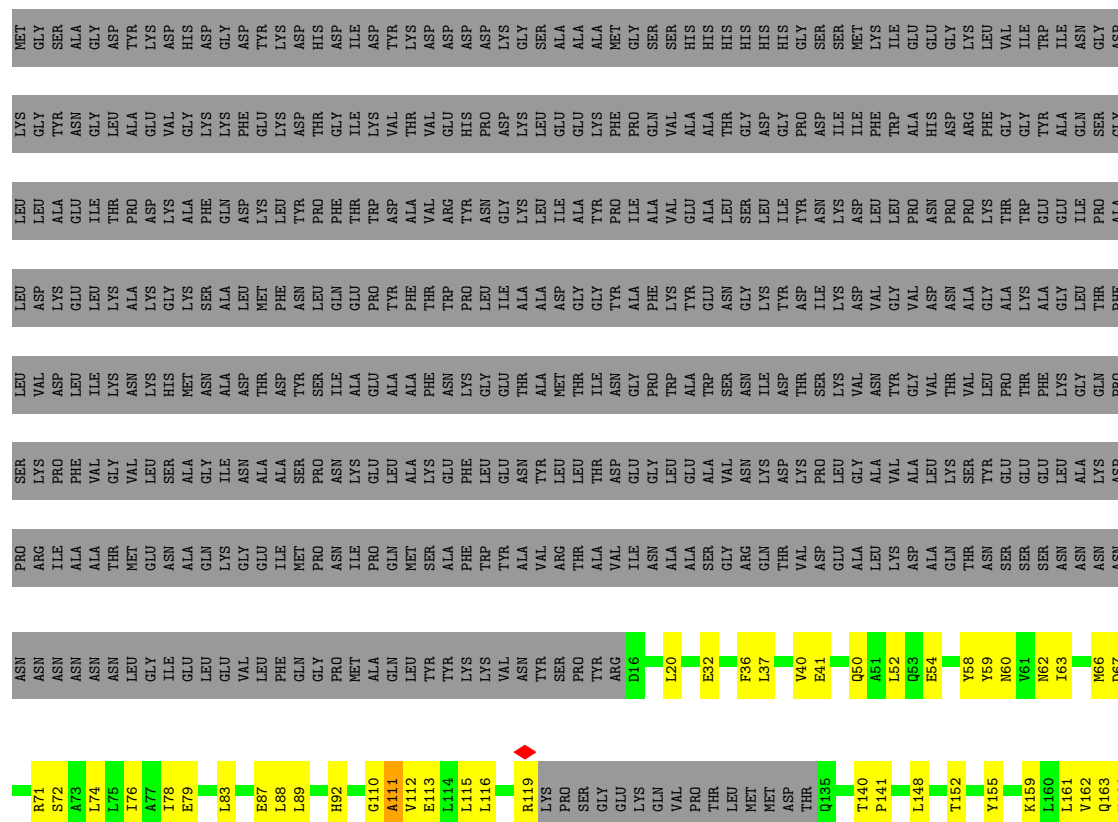
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			39	34	5	
5	B	1	Total	C	O	0
			39	34	5	
5	C	1	Total	C	O	0
			39	34	5	
5	C	1	Total	C	O	0
			39	34	5	

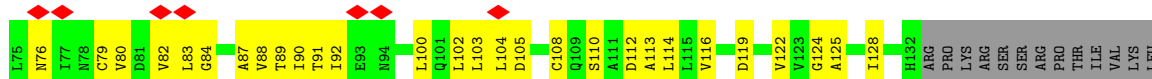


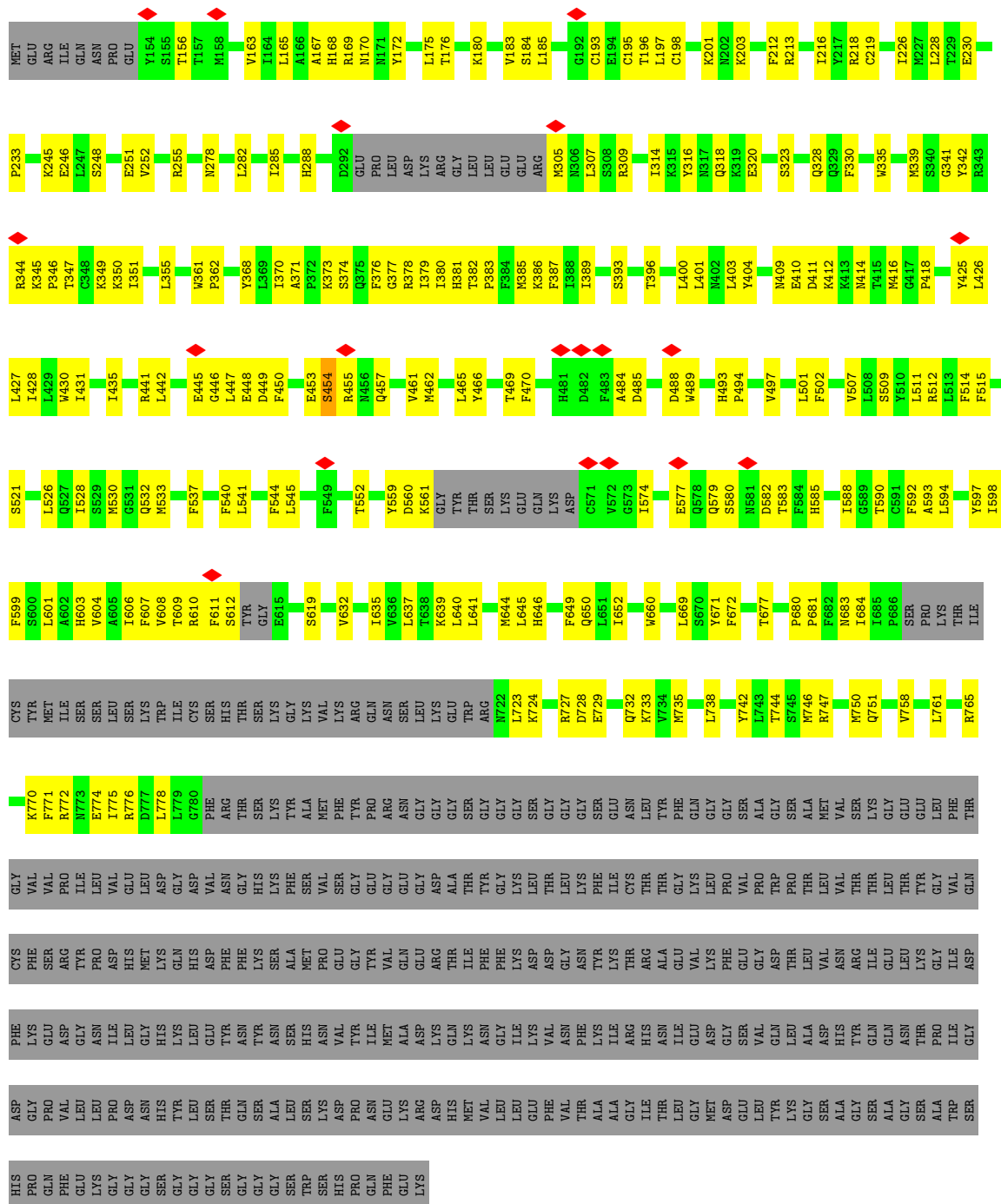


• Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Short transient receptor potential channel 5

Chain D: 38% 19% 43%







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	143788	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.516	Depositor
Minimum map value	-0.257	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	332.0, 332.0, 332.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: Y01, CA, YZY

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	0.66	0/5695	0.74	5/7725 (0.1%)
1	C	0.64	0/5695	0.70	3/7725 (0.0%)
1	D	0.67	1/5695 (0.0%)	0.70	7/7725 (0.1%)
2	B	0.64	0/5346	0.72	2/7228 (0.0%)
All	All	0.65	1/22431 (0.0%)	0.72	17/30403 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	385	SER	C-N	-5.08	1.26	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	GLY	N-CA-C	-7.97	103.06	115.73
1	D	111	ALA	N-CA-C	-7.04	104.81	113.19
1	A	109	VAL	N-CA-C	-6.36	106.25	111.91
2	B	608	VAL	N-CA-C	-6.17	105.70	112.80
1	C	110	GLY	N-CA-C	-5.99	106.92	114.16
2	B	454	SER	N-CA-C	5.81	117.29	111.07
1	A	457	TYR	N-CA-C	-5.61	105.17	111.28
1	D	341	PHE	CA-C-N	-5.24	113.23	119.05
1	D	341	PHE	C-N-CA	-5.24	113.23	119.05
1	D	457	TYR	N-CA-C	-5.24	105.47	111.07
1	A	658	PRO	CA-C-N	-5.11	115.11	120.38
1	A	658	PRO	C-N-CA	-5.11	115.11	120.38
1	D	658	PRO	N-CA-C	5.06	116.88	110.70
1	D	436	ASN	CA-C-N	-5.05	113.87	120.44
1	D	436	ASN	C-N-CA	-5.05	113.87	120.44
1	C	341	PHE	CA-C-N	-5.04	113.72	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	341	PHE	C-N-CA	-5.04	113.72	118.97

There are no chirality outliers.

There are no planarity outliers.

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	5563	0	5567	213	0
1	C	5563	0	5567	216	0
1	D	5563	0	5567	189	0
2	B	5239	0	5268	246	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	35	0	49	4	0
4	C	35	0	49	4	0
4	D	35	0	49	2	0
5	A	39	0	61	2	0
5	B	39	0	61	18	0
5	C	78	0	122	2	0
All	All	22192	0	22360	813	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 18.

All (813) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:592:PHE:HE1	5:B:1101:YZY:C4	1.60	1.12
2:B:592:PHE:CE1	5:B:1101:YZY:C5	2.43	1.01
1:A:20:LEU:HD11	2:B:185:LEU:HG	1.46	0.97
2:B:592:PHE:CE1	5:B:1101:YZY:C4	2.49	0.95
2:B:592:PHE:HE1	5:B:1101:YZY:C3	1.79	0.94
2:B:729:GLU:HG3	2:B:733:LYS:HE2	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:PHE:HB3	1:C:322:TRP:HB2	1.54	0.88
2:B:592:PHE:CD1	5:B:1101:YZY:H52	2.09	0.86
2:B:592:PHE:CE1	5:B:1101:YZY:C3	2.62	0.81
2:B:639:LYS:HD2	1:C:621:ILE:HG12	1.60	0.81
1:A:464:ARG:HH21	1:A:473:HIS:HD2	1.30	0.79
2:B:592:PHE:CE1	5:B:1101:YZY:H52	2.17	0.79
1:C:435:TRP:HZ3	1:C:492:ARG:HA	1.48	0.78
2:B:76:ASN:HB3	2:B:79:CYS:HB2	1.65	0.77
1:C:535:LEU:HD23	1:C:604:MET:HE3	1.66	0.77
1:D:535:LEU:HD23	1:D:604:MET:HE3	1.66	0.76
1:D:517:ILE:HG12	1:D:624:MET:HE2	1.69	0.75
1:A:327:TRP:CE2	1:A:328:VAL:HG23	2.21	0.75
1:D:387:HIS:HA	1:D:390:ARG:HB2	1.67	0.74
2:B:592:PHE:HE1	5:B:1101:YZY:H42	1.52	0.74
2:B:416:MET:HE2	2:B:489:TRP:CD1	2.23	0.74
2:B:373:LYS:HA	2:B:378:ARG:HE	1.52	0.73
1:A:386:GLN:HB2	1:A:388:ILE:HG12	1.68	0.73
1:A:656:THR:HG23	1:A:661:PHE:HD1	1.54	0.73
1:A:512:ARG:HB2	1:A:631:ILE:HD13	1.70	0.73
2:B:454:SER:HA	2:B:457:GLN:HG2	1.71	0.72
1:C:497:PHE:HE1	4:C:802:Y01:HAQ2	1.55	0.71
1:A:658:PRO:HA	1:A:661:PHE:HB2	1.73	0.71
2:B:305:MET:HA	2:B:305:MET:HE2	1.72	0.70
2:B:465:LEU:O	2:B:469:THR:HG23	1.92	0.70
1:D:319:PHE:HZ	1:D:365:ILE:HD11	1.57	0.69
1:D:657:LEU:HD12	1:D:657:LEU:H	1.58	0.69
1:D:703:HIS:NE2	1:D:707:LEU:HD21	2.08	0.69
1:D:360:ILE:HD11	1:D:369:CYS:SG	2.33	0.69
1:D:161:LEU:O	1:D:164:LYS:HG2	1.94	0.68
1:D:326:HIS:HB3	1:D:329:VAL:HG23	1.74	0.68
1:A:369:CYS:HB3	1:A:657:LEU:HD11	1.74	0.68
2:B:582:ASP:HA	2:B:585:HIS:ND1	2.09	0.68
1:C:174:ILE:HD12	1:C:174:ILE:H	1.59	0.68
1:C:326:HIS:HB3	1:C:329:VAL:HG23	1.74	0.68
1:C:369:CYS:HB3	1:C:657:LEU:HD21	1.76	0.68
1:C:263:ARG:O	1:C:266:GLU:HG2	1.94	0.68
1:C:373:SER:HB3	1:C:657:LEU:HD23	1.75	0.67
1:D:366:LYS:HA	1:D:369:CYS:SG	2.33	0.67
1:A:324:ARG:HD2	1:D:175:ARG:HA	1.75	0.66
1:D:319:PHE:CZ	1:D:365:ILE:HD11	2.31	0.66
1:C:327:TRP:HA	1:C:330:LYS:HE2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:SER:O	2:B:255:ARG:HG2	1.96	0.65
1:A:175:ARG:HA	2:B:344:ARG:HG2	1.78	0.65
1:D:176:CYS:HB2	1:D:179:VAL:HG23	1.78	0.65
2:B:119:ASP:HA	2:B:169:ARG:HD2	1.77	0.65
2:B:592:PHE:CE1	5:B:1101:YZY:H42	2.29	0.64
1:D:464:ARG:HH21	1:D:468:GLU:HB3	1.62	0.64
2:B:400:LEU:HB2	2:B:427:LEU:HD21	1.79	0.64
2:B:361:TRP:HB2	2:B:389:ILE:HG23	1.78	0.64
2:B:561:LYS:HA	1:C:390:ARG:HH12	1.63	0.64
2:B:431:ILE:HD13	2:B:466:TYR:HB3	1.78	0.64
1:A:179:VAL:HG23	1:A:182:VAL:HG22	1.80	0.64
1:C:657:LEU:H	1:C:657:LEU:HD12	1.62	0.63
1:A:331:LEU:O	1:A:335:MET:HG2	1.99	0.63
1:D:331:LEU:O	1:D:335:MET:HG2	1.99	0.63
1:C:146:ILE:HB	1:C:166:VAL:HG21	1.79	0.63
1:C:662:ASN:O	1:C:663:ILE:C	2.41	0.63
1:A:464:ARG:HH21	1:A:473:HIS:CD2	2.16	0.62
1:A:734:THR:O	1:A:735:ASN:OD1	2.17	0.62
2:B:102:LEU:HA	2:B:105:ASP:HB2	1.81	0.62
1:A:33:GLU:HG2	1:A:61:VAL:HG13	1.79	0.62
1:A:66:MET:HE3	1:A:72:SER:HB3	1.81	0.62
1:A:322:TRP:O	1:A:330:LYS:HE2	1.99	0.62
1:A:325:LYS:O	1:A:330:LYS:HE3	1.99	0.62
1:A:319:PHE:HZ	1:A:365:ILE:HD11	1.65	0.62
1:C:656:THR:HG23	1:C:661:PHE:HA	1.82	0.62
2:B:176:THR:HG22	2:B:180:LYS:HE2	1.82	0.61
1:D:508:ILE:HG21	1:D:638:GLU:HB3	1.81	0.61
1:D:381:LEU:HD23	1:D:407:ILE:HD13	1.83	0.61
2:B:195:CYS:HB3	2:B:197:LEU:HG	1.81	0.61
1:C:658:PRO:HA	1:C:661:PHE:HB2	1.82	0.61
1:A:175:ARG:HH21	2:B:346:PRO:HA	1.66	0.60
2:B:650:GLN:HE22	1:C:629:GLN:HE21	1.50	0.60
2:B:282:LEU:HD21	2:B:330:PHE:HB2	1.84	0.60
1:A:656:THR:HG23	1:A:661:PHE:CD1	2.36	0.60
1:A:18:ILE:HG12	2:B:185:LEU:O	2.00	0.60
1:D:180:GLU:HA	1:D:183:SER:HB3	1.83	0.60
1:A:497:PHE:HE1	4:A:802:Y01:HAQ2	1.66	0.60
2:B:772:ARG:HA	1:C:753:PHE:CE1	2.36	0.60
1:C:176:CYS:O	1:C:179:VAL:HG12	2.01	0.60
1:C:459:LYS:HG3	1:C:460:TYR:HD2	1.67	0.60
1:C:590:VAL:O	1:C:593:ARG:HD2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:PRO:O	1:C:346:ILE:HG13	2.02	0.60
1:D:408:LEU:HB3	1:D:409:PRO:HD3	1.83	0.60
1:C:634:HIS:HB3	1:C:637:ILE:HD11	1.84	0.60
1:A:401:THR:HG23	1:A:404:GLU:H	1.67	0.59
2:B:540:PHE:CZ	2:B:637:LEU:HB3	2.36	0.59
1:C:225:TRP:HZ3	1:C:297:HIS:HD1	1.50	0.59
1:D:155:TYR:CE1	1:D:211:LEU:HG	2.37	0.59
2:B:646:HIS:O	2:B:650:GLN:HG3	2.03	0.59
1:C:236:GLU:CD	1:C:236:GLU:H	2.10	0.59
2:B:335:TRP:HE3	2:B:672:PHE:HE1	1.51	0.59
1:D:345:SER:OG	1:D:657:LEU:HD13	2.02	0.59
1:A:394:HIS:ND1	1:A:465:PRO:HA	2.16	0.59
2:B:680:PRO:HA	2:B:683:ASN:ND2	2.18	0.59
1:A:543:GLU:HB3	1:A:566:SER:HB2	1.83	0.59
1:C:495:SER:HA	1:C:507:GLN:HE22	1.66	0.59
1:D:369:CYS:SG	1:D:657:LEU:HD11	2.43	0.59
1:A:304:GLN:HE22	1:A:306:ASN:CG	2.10	0.59
1:A:464:ARG:HG3	1:A:469:TRP:NE1	2.18	0.59
2:B:580:SER:O	2:B:583:THR:HG23	2.02	0.59
1:C:268:ILE:HD11	1:C:720:LEU:HD11	1.85	0.59
1:A:497:PHE:HE1	4:A:802:Y01:CAQ	2.16	0.58
1:C:514:LEU:HD23	1:C:517:ILE:HD12	1.85	0.58
1:C:108:VAL:HG13	1:C:110:GLY:H	1.69	0.58
1:C:155:TYR:CE1	1:C:211:LEU:HG	2.38	0.58
1:A:322:TRP:HD1	1:A:325:LYS:HZ2	1.51	0.58
2:B:540:PHE:CE1	2:B:637:LEU:HB3	2.38	0.58
1:A:254:ASP:O	1:A:258:GLN:HG2	2.03	0.58
1:A:377:PHE:HE1	1:A:407:ILE:HG23	1.68	0.58
1:D:76:ILE:O	1:D:79:GLU:HG2	2.03	0.58
1:A:319:PHE:CZ	1:A:365:ILE:HD11	2.39	0.58
2:B:196:THR:O	2:B:197:LEU:C	2.46	0.58
2:B:724:LYS:HA	2:B:727:ARG:NE	2.18	0.58
1:D:520:PHE:CZ	1:D:616:LEU:HB3	2.37	0.58
2:B:635:ILE:O	2:B:639:LYS:HG2	2.03	0.58
1:C:508:ILE:HG21	1:C:638:GLU:HB3	1.85	0.58
2:B:644:MET:HA	1:C:628:TYR:CZ	2.39	0.58
1:A:579:VAL:HA	1:A:613:LEU:HD21	1.86	0.58
2:B:56:ASP:HB2	2:B:90:ILE:HD11	1.86	0.58
1:A:168:ILE:HG13	1:D:20:LEU:HD11	1.85	0.57
1:A:268:ILE:HD11	1:A:720:LEU:HD11	1.85	0.57
1:A:508:ILE:O	1:A:512:ARG:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:559:TYR:HA	2:B:610:ARG:HH22	1.69	0.57
2:B:592:PHE:CE1	5:B:1101:YZY:H51	2.33	0.57
1:A:176:CYS:O	1:A:179:VAL:HG22	2.03	0.57
2:B:335:TRP:HA	2:B:383:PRO:HG2	1.84	0.57
2:B:314:ILE:HD12	2:B:669:LEU:HD22	1.85	0.57
2:B:544:PHE:CZ	2:B:598:ILE:HD11	2.39	0.57
2:B:724:LYS:HA	2:B:727:ARG:HE	1.68	0.57
1:C:406:MET:O	1:C:409:PRO:HD2	2.04	0.57
1:D:517:ILE:O	1:D:521:LEU:HG	2.04	0.57
2:B:378:ARG:HA	2:B:381:HIS:ND1	2.20	0.57
1:C:45:TYR:HE1	1:C:49:LYS:HD2	1.70	0.57
1:C:188:ASP:HA	1:D:262:SER:OG	2.03	0.57
1:C:319:PHE:CB	1:C:322:TRP:HB2	2.32	0.57
1:D:392:ASP:HB3	1:D:394:HIS:CD2	2.40	0.57
1:D:657:LEU:HD12	1:D:657:LEU:N	2.20	0.57
2:B:52:LEU:HG	2:B:53:LEU:H	1.69	0.57
2:B:376:PHE:HA	2:B:379:ILE:HG12	1.87	0.57
2:B:744:THR:HG22	2:B:747:ARG:HH21	1.69	0.57
1:C:520:PHE:HB2	1:C:623:MET:HE1	1.86	0.57
1:C:703:HIS:O	1:C:707:LEU:HG	2.05	0.57
2:B:425:TYR:O	2:B:428:ILE:HB	2.04	0.56
2:B:347:THR:O	2:B:351:ILE:HG12	2.04	0.56
1:C:236:GLU:HG2	1:C:237:PHE:HD1	1.70	0.56
1:C:657:LEU:HD12	1:C:657:LEU:N	2.21	0.56
1:D:41:GLU:HG2	1:D:76:ILE:HG21	1.88	0.56
2:B:598:ILE:HG21	5:B:1101:YZY:H171	1.88	0.56
1:C:416:TRP:HA	1:C:419:ILE:HD12	1.86	0.56
1:D:345:SER:O	1:D:349:LEU:HG	2.04	0.56
2:B:560:ASP:HB3	1:C:387:HIS:CE1	2.40	0.56
1:C:435:TRP:HH2	1:C:494:ILE:HB	1.71	0.56
1:D:506:LEU:O	1:D:510:LEU:HG	2.06	0.56
1:A:520:PHE:CZ	1:A:616:LEU:HB3	2.41	0.56
2:B:91:THR:OG1	2:B:100:LEU:HD21	2.06	0.56
2:B:598:ILE:HD13	5:B:1101:YZY:H171	1.88	0.56
1:C:89:LEU:O	1:C:94:VAL:HG23	2.05	0.56
1:C:517:ILE:O	1:C:521:LEU:HG	2.06	0.56
1:D:406:MET:O	1:D:409:PRO:HD2	2.06	0.56
1:C:290:LEU:HD21	1:C:311:LEU:HD11	1.87	0.56
1:A:754:ARG:HA	2:B:771:PHE:CZ	2.41	0.56
1:D:640:LYS:O	1:D:644:THR:HG23	2.06	0.56
1:A:738:LEU:HD22	1:D:743:PHE:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:GLY:C	1:D:112:VAL:H	2.13	0.56
1:C:497:PHE:HE1	4:C:802:Y01:CAQ	2.18	0.55
1:C:519:LYS:HA	1:C:522:PHE:CD2	2.41	0.55
2:B:335:TRP:CE3	2:B:383:PRO:HB2	2.41	0.55
1:C:179:VAL:HG13	1:C:182:VAL:H	1.70	0.55
1:A:423:TRP:HD1	1:A:424:ASP:OD1	1.90	0.55
1:A:464:ARG:HG3	1:A:469:TRP:CD1	2.41	0.55
1:A:464:ARG:CZ	1:A:469:TRP:HA	2.36	0.55
1:A:517:ILE:O	1:A:521:LEU:HG	2.06	0.55
1:C:381:LEU:HD23	1:C:407:ILE:HD13	1.89	0.55
1:C:470:GLU:CD	1:C:470:GLU:H	2.14	0.55
2:B:592:PHE:CE1	5:B:1101:YZY:O2	2.60	0.55
1:C:348:TYR:HE1	1:C:361:LYS:HE2	1.71	0.55
1:C:464:ARG:HG3	1:C:469:TRP:NE1	2.21	0.55
1:A:290:LEU:HD21	1:A:311:LEU:HD11	1.89	0.55
1:A:290:LEU:CD2	1:A:311:LEU:HD21	2.36	0.55
2:B:156:THR:HB	2:B:212:PHE:HD1	1.72	0.55
2:B:380:ILE:HD13	2:B:677:THR:HG22	1.89	0.55
1:C:435:TRP:CZ3	1:C:492:ARG:HA	2.37	0.55
1:A:311:LEU:HD22	1:A:651:PHE:HE2	1.72	0.55
1:A:406:MET:O	1:A:409:PRO:HD2	2.06	0.55
1:C:418:GLU:O	1:C:422:MET:HG3	2.07	0.55
1:D:52:LEU:HD11	1:D:89:LEU:HD23	1.88	0.55
1:D:355:ASN:HA	1:D:358:LEU:HD12	1.88	0.55
1:D:449:THR:O	1:D:453:LYS:HG2	2.07	0.55
1:A:734:THR:C	1:A:735:ASN:OD1	2.49	0.55
1:D:369:CYS:HB2	1:D:657:LEU:HD21	1.89	0.55
1:D:415:ILE:O	1:D:419:ILE:HG12	2.06	0.55
1:C:258:GLN:HB3	1:C:723:ARG:HG3	1.88	0.55
1:D:322:TRP:HE3	1:D:325:LYS:HZ2	1.55	0.55
1:A:520:PHE:HD1	2:B:530:MET:HE1	1.72	0.55
1:A:471:MET:HE3	1:A:472:TRP:NE1	2.23	0.54
2:B:454:SER:O	2:B:457:GLN:HG2	2.07	0.54
1:C:405:TRP:O	1:C:409:PRO:HD3	2.06	0.54
1:A:373:SER:HB3	1:A:657:LEU:HD23	1.89	0.54
2:B:288:HIS:O	2:B:309:ARG:HG2	2.07	0.54
2:B:592:PHE:HD1	5:B:1101:YZY:H52	1.70	0.54
1:C:174:ILE:HG22	1:C:175:ARG:HG3	1.89	0.54
2:B:541:LEU:O	2:B:545:LEU:HG	2.08	0.54
2:B:746:MET:HB3	2:B:750:MET:HE3	1.90	0.54
1:C:319:PHE:HZ	1:C:365:ILE:HD11	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:GLU:OE1	1:D:60:ASN:HB2	2.06	0.54
1:A:108:VAL:HG12	1:A:110:GLY:H	1.72	0.54
2:B:532:GLN:HB2	2:B:652:ILE:HD13	1.89	0.54
1:A:324:ARG:HB3	1:D:175:ARG:HG2	1.89	0.54
1:A:326:HIS:HB3	1:A:329:VAL:HG23	1.90	0.54
1:C:420:LYS:HD3	1:C:661:PHE:CZ	2.42	0.54
1:A:705:ASP:O	1:A:709:GLN:HG2	2.08	0.54
1:A:322:TRP:CD1	1:A:325:LYS:HZ2	2.26	0.54
1:A:523:ILE:HG23	2:B:514:PHE:HE2	1.72	0.54
1:C:464:ARG:HD3	1:C:468:GLU:HB2	1.89	0.54
2:B:361:TRP:N	2:B:362:PRO:HD2	2.23	0.53
1:D:110:GLY:C	1:D:112:VAL:N	2.66	0.53
2:B:552:THR:HG23	2:B:590:THR:HB	1.89	0.53
1:D:321:GLY:O	1:D:325:LYS:HG3	2.08	0.53
1:A:703:HIS:O	1:A:707:LEU:HG	2.09	0.53
1:D:348:TYR:HE1	1:D:361:LYS:HE2	1.74	0.53
1:A:37:LEU:HD13	1:A:67:ASP:OD1	2.08	0.53
1:A:155:TYR:CE1	1:A:211:LEU:HG	2.43	0.53
1:A:180:GLU:HA	1:A:183:SER:HB3	1.91	0.53
2:B:598:ILE:HG21	5:B:1101:YZY:C17	2.39	0.53
1:D:392:ASP:HB2	1:D:395:VAL:HG12	1.90	0.53
1:A:377:PHE:CE1	1:A:407:ILE:HG23	2.44	0.53
1:C:743:PHE:HB2	1:D:738:LEU:HD22	1.90	0.53
1:A:381:LEU:HD23	1:A:407:ILE:HD13	1.91	0.53
4:A:802:Y01:OAH	4:A:802:Y01:OAW	2.27	0.53
2:B:598:ILE:HD13	5:B:1101:YZY:H151	1.91	0.53
1:C:473:HIS:CG	1:C:474:PRO:HD2	2.44	0.53
1:A:74:LEU:O	1:A:78:ILE:HG13	2.09	0.53
1:A:327:TRP:CZ2	1:A:328:VAL:CG2	2.92	0.53
1:A:410:TRP:H	1:A:410:TRP:CD1	2.27	0.53
2:B:469:THR:HG21	2:B:502:PHE:HA	1.90	0.53
1:C:17:ARG:NH1	1:D:169:PRO:HG3	2.24	0.52
2:B:361:TRP:HH2	2:B:681:PRO:HG3	1.74	0.52
1:D:348:TYR:HB2	1:D:360:ILE:HG21	1.91	0.52
1:D:657:LEU:H	1:D:657:LEU:CD1	2.22	0.52
1:A:504:GLY:O	1:A:508:ILE:HG12	2.09	0.52
1:A:741:GLU:HB3	2:B:751:GLN:HG3	1.90	0.52
2:B:410:GLU:H	2:B:410:GLU:CD	2.17	0.52
1:C:501:SER:HA	1:C:639:TRP:CZ2	2.43	0.52
1:D:650:TYR:C	1:D:652:ASP:H	2.15	0.52
1:A:29:LEU:HD13	1:A:37:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:O	1:A:87:GLU:HG3	2.09	0.52
2:B:100:LEU:HD22	2:B:104:LEU:HD11	1.91	0.52
2:B:285:ILE:HD11	2:B:738:LEU:HD11	1.91	0.52
2:B:588:ILE:HG22	2:B:592:PHE:CZ	2.44	0.52
1:C:159:LYS:O	1:C:163:GLN:HG3	2.08	0.52
1:D:199:ILE:O	1:D:203:LEU:HG	2.09	0.52
1:A:707:LEU:O	1:A:711:GLN:HG3	2.09	0.52
1:C:417:GLY:O	1:C:421:GLU:HG3	2.09	0.52
1:C:458:VAL:HG23	1:C:459:LYS:H	1.75	0.52
1:C:641:PHE:O	1:C:645:LYS:HG3	2.10	0.52
1:D:322:TRP:HA	1:D:325:LYS:HD2	1.91	0.52
2:B:195:CYS:C	2:B:197:LEU:N	2.66	0.52
2:B:462:MET:HE1	2:B:512:ARG:HD2	1.91	0.52
2:B:644:MET:HA	1:C:628:TYR:CE2	2.44	0.52
1:C:290:LEU:HD11	1:C:302:VAL:HG13	1.92	0.52
1:A:342:PRO:O	1:A:346:ILE:HG13	2.09	0.52
1:A:520:PHE:CE1	1:A:616:LEU:HB3	2.45	0.52
2:B:70:ASN:O	2:B:71:SER:C	2.51	0.52
2:B:683:ASN:OD1	2:B:684:ILE:N	2.42	0.52
1:C:76:ILE:O	1:C:79:GLU:HG2	2.10	0.52
1:D:37:LEU:O	1:D:41:GLU:HG3	2.10	0.52
1:A:328:VAL:O	1:A:332:LEU:HG	2.10	0.52
1:A:395:VAL:HG13	1:A:398:PRO:HB3	1.92	0.52
1:A:506:LEU:O	1:A:510:LEU:HG	2.09	0.52
1:D:589:ASN:HA	1:D:598:GLU:HG2	1.91	0.52
2:B:226:ILE:HG23	2:B:230:GLU:HG3	1.92	0.52
2:B:454:SER:O	2:B:455:ARG:C	2.52	0.52
1:C:319:PHE:CZ	1:C:365:ILE:HD11	2.45	0.52
1:C:385:SER:C	1:C:387:HIS:H	2.17	0.52
1:C:754:ARG:O	1:C:758:LEU:HG	2.09	0.52
1:C:331:LEU:O	1:C:335:MET:HG2	2.10	0.52
4:C:802:Y01:OAW	4:C:802:Y01:OAH	2.27	0.52
2:B:412:LYS:HD3	2:B:418:PRO:HB2	1.92	0.51
1:D:373:SER:HB2	1:D:657:LEU:HD23	1.92	0.51
4:D:802:Y01:OAH	4:D:802:Y01:OAW	2.27	0.51
2:B:307:LEU:HD21	2:B:330:PHE:HE1	1.75	0.51
2:B:339:MET:HG3	2:B:385:MET:HE2	1.92	0.51
1:D:565:PHE:HD1	1:D:571:THR:HG23	1.75	0.51
1:A:380:MET:HE2	1:A:380:MET:HA	1.92	0.51
2:B:112:ASP:O	2:B:116:VAL:HG23	2.10	0.51
2:B:453:GLU:OE2	2:B:455:ARG:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:TRP:HA	1:D:330:LYS:HE2	1.92	0.51
1:D:430:TYR:CE1	1:D:436:ASN:HB3	2.45	0.51
2:B:431:ILE:O	2:B:435:ILE:HG13	2.11	0.51
2:B:574:ILE:HD12	2:B:574:ILE:H	1.75	0.51
1:A:511:GLY:HA2	1:A:514:LEU:HD12	1.93	0.51
1:A:641:PHE:O	1:A:645:LYS:HG3	2.11	0.51
2:B:252:VAL:HA	2:B:255:ARG:HG3	1.92	0.51
1:C:640:LYS:O	1:C:644:THR:HG23	2.11	0.51
2:B:87:ALA:HB3	2:B:108:CYS:SG	2.51	0.51
2:B:577:GLU:CD	2:B:577:GLU:H	2.19	0.51
2:B:592:PHE:CD1	5:B:1101:YZY:C5	2.79	0.51
1:C:514:LEU:O	1:C:518:LEU:HG	2.11	0.51
1:A:465:PRO:HB3	1:A:467:GLU:OE2	2.11	0.51
2:B:462:MET:HE2	2:B:509:SER:HA	1.93	0.51
1:C:416:TRP:NE1	1:C:420:LYS:HD2	2.25	0.51
1:C:433:ASP:HB3	1:C:436:ASN:ND2	2.25	0.51
2:B:58:GLY:O	2:B:770:LYS:HE2	2.10	0.51
1:D:83:LEU:O	1:D:87:GLU:HG3	2.11	0.51
1:A:537:GLN:HE22	2:B:404:TYR:HE2	1.56	0.51
2:B:771:PHE:CZ	2:B:775:ILE:HD11	2.46	0.51
1:C:24:ARG:NH2	1:D:213:SER:O	2.44	0.51
2:B:574:ILE:HG23	2:B:604:VAL:HG22	1.93	0.51
1:C:707:LEU:O	1:C:711:GLN:HG3	2.11	0.51
1:D:62:ASN:O	1:D:63:ILE:C	2.54	0.51
1:D:348:TYR:CE1	1:D:361:LYS:HE2	2.46	0.51
1:A:471:MET:HE3	1:A:472:TRP:HE1	1.76	0.50
2:B:307:LEU:HD21	2:B:330:PHE:CE1	2.46	0.50
1:C:63:ILE:HG21	1:C:94:VAL:HG22	1.93	0.50
1:A:173:GLN:O	1:A:176:CYS:HB2	2.11	0.50
1:A:315:TRP:HE3	1:A:651:PHE:CE1	2.29	0.50
1:A:418:GLU:O	1:A:422:MET:HG3	2.11	0.50
1:A:514:LEU:O	1:A:518:LEU:HG	2.11	0.50
1:C:761:LEU:HD22	1:D:761:LEU:HD21	1.92	0.50
2:B:88:VAL:O	2:B:92:ILE:HG13	2.11	0.50
2:B:346:PRO:HD2	2:B:349:LYS:HD2	1.93	0.50
1:D:236:GLU:CD	1:D:236:GLU:H	2.19	0.50
1:D:703:HIS:O	1:D:707:LEU:HG	2.11	0.50
1:A:519:LYS:HA	1:A:522:PHE:CD2	2.47	0.50
1:D:66:MET:HE3	1:D:72:SER:HB3	1.92	0.50
1:A:257:ASP:OD1	1:A:304:GLN:HG3	2.11	0.50
2:B:609:THR:HA	2:B:619:SER:OG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:GLY:O	1:D:341:PHE:HD2	1.94	0.50
1:D:519:LYS:HA	1:D:522:PHE:CD2	2.47	0.50
1:A:188:ASP:OD2	2:B:278:ASN:HB2	2.12	0.50
2:B:342:TYR:O	2:B:350:LYS:HD3	2.11	0.50
2:B:351:ILE:O	2:B:355:LEU:HG	2.11	0.50
2:B:729:GLU:O	2:B:733:LYS:HG3	2.12	0.50
2:B:122:VAL:HB	2:B:125:ALA:HB3	1.93	0.50
1:A:54:GLU:HB3	1:A:58:TYR:HD2	1.77	0.50
1:A:551:ASN:O	1:A:552:ASN:C	2.55	0.50
2:B:233:PRO:HD2	2:B:735:MET:HG2	1.93	0.50
1:D:410:TRP:H	1:D:410:TRP:CD1	2.29	0.50
1:C:411:VAL:O	1:C:415:ILE:HG12	2.12	0.50
1:D:467:GLU:H	1:D:467:GLU:CD	2.19	0.50
2:B:80:VAL:HB	2:B:84:GLY:HA2	1.94	0.49
1:C:626:ASN:HD22	1:D:628:TYR:HE2	1.59	0.49
1:D:389:VAL:HB	1:D:401:THR:HB	1.94	0.49
1:A:393:LEU:HD22	1:D:541:TYR:HD1	1.77	0.49
1:A:487:ILE:HD11	1:D:604:MET:SD	2.53	0.49
1:A:497:PHE:CE1	4:A:802:Y01:HAQ2	2.47	0.49
1:A:600:VAL:O	1:A:604:MET:HG3	2.12	0.49
2:B:454:SER:HA	2:B:457:GLN:CG	2.41	0.49
2:B:560:ASP:O	2:B:561:LYS:C	2.53	0.49
1:D:290:LEU:CD2	1:D:311:LEU:HD21	2.42	0.49
1:A:354:SER:O	1:A:358:LEU:HG	2.12	0.49
1:A:644:THR:O	1:A:648:MET:HG2	2.12	0.49
1:D:159:LYS:HE2	1:D:211:LEU:HD21	1.93	0.49
1:A:159:LYS:O	1:A:163:GLN:HG3	2.13	0.49
1:A:611:ILE:O	1:A:615:VAL:HB	2.13	0.49
1:C:585:LEU:O	1:C:588:THR:HG22	2.13	0.49
1:A:341:PHE:N	1:A:342:PRO:HD2	2.28	0.49
2:B:574:ILE:CG2	2:B:604:VAL:HG22	2.42	0.49
1:D:620:LEU:HG	1:D:624:MET:HE3	1.95	0.49
1:D:650:TYR:C	1:D:652:ASP:N	2.68	0.49
1:D:704:ALA:O	1:D:708:ILE:HG13	2.12	0.49
1:A:585:LEU:O	1:A:588:THR:HG22	2.12	0.49
2:B:361:TRP:CD1	2:B:362:PRO:HD3	2.48	0.49
1:D:119:ARG:NE	1:D:119:ARG:HA	2.28	0.49
2:B:100:LEU:HA	2:B:103:LEU:HB3	1.95	0.49
2:B:387:PHE:HD1	2:B:671:TYR:CZ	2.30	0.49
2:B:484:ALA:HB1	2:B:488:ASP:OD2	2.13	0.49
1:C:410:TRP:CD1	1:C:410:TRP:H	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:626:ASN:O	1:D:630:LEU:HG	2.13	0.49
1:D:707:LEU:O	1:D:711:GLN:HG3	2.13	0.49
2:B:646:HIS:CD2	2:B:650:GLN:HE21	2.31	0.49
1:C:657:LEU:H	1:C:657:LEU:CD1	2.26	0.49
1:D:357:GLY:O	1:D:360:ILE:HG22	2.13	0.49
1:C:100:LEU:O	1:C:104:ILE:HG13	2.12	0.49
1:D:551:ASN:O	1:D:552:ASN:C	2.56	0.49
1:C:475:THR:O	1:C:479:GLU:HG3	2.13	0.48
1:D:171:PRO:HG3	1:D:199:ILE:HG21	1.94	0.48
1:D:179:VAL:O	1:D:180:GLU:HB3	2.12	0.48
1:A:341:PHE:CD2	1:A:342:PRO:HD3	2.47	0.48
1:A:365:ILE:O	1:A:366:LYS:C	2.53	0.48
1:C:270:ASN:OD1	1:C:287:LEU:HD23	2.12	0.48
1:C:387:HIS:CD2	1:C:390:ARG:HH21	2.32	0.48
1:C:551:ASN:O	1:C:552:ASN:C	2.56	0.48
1:A:174:ILE:HG21	1:A:233:VAL:HG21	1.94	0.48
1:A:560:LYS:NZ	2:B:577:GLU:HB3	2.28	0.48
2:B:521:SER:HA	2:B:660:TRP:CZ2	2.49	0.48
1:C:402:VAL:HA	1:C:405:TRP:HD1	1.77	0.48
1:C:588:THR:HG21	1:D:557:ARG:HD2	1.94	0.48
2:B:113:ALA:O	2:B:114:LEU:C	2.55	0.48
1:D:520:PHE:HZ	1:D:616:LEU:HB3	1.77	0.48
1:D:613:LEU:O	1:D:617:LEU:HB3	2.12	0.48
1:A:72:SER:O	1:A:76:ILE:HG13	2.14	0.48
1:A:730:ARG:O	1:A:734:THR:HG23	2.12	0.48
1:C:390:ARG:NH1	1:C:393:LEU:HD21	2.28	0.48
1:D:535:LEU:CD2	1:D:604:MET:HE3	2.38	0.48
1:A:738:LEU:HD21	1:D:739:THR:O	2.13	0.48
1:D:389:VAL:HG21	1:D:402:VAL:HB	1.96	0.48
1:D:514:LEU:HD23	1:D:517:ILE:HD12	1.94	0.48
2:B:102:LEU:C	2:B:105:ASP:H	2.22	0.48
2:B:195:CYS:SG	2:B:197:LEU:HG	2.54	0.48
2:B:320:GLU:H	2:B:320:GLU:CD	2.22	0.48
2:B:416:MET:HE3	2:B:484:ALA:HB3	1.95	0.48
2:B:493:HIS:CG	2:B:494:PRO:HD2	2.48	0.48
1:C:62:ASN:O	1:C:63:ILE:C	2.56	0.48
1:D:67:ASP:HB2	1:D:71:ARG:HG3	1.94	0.48
1:A:327:TRP:CZ2	1:A:328:VAL:HG23	2.49	0.48
1:A:369:CYS:HB3	1:A:657:LEU:HD21	1.96	0.48
1:D:662:ASN:O	1:D:663:ILE:C	2.56	0.48
1:A:360:ILE:HA	1:A:365:ILE:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:370:ILE:HG13	2:B:371:ALA:N	2.29	0.48
2:B:385:MET:O	2:B:386:LYS:C	2.53	0.48
1:C:179:VAL:HG22	1:C:181:CYS:HB2	1.96	0.48
1:C:438:MET:HE2	1:C:488:LEU:O	2.14	0.48
1:C:471:MET:HE3	1:C:472:TRP:NE1	2.29	0.48
1:A:451:SER:O	1:A:455:VAL:HG23	2.13	0.48
1:A:657:LEU:HD12	1:A:657:LEU:N	2.29	0.48
2:B:374:SER:O	2:B:378:ARG:HG2	2.14	0.48
1:C:72:SER:O	1:C:76:ILE:HG13	2.14	0.48
1:D:263:ARG:O	1:D:267:ILE:HG13	2.13	0.48
1:D:354:SER:O	1:D:358:LEU:HG	2.14	0.48
2:B:611:PHE:O	2:B:612:SER:C	2.57	0.47
1:C:435:TRP:CH2	1:C:494:ILE:HB	2.48	0.47
1:D:501:SER:HA	1:D:639:TRP:CZ2	2.49	0.47
2:B:252:VAL:O	2:B:255:ARG:HG3	2.14	0.47
1:C:459:LYS:HG3	1:C:460:TYR:CD2	2.47	0.47
1:D:460:TYR:CE1	1:D:474:PRO:HG3	2.49	0.47
1:A:270:ASN:OD1	1:A:287:LEU:HD23	2.14	0.47
1:A:534:GLY:C	1:A:604:MET:HE1	2.38	0.47
2:B:88:VAL:HG11	2:B:110:SER:HB3	1.95	0.47
1:C:377:PHE:CE1	1:C:407:ILE:HG23	2.50	0.47
1:C:459:LYS:O	1:C:460:TYR:C	2.56	0.47
1:D:112:VAL:O	1:D:116:LEU:HD13	2.14	0.47
1:C:345:SER:OG	1:C:657:LEU:HD13	2.12	0.47
1:C:576:PHE:CE2	5:C:804:YZY:H192	2.49	0.47
1:D:50:GLN:HG2	1:D:54:GLU:OE2	2.14	0.47
1:D:111:ALA:C	1:D:113:GLU:N	2.71	0.47
1:D:446:TYR:O	1:D:450:ILE:HG13	2.15	0.47
1:A:442:MET:HG3	1:A:446:TYR:CE2	2.49	0.47
2:B:761:LEU:HD22	1:C:742:ASN:HB3	1.96	0.47
1:C:156:GLU:O	1:C:160:LEU:HG	2.14	0.47
1:C:377:PHE:HE1	1:C:407:ILE:HG23	1.78	0.47
1:D:410:TRP:CZ3	1:D:659:PRO:HG3	2.49	0.47
1:A:162:VAL:HA	1:A:166:VAL:CG2	2.45	0.47
1:A:420:LYS:HD3	1:A:661:PHE:CZ	2.49	0.47
1:A:442:MET:HG3	1:A:446:TYR:HE2	1.80	0.47
1:A:464:ARG:HG3	1:A:469:TRP:HE1	1.79	0.47
1:C:369:CYS:HB3	1:C:657:LEU:HD11	1.97	0.47
1:C:595:GLU:HB2	1:D:471:MET:HE3	1.97	0.47
1:D:400:PRO:HB2	1:D:405:TRP:CE2	2.49	0.47
1:A:67:ASP:OD2	1:A:76:ILE:HD11	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:PHE:O	1:A:322:TRP:HB2	2.15	0.47
1:A:330:LYS:O	1:A:331:LEU:C	2.58	0.47
2:B:341:GLY:HA2	2:B:344:ARG:NH1	2.30	0.47
2:B:426:LEU:HG	2:B:430:TRP:HE1	1.79	0.47
1:C:179:VAL:HG22	1:C:181:CYS:H	1.78	0.47
1:C:236:GLU:O	1:C:237:PHE:HB2	2.15	0.47
1:C:268:ILE:CD1	1:C:720:LEU:HD11	2.44	0.47
1:C:290:LEU:O	1:C:294:ILE:HG13	2.15	0.47
1:D:517:ILE:CG1	1:D:624:MET:HE2	2.43	0.47
1:A:446:TYR:CE2	1:A:485:SER:HB2	2.49	0.47
1:A:753:PHE:CE1	1:D:754:ARG:HA	2.50	0.47
1:C:50:GLN:HG2	1:C:54:GLU:OE2	2.14	0.47
1:C:541:TYR:HD1	1:D:393:LEU:HD22	1.79	0.47
1:C:588:THR:CG2	1:D:557:ARG:HD2	2.45	0.47
1:D:159:LYS:O	1:D:163:GLN:HG3	2.15	0.47
1:D:387:HIS:O	1:D:388:ILE:C	2.57	0.47
1:D:458:VAL:O	1:D:459:LYS:HB3	2.14	0.47
1:A:54:GLU:HB3	1:A:58:TYR:CD2	2.50	0.47
1:C:148:LEU:O	1:C:152:THR:HG23	2.15	0.47
1:C:326:HIS:O	1:C:327:TRP:C	2.55	0.47
1:D:290:LEU:HD21	1:D:311:LEU:HD11	1.97	0.47
1:A:446:TYR:O	1:A:450:ILE:HG12	2.15	0.47
2:B:102:LEU:O	2:B:103:LEU:C	2.58	0.47
2:B:165:LEU:O	2:B:169:ARG:HG2	2.14	0.47
2:B:168:HIS:CD2	2:B:218:ARG:HG2	2.50	0.47
2:B:201:LYS:C	2:B:203:LYS:N	2.71	0.47
2:B:601:LEU:HB2	2:B:603:HIS:NE2	2.30	0.47
1:C:108:VAL:HG22	1:C:109:VAL:N	2.30	0.47
1:D:358:LEU:HD23	1:D:361:LYS:NZ	2.30	0.47
1:C:186:GLU:OE1	1:C:186:GLU:N	2.49	0.46
1:A:725:VAL:O	1:A:729:ILE:HG12	2.15	0.46
2:B:579:GLN:HE22	2:B:604:VAL:HA	1.80	0.46
1:C:448:ALA:O	1:C:449:THR:C	2.59	0.46
1:A:199:ILE:O	1:A:203:LEU:HG	2.15	0.46
1:A:417:GLY:HA2	1:A:661:PHE:HE2	1.81	0.46
2:B:282:LEU:CD2	2:B:330:PHE:HB2	2.45	0.46
2:B:285:ILE:CD1	2:B:738:LEU:HD11	2.46	0.46
2:B:533:MET:SD	2:B:649:PHE:HD2	2.38	0.46
1:D:391:THR:O	1:D:392:ASP:C	2.59	0.46
2:B:201:LYS:C	2:B:203:LYS:H	2.22	0.46
2:B:377:GLY:O	2:B:380:ILE:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:649:PHE:O	2:B:650:GLN:C	2.59	0.46
1:C:18:ILE:HD11	1:D:170:ARG:HA	1.96	0.46
1:D:584:ASN:HD22	1:D:586:TYR:HE2	1.62	0.46
1:A:754:ARG:O	1:A:758:LEU:HG	2.16	0.46
2:B:185:LEU:HD11	2:B:219:CYS:SG	2.56	0.46
2:B:728:ASP:O	2:B:732:GLN:HG2	2.14	0.46
1:C:328:VAL:O	1:C:332:LEU:HG	2.16	0.46
1:C:509:SER:HA	1:C:631:ILE:HG21	1.97	0.46
1:A:408:LEU:O	1:A:412:LEU:HG	2.15	0.46
1:A:493:LEU:HA	1:A:496:LEU:HD13	1.97	0.46
1:A:497:PHE:HB2	1:A:507:GLN:OE1	2.15	0.46
2:B:176:THR:O	2:B:180:LYS:HG2	2.16	0.46
2:B:203:LYS:HE2	2:B:203:LYS:HB3	1.78	0.46
2:B:461:VAL:O	2:B:462:MET:C	2.59	0.46
1:C:45:TYR:CE1	1:C:49:LYS:HD2	2.50	0.46
1:C:719:ASN:O	1:C:723:ARG:HG2	2.15	0.46
1:D:358:LEU:HA	1:D:361:LYS:HE3	1.96	0.46
1:D:514:LEU:O	1:D:518:LEU:HG	2.15	0.46
1:D:641:PHE:O	1:D:645:LYS:HG3	2.15	0.46
2:B:592:PHE:CD1	5:B:1101:YZY:O2	2.68	0.46
1:C:222:ARG:O	1:C:226:GLU:HG3	2.16	0.46
1:C:466:ARG:HA	1:C:469:TRP:CD1	2.51	0.46
1:C:656:THR:CG2	1:C:661:PHE:HA	2.45	0.46
1:D:236:GLU:O	1:D:237:PHE:HB2	2.15	0.46
1:A:367:PHE:O	1:A:371:THR:HG23	2.16	0.46
2:B:54:ALA:O	2:B:55:CYS:C	2.58	0.46
2:B:507:VAL:O	2:B:511:LEU:HG	2.16	0.46
1:C:161:LEU:HA	1:C:164:LYS:NZ	2.30	0.46
1:D:164:LYS:HE2	1:D:164:LYS:HB3	1.73	0.46
1:D:429:GLU:O	1:D:432:HIS:HB3	2.16	0.46
1:A:76:ILE:O	1:A:79:GLU:HG2	2.16	0.46
1:A:162:VAL:HA	1:A:166:VAL:HG21	1.98	0.46
1:A:235:ASN:O	1:A:238:LYS:HB2	2.15	0.46
1:A:304:GLN:OE1	1:A:306:ASN:N	2.49	0.46
2:B:67:LEU:O	2:B:70:ASN:HB2	2.16	0.46
2:B:396:THR:O	2:B:400:LEU:HG	2.15	0.46
1:C:304:GLN:HG2	1:C:305:PRO:HD2	1.98	0.46
1:D:242:GLU:O	1:D:246:GLN:HG2	2.16	0.46
1:A:309:GLN:O	1:A:313:THR:HG23	2.15	0.46
2:B:169:ARG:O	2:B:170:ASN:C	2.57	0.46
2:B:409:ASN:OD1	2:B:412:LYS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:641:LEU:O	2:B:645:LEU:HG	2.16	0.46
2:B:650:GLN:NE2	1:C:629:GLN:HE21	2.12	0.46
1:C:341:PHE:HD1	1:C:657:LEU:HD22	1.80	0.46
1:A:415:ILE:O	1:A:419:ILE:HG13	2.17	0.45
2:B:82:VAL:HB	2:B:83:LEU:HD12	1.97	0.45
2:B:382:THR:O	2:B:383:PRO:C	2.57	0.45
2:B:742:TYR:O	2:B:746:MET:HG2	2.16	0.45
1:D:631:ILE:HA	1:D:634:HIS:NE2	2.31	0.45
1:C:472:TRP:HB3	1:C:477:ILE:HD11	1.98	0.45
1:C:704:ALA:O	1:C:708:ILE:HG13	2.16	0.45
1:D:510:LEU:O	1:D:514:LEU:HG	2.17	0.45
1:A:317:ASP:OD1	1:A:363:PRO:HD2	2.17	0.45
1:A:438:MET:HE1	1:A:491:LEU:HB2	1.98	0.45
1:C:62:ASN:OD1	1:C:65:CYS:HB3	2.16	0.45
1:C:458:VAL:HG23	1:C:459:LYS:N	2.32	0.45
1:D:283:LYS:HG3	1:D:284:TYR:O	2.17	0.45
1:A:389:VAL:O	1:A:390:ARG:C	2.59	0.45
2:B:574:ILE:HD11	2:B:593:ALA:HB2	1.98	0.45
2:B:758:VAL:HA	1:C:738:LEU:HD21	1.96	0.45
1:C:450:ILE:O	1:C:454:ILE:HG13	2.16	0.45
1:D:341:PHE:N	1:D:342:PRO:HD2	2.31	0.45
1:D:430:TYR:CZ	1:D:436:ASN:HB3	2.51	0.45
2:B:469:THR:HG21	2:B:502:PHE:CA	2.46	0.45
2:B:599:PHE:HB2	2:B:603:HIS:NE2	2.31	0.45
1:D:369:CYS:HB2	1:D:657:LEU:HD11	1.97	0.45
1:A:626:ASN:ND2	2:B:649:PHE:CD1	2.85	0.45
2:B:632:VAL:HG13	5:C:804:YZY:H331	1.99	0.45
1:C:74:LEU:O	1:C:78:ILE:HG13	2.16	0.45
1:D:480:ALA:O	1:D:484:ILE:HG13	2.16	0.45
1:A:480:ALA:O	1:A:484:ILE:HG13	2.17	0.45
1:C:377:PHE:CE2	1:C:381:LEU:HD11	2.51	0.45
1:C:753:PHE:O	1:C:757:VAL:HG23	2.16	0.45
1:D:508:ILE:HG21	1:D:638:GLU:CB	2.45	0.45
1:A:100:LEU:O	1:A:104:ILE:HG13	2.16	0.45
1:A:526:LEU:HD23	2:B:514:PHE:CD1	2.51	0.45
2:B:361:TRP:HE1	2:B:396:THR:HG21	1.81	0.45
1:C:416:TRP:HD1	1:C:661:PHE:CE2	2.34	0.45
1:C:537:GLN:OE1	1:D:385:SER:HB3	2.16	0.45
1:A:304:GLN:OE1	1:A:306:ASN:HB2	2.17	0.45
2:B:528:ILE:O	2:B:532:GLN:HG2	2.17	0.45
1:C:341:PHE:N	1:C:342:PRO:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:544:THR:HG21	1:C:591:LYS:NZ	2.31	0.45
1:A:335:MET:HE3	1:A:339:PHE:CZ	2.51	0.45
1:A:417:GLY:HA2	1:A:661:PHE:CE2	2.52	0.45
1:C:446:TYR:O	1:C:450:ILE:HG13	2.17	0.45
1:C:510:LEU:O	1:C:514:LEU:HG	2.17	0.45
1:C:526:LEU:HD23	1:D:494:ILE:HG12	1.99	0.45
1:D:72:SER:O	1:D:76:ILE:HG13	2.17	0.45
1:D:628:TYR:O	1:D:629:GLN:C	2.60	0.45
1:A:296:TYR:HB3	1:A:298:GLN:HE21	1.81	0.44
1:C:400:PRO:HB3	1:C:404:GLU:HG2	1.99	0.44
1:C:415:ILE:O	1:C:419:ILE:HG13	2.18	0.44
1:D:140:THR:HB	1:D:141:PRO:HD2	1.99	0.44
1:A:179:VAL:C	1:A:181:CYS:N	2.70	0.44
1:D:342:PRO:O	1:D:346:ILE:HG13	2.17	0.44
1:D:754:ARG:O	1:D:758:LEU:HG	2.17	0.44
1:A:268:ILE:CD1	1:A:720:LEU:HD11	2.47	0.44
1:A:348:TYR:HB2	1:A:360:ILE:HG21	2.00	0.44
2:B:195:CYS:O	2:B:196:THR:C	2.59	0.44
2:B:428:ILE:HD11	2:B:470:PHE:CG	2.53	0.44
2:B:770:LYS:NZ	2:B:770:LYS:HB3	2.33	0.44
1:C:298:GLN:O	1:C:302:VAL:HG23	2.17	0.44
1:C:335:MET:HB3	1:C:339:PHE:CZ	2.53	0.44
1:C:627:SER:O	1:C:631:ILE:HG12	2.17	0.44
1:A:718:ARG:O	1:A:722:LYS:HG3	2.16	0.44
2:B:79:CYS:SG	2:B:80:VAL:N	2.91	0.44
2:B:102:LEU:O	2:B:105:ASP:N	2.50	0.44
2:B:683:ASN:OD1	2:B:683:ASN:C	2.61	0.44
1:C:254:ASP:O	1:C:258:GLN:HG2	2.17	0.44
1:C:455:VAL:O	1:C:459:LYS:HG2	2.18	0.44
1:D:360:ILE:HD12	1:D:365:ILE:HG22	1.99	0.44
1:D:414:PHE:O	1:D:418:GLU:HG2	2.17	0.44
1:A:315:TRP:HZ3	1:A:650:TYR:HB2	1.82	0.44
2:B:455:ARG:HD3	2:B:515:PHE:CG	2.52	0.44
1:C:263:ARG:O	1:C:267:ILE:HG13	2.18	0.44
1:C:637:ILE:HG13	1:C:638:GLU:N	2.33	0.44
1:D:88:LEU:O	1:D:92:HIS:HD2	2.01	0.44
1:A:322:TRP:HA	1:A:325:LYS:CD	2.47	0.44
1:A:354:SER:O	1:A:355:ASN:C	2.61	0.44
2:B:124:GLY:O	2:B:128:ILE:HG13	2.17	0.44
2:B:213:ARG:HD2	2:B:251:GLU:OE2	2.17	0.44
2:B:594:LEU:HA	2:B:597:TYR:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:658:PRO:N	1:C:659:PRO:HD2	2.33	0.44
1:D:225:TRP:NE1	1:D:229:GLU:OE2	2.51	0.44
1:A:242:GLU:O	1:A:246:GLN:HG3	2.18	0.44
2:B:167:ALA:HA	2:B:175:LEU:HD11	2.00	0.44
2:B:560:ASP:OD2	1:C:387:HIS:ND1	2.51	0.44
1:C:177:ASN:HB3	1:D:324:ARG:NH2	2.33	0.44
1:C:257:ASP:OD1	1:C:304:GLN:HG3	2.16	0.44
1:A:539:TYR:OH	1:A:601:GLY:HA3	2.18	0.44
1:A:658:PRO:N	1:A:659:PRO:HD2	2.33	0.44
2:B:195:CYS:CB	2:B:197:LEU:HG	2.47	0.44
2:B:441:ARG:HG3	2:B:445:GLU:CD	2.43	0.44
1:C:341:PHE:CD2	1:C:342:PRO:HD3	2.53	0.44
1:C:415:ILE:CD1	1:C:443:ASN:HB3	2.47	0.44
1:D:497:PHE:CD2	1:D:503:LEU:HB3	2.53	0.44
1:A:416:TRP:HE3	1:A:419:ILE:HD12	1.83	0.44
2:B:469:THR:HG22	2:B:501:LEU:HB2	2.00	0.44
1:C:83:LEU:O	1:C:87:GLU:HG3	2.18	0.44
1:C:328:VAL:O	1:C:329:VAL:C	2.61	0.44
1:D:327:TRP:CD1	1:D:328:VAL:HG23	2.52	0.44
1:A:86:MET:HE2	1:A:86:MET:HB3	1.83	0.43
1:A:304:GLN:HG2	1:A:305:PRO:HD2	2.00	0.43
1:A:326:HIS:ND1	1:A:328:VAL:HB	2.33	0.43
1:A:467:GLU:CD	1:A:467:GLU:H	2.24	0.43
1:A:623:MET:HE2	2:B:526:LEU:HD11	1.99	0.43
1:C:158:ILE:O	1:C:162:VAL:HG23	2.18	0.43
1:C:177:ASN:O	1:C:178:CYS:C	2.60	0.43
1:C:539:TYR:OH	1:C:601:GLY:HA3	2.18	0.43
1:C:558:CYS:O	1:C:559:GLU:C	2.60	0.43
1:D:341:PHE:HB2	1:D:657:LEU:HD21	2.00	0.43
1:D:341:PHE:HD1	1:D:657:LEU:HD22	1.83	0.43
1:D:365:ILE:O	1:D:366:LYS:C	2.61	0.43
1:D:417:GLY:O	1:D:421:GLU:HG3	2.19	0.43
1:D:422:MET:HE2	1:D:430:TYR:CE1	2.53	0.43
1:A:351:SER:O	1:A:352:PRO:C	2.60	0.43
1:A:355:ASN:HA	1:A:358:LEU:HD12	2.00	0.43
2:B:193:CYS:HB3	2:B:198:CYS:SG	2.59	0.43
2:B:368:TYR:CZ	2:B:677:THR:HG21	2.53	0.43
1:C:235:ASN:O	1:C:238:LYS:HB2	2.18	0.43
1:D:148:LEU:O	1:D:152:THR:HG23	2.18	0.43
1:D:376:THR:O	1:D:380:MET:HG2	2.18	0.43
1:A:154:ASN:O	1:A:158:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:MET:HE3	2:B:537:PHE:CE1	2.53	0.43
2:B:316:TYR:HB3	2:B:318:GLN:HE21	1.84	0.43
2:B:380:ILE:HG13	2:B:389:ILE:HD12	2.00	0.43
2:B:772:ARG:HG2	2:B:776:ARG:HH12	1.82	0.43
1:C:497:PHE:HB2	1:C:507:GLN:OE1	2.18	0.43
1:A:148:LEU:O	1:A:152:THR:HG23	2.17	0.43
1:A:704:ALA:O	1:A:708:ILE:HG13	2.17	0.43
2:B:449:ASP:N	2:B:449:ASP:OD1	2.51	0.43
1:C:23:VAL:HG23	1:C:24:ARG:N	2.34	0.43
1:C:63:ILE:CG2	1:C:94:VAL:HG22	2.48	0.43
1:D:58:TYR:O	1:D:59:TYR:C	2.61	0.43
1:A:327:TRP:CH2	1:A:328:VAL:HG22	2.53	0.43
1:A:408:LEU:O	1:A:409:PRO:C	2.61	0.43
2:B:245:LYS:O	2:B:246:GLU:C	2.60	0.43
2:B:559:TYR:HA	2:B:610:ARG:NH2	2.32	0.43
1:A:240:GLU:OE1	1:A:240:GLU:N	2.48	0.43
2:B:172:TYR:CE1	2:B:228:LEU:HG	2.54	0.43
2:B:607:PHE:CZ	1:C:559:GLU:HA	2.53	0.43
2:B:761:LEU:O	2:B:765:ARG:HG3	2.19	0.43
1:C:86:MET:HE2	1:C:86:MET:HB3	1.89	0.43
1:C:393:LEU:HA	1:C:466:ARG:HH21	1.83	0.43
1:D:317:ASP:OD1	1:D:363:PRO:HD2	2.18	0.43
1:D:322:TRP:HA	1:D:325:LYS:CD	2.47	0.43
1:A:458:VAL:O	1:A:459:LYS:HB2	2.19	0.43
2:B:361:TRP:CG	2:B:362:PRO:HD3	2.54	0.43
1:C:378:LEU:HA	1:C:381:LEU:HD12	2.00	0.43
1:D:52:LEU:HD12	1:D:88:LEU:HG	2.00	0.43
1:D:408:LEU:O	1:D:409:PRO:C	2.61	0.43
2:B:442:LEU:HD12	2:B:446:GLY:O	2.19	0.43
1:C:52:LEU:HB3	1:C:92:HIS:CD2	2.54	0.43
1:C:108:VAL:HG22	1:C:109:VAL:H	1.82	0.43
1:C:184:SER:O	1:C:187:VAL:N	2.49	0.43
1:C:319:PHE:O	1:C:320:PRO:C	2.62	0.43
1:C:379:PHE:CZ	1:C:383:LEU:HD21	2.53	0.43
1:C:467:GLU:H	1:C:467:GLU:CD	2.27	0.43
1:C:544:THR:HG21	1:C:591:LYS:HZ2	1.82	0.43
1:A:90:LEU:HD11	1:A:114:LEU:HD23	2.00	0.43
1:A:174:ILE:HG22	1:A:175:ARG:HG3	2.01	0.43
1:A:236:GLU:CD	1:A:236:GLU:H	2.26	0.43
1:A:338:GLY:O	1:A:341:PHE:HD2	2.01	0.43
1:A:408:LEU:HB3	1:A:409:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:738:LEU:O	1:D:738:LEU:HG	2.18	0.43
1:D:36:PHE:O	1:D:40:VAL:HG23	2.18	0.43
1:D:74:LEU:O	1:D:78:ILE:HG13	2.19	0.43
1:D:176:CYS:HB2	1:D:179:VAL:CG2	2.45	0.43
1:D:235:ASN:O	1:D:238:LYS:HB2	2.18	0.43
1:A:179:VAL:CG2	1:A:182:VAL:HG13	2.48	0.43
1:A:346:ILE:O	1:A:347:ALA:C	2.62	0.43
1:C:385:SER:C	1:C:387:HIS:N	2.71	0.43
1:C:408:LEU:O	1:C:412:LEU:HG	2.18	0.43
1:C:420:LYS:HE3	1:C:420:LYS:HB3	1.92	0.43
1:D:633:ASP:OD1	1:D:634:HIS:N	2.52	0.43
1:A:501:SER:HA	1:A:639:TRP:CZ2	2.54	0.42
1:A:640:LYS:O	1:A:644:THR:HG23	2.19	0.42
2:B:163:VAL:HG21	2:B:183:VAL:HG11	2.01	0.42
2:B:401:LEU:O	2:B:404:TYR:HB3	2.18	0.42
2:B:540:PHE:CD2	2:B:641:LEU:HD22	2.54	0.42
1:A:63:ILE:HD11	1:A:93:SER:O	2.19	0.42
1:A:573:GLN:HG2	5:A:803:YZY:H52	2.01	0.42
2:B:55:CYS:SG	2:B:90:ILE:HD13	2.59	0.42
2:B:723:LEU:O	2:B:727:ARG:HG3	2.20	0.42
1:C:326:HIS:HE1	1:C:328:VAL:HG23	1.84	0.42
1:A:62:ASN:OD1	1:A:65:CYS:HB3	2.18	0.42
2:B:393:SER:OG	2:B:680:PRO:HD2	2.19	0.42
1:C:469:TRP:CD1	1:C:469:TRP:N	2.87	0.42
1:C:520:PHE:CZ	1:C:616:LEU:HB3	2.55	0.42
1:D:112:VAL:HG23	1:D:115:LEU:HD12	2.01	0.42
1:D:341:PHE:CD2	1:D:342:PRO:HD3	2.54	0.42
1:A:523:ILE:HG23	2:B:514:PHE:CE2	2.53	0.42
2:B:724:LYS:HG3	2:B:727:ARG:HH21	1.85	0.42
1:D:366:LYS:O	1:D:369:CYS:SG	2.78	0.42
2:B:53:LEU:O	2:B:54:ALA:C	2.62	0.42
1:D:407:ILE:O	1:D:408:LEU:C	2.62	0.42
1:D:617:LEU:O	1:D:618:ASN:C	2.62	0.42
1:A:596:PHE:CE2	2:B:497:VAL:HA	2.55	0.42
2:B:410:GLU:HG2	2:B:411:ASP:OD1	2.20	0.42
1:C:322:TRP:HZ2	1:C:334:CYS:SG	2.43	0.42
1:C:644:THR:O	1:C:645:LYS:C	2.59	0.42
2:B:644:MET:HG2	1:C:628:TYR:CE1	2.55	0.42
1:C:180:GLU:O	1:C:183:SER:HB3	2.19	0.42
1:C:296:TYR:HB3	1:C:298:GLN:HE21	1.85	0.42
1:C:449:THR:O	1:C:453:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:PRO:O	1:A:364:PHE:C	2.63	0.42
1:C:420:LYS:HD3	1:C:661:PHE:HZ	1.85	0.42
2:B:341:GLY:O	2:B:345:LYS:HG3	2.20	0.42
2:B:599:PHE:HB2	2:B:603:HIS:CD2	2.55	0.42
4:C:802:Y01:HAE2	4:C:802:Y01:HBB	1.85	0.42
1:C:416:TRP:HE1	1:C:420:LYS:HD2	1.83	0.42
2:B:428:ILE:HD11	2:B:470:PHE:CD1	2.54	0.41
1:C:348:TYR:HB2	1:C:360:ILE:HG21	2.02	0.41
1:D:162:VAL:HA	1:D:166:VAL:CG2	2.50	0.41
1:C:340:LEU:C	1:C:342:PRO:HD2	2.45	0.41
4:D:802:Y01:HAE2	4:D:802:Y01:HBB	1.85	0.41
1:A:416:TRP:CE2	1:A:420:LYS:HD2	2.55	0.41
2:B:368:TYR:CD2	2:B:380:ILE:HG21	2.56	0.41
1:C:338:GLY:O	1:C:341:PHE:HD2	2.03	0.41
1:A:236:GLU:O	1:A:237:PHE:HB2	2.20	0.41
1:A:290:LEU:O	1:A:294:ILE:HG13	2.20	0.41
2:B:448:GLU:H	2:B:448:GLU:CD	2.27	0.41
1:A:179:VAL:HG23	1:A:182:VAL:HG13	2.01	0.41
1:A:387:HIS:O	1:A:388:ILE:C	2.62	0.41
1:A:576:PHE:CE2	5:A:803:YZY:H192	2.56	0.41
1:A:746:LEU:HG	1:D:743:PHE:HE1	1.85	0.41
2:B:400:LEU:HA	2:B:403:LEU:HG	2.02	0.41
2:B:426:LEU:O	2:B:427:LEU:C	2.62	0.41
1:A:69:LEU:HD23	2:B:747:ARG:HD3	2.02	0.41
2:B:88:VAL:HG13	2:B:89:THR:N	2.35	0.41
1:C:322:TRP:HA	1:C:325:LYS:HD2	2.01	0.41
1:A:558:CYS:O	1:A:559:GLU:C	2.61	0.41
1:A:460:TYR:CE2	1:A:474:PRO:HG3	2.56	0.41
2:B:447:LEU:HD23	2:B:447:LEU:C	2.45	0.41
1:A:414:PHE:O	1:A:418:GLU:HG2	2.21	0.41
2:B:323:SER:HA	2:B:328:GLN:OE1	2.21	0.41
1:C:58:TYR:O	1:C:59:TYR:C	2.63	0.41
1:C:408:LEU:HB3	1:C:409:PRO:HD3	2.03	0.41
1:D:348:TYR:CB	1:D:360:ILE:HG21	2.51	0.41
1:D:377:PHE:CE1	1:D:407:ILE:HG23	2.56	0.41
1:D:402:VAL:O	1:D:406:MET:HG3	2.21	0.41
1:A:17:ARG:NH1	2:B:184:SER:O	2.54	0.41
1:C:351:SER:O	1:C:352:PRO:C	2.62	0.41
1:C:416:TRP:O	1:C:420:LYS:HG3	2.21	0.41
1:D:286:ASP:O	1:D:287:LEU:C	2.62	0.41
1:D:593:ARG:HD2	1:D:593:ARG:HA	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ASP:O	1:A:291:LYS:HE3	2.20	0.40
1:A:657:LEU:H	1:A:657:LEU:CD1	2.34	0.40
2:B:526:LEU:O	2:B:530:MET:HG3	2.21	0.40
1:D:601:GLY:HA2	1:D:604:MET:HE2	2.02	0.40
1:C:464:ARG:HG3	1:C:469:TRP:HE1	1.84	0.40
1:D:413:GLY:O	1:D:414:PHE:C	2.63	0.40
1:D:475:THR:O	1:D:479:GLU:HG3	2.22	0.40
2:B:55:CYS:HB2	2:B:91:THR:CG2	2.51	0.40
2:B:346:PRO:O	2:B:347:THR:C	2.64	0.40
2:B:441:ARG:HD2	2:B:450:PHE:CE1	2.56	0.40
1:C:404:GLU:O	1:C:405:TRP:C	2.64	0.40
1:D:218:LEU:HD21	1:D:222:ARG:NH2	2.36	0.40
1:D:466:ARG:HD3	1:D:469:TRP:CE3	2.56	0.40
1:D:473:HIS:O	1:D:474:PRO:C	2.63	0.40
1:A:369:CYS:CB	1:A:657:LEU:HD11	2.46	0.40
1:A:386:GLN:C	1:A:388:ILE:H	2.30	0.40
1:A:410:TRP:O	1:A:411:VAL:C	2.64	0.40
2:B:381:HIS:O	2:B:382:THR:C	2.64	0.40
2:B:640:LEU:O	2:B:644:MET:HG3	2.21	0.40
2:B:750:MET:O	2:B:751:GLN:C	2.65	0.40
2:B:774:GLU:O	2:B:778:LEU:HD23	2.21	0.40
1:C:546:ALA:O	1:C:552:ASN:HA	2.21	0.40
1:A:98:ASP:O	1:A:102:TYR:HD2	2.05	0.40
2:B:212:PHE:CZ	2:B:216:ILE:HD11	2.56	0.40
2:B:414:ASN:ND2	2:B:485:ASP:HA	2.37	0.40
1:D:250:LEU:HD12	1:D:253:LYS:HD3	2.02	0.40
1:D:315:TRP:CE3	1:D:363:PRO:HB2	2.57	0.40
1:D:434:TRP:O	1:D:437:LEU:HB3	2.21	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	678/1203 (56%)	654 (96%)	24 (4%)	0	100	100
1	C	678/1203 (56%)	657 (97%)	21 (3%)	0	100	100
1	D	678/1203 (56%)	654 (96%)	24 (4%)	0	100	100
2	B	639/1504 (42%)	605 (95%)	34 (5%)	0	100	100
All	All	2673/5113 (52%)	2570 (96%)	103 (4%)	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	605/1040 (58%)	603 (100%)	2 (0%)	91	96
1	C	605/1040 (58%)	602 (100%)	3 (0%)	86	94
1	D	605/1040 (58%)	605 (100%)	0	100	100
2	B	580/1291 (45%)	579 (100%)	1 (0%)	92	97
All	All	2395/4411 (54%)	2389 (100%)	6 (0%)	90	96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	395	VAL
1	A	589	ASN
2	B	606	ILE
1	C	18	ILE
1	C	109	VAL
1	C	395	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	309	GLN

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Mol	Chain	Res	Type
1	A	387	HIS
1	A	552	ASN
2	B	618	GLN
2	B	646	HIS
2	B	650	GLN
2	B	655	HIS
1	C	163	GLN
1	C	386	GLN
1	C	396	GLN
1	C	507	GLN
1	C	573	GLN
1	C	626	ASN
1	D	192	HIS

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](#)

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	Y01	D	802	-	38,38,38	0.96	1 (2%)	57,57,57	1.35	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	Y01	C	802	-	38,38,38	0.97	1 (2%)	57,57,57	1.34	7 (12%)
5	YZY	C	804	-	38,38,41	1.38	6 (15%)	40,40,43	1.72	7 (17%)
4	Y01	A	802	-	38,38,38	0.97	1 (2%)	57,57,57	1.34	8 (14%)
5	YZY	C	803	-	38,38,41	1.38	6 (15%)	40,40,43	1.73	7 (17%)
5	YZY	A	803	-	38,38,41	1.38	6 (15%)	40,40,43	1.73	7 (17%)
5	YZY	B	1101	-	38,38,41	1.38	6 (15%)	40,40,43	1.73	7 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	Y01	D	802	-	-	5/19/77/77	0/4/4/4
4	Y01	C	802	-	-	6/19/77/77	0/4/4/4
5	YZY	C	804	-	-	17/40/40/43	-
4	Y01	A	802	-	-	5/19/77/77	0/4/4/4
5	YZY	C	803	-	-	17/40/40/43	-
5	YZY	A	803	-	-	17/40/40/43	-
5	YZY	B	1101	-	-	17/40/40/43	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	802	Y01	OAW-CAY	4.18	1.46	1.34
4	C	802	Y01	OAW-CAY	4.16	1.46	1.34
4	D	802	Y01	OAW-CAY	4.13	1.46	1.34
5	C	804	YZY	O2-C3	3.75	1.44	1.34
5	C	803	YZY	O2-C3	3.75	1.44	1.34
5	A	803	YZY	O2-C3	3.70	1.44	1.34
5	B	1101	YZY	O2-C3	3.69	1.44	1.34
5	B	1101	YZY	C13-C12	-3.62	1.31	1.51
5	C	804	YZY	C13-C12	-3.60	1.31	1.51
5	A	803	YZY	C13-C12	-3.59	1.31	1.51
5	C	803	YZY	C13-C12	-3.59	1.31	1.51
5	B	1101	YZY	C29-C28	3.15	1.50	1.31
5	A	803	YZY	C29-C28	3.15	1.50	1.31
5	C	803	YZY	C29-C28	3.15	1.50	1.31
5	C	804	YZY	C29-C28	3.13	1.49	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	804	YZY	C30-C29	-3.06	1.32	1.50
5	C	803	YZY	C30-C29	-3.06	1.32	1.50
5	B	1101	YZY	C30-C29	-3.05	1.32	1.50
5	A	803	YZY	C30-C29	-3.04	1.33	1.50
5	B	1101	YZY	O4-C20	2.97	1.42	1.33
5	A	803	YZY	O4-C20	2.96	1.42	1.33
5	C	803	YZY	O4-C20	2.94	1.41	1.33
5	C	804	YZY	O4-C20	2.90	1.41	1.33
5	C	804	YZY	O2-C2	-2.43	1.40	1.46
5	C	803	YZY	O2-C2	-2.41	1.40	1.46
5	B	1101	YZY	O2-C2	-2.39	1.40	1.46
5	A	803	YZY	O2-C2	-2.34	1.40	1.46

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1101	YZY	O2-C3-C4	6.37	125.23	111.50
5	A	803	YZY	O2-C3-C4	6.34	125.16	111.50
5	C	803	YZY	O2-C3-C4	6.34	125.16	111.50
5	C	804	YZY	O2-C3-C4	6.34	125.16	111.50
5	C	803	YZY	O4-C20-C21	4.80	126.99	111.91
5	A	803	YZY	O4-C20-C21	4.79	126.93	111.91
5	B	1101	YZY	O4-C20-C21	4.79	126.93	111.91
5	C	804	YZY	O4-C20-C21	4.76	126.84	111.91
4	D	802	Y01	OAW-CAY-CAM	4.21	120.58	111.50
4	A	802	Y01	OAW-CAY-CAM	4.20	120.55	111.50
4	C	802	Y01	OAW-CAY-CAM	4.20	120.55	111.50
4	D	802	Y01	CAV-CAZ-CBH	3.93	121.64	116.42
4	C	802	Y01	CAV-CAZ-CBH	3.89	121.58	116.42
4	A	802	Y01	CAV-CAZ-CBH	3.85	121.53	116.42
5	A	803	YZY	O4-C20-O5	-3.64	114.42	123.59
5	B	1101	YZY	O4-C20-O5	-3.63	114.44	123.59
5	C	803	YZY	O4-C20-O5	-3.62	114.45	123.59
5	C	804	YZY	O4-C20-O5	-3.60	114.50	123.59
4	C	802	Y01	CBD-CAK-CAI	-2.49	109.15	112.73
4	D	802	Y01	CBD-CAK-CAI	-2.47	109.19	112.73
4	A	802	Y01	CBD-CAK-CAI	-2.41	109.27	112.73
5	B	1101	YZY	O2-C3-O3	-2.36	118.00	123.70
5	C	803	YZY	O2-C3-O3	-2.36	118.01	123.70
5	A	803	YZY	O2-C3-O3	-2.34	118.04	123.70
5	C	804	YZY	O2-C3-O3	-2.33	118.08	123.70
5	A	803	YZY	C31-C30-C29	2.31	125.68	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	802	Y01	CAV-CAZ-CAI	-2.31	117.28	120.61
4	D	802	Y01	CAV-CAZ-CAI	-2.31	117.28	120.61
5	C	803	YZY	C31-C30-C29	2.31	125.67	112.43
5	C	804	YZY	C31-C30-C29	2.30	125.63	112.43
5	B	1101	YZY	C31-C30-C29	2.30	125.61	112.43
4	C	802	Y01	CAV-CAZ-CAI	-2.29	117.31	120.61
4	C	802	Y01	CBC-OAW-CAY	-2.14	112.52	117.79
4	A	802	Y01	CBC-OAW-CAY	-2.14	112.53	117.79
4	D	802	Y01	CBC-OAW-CAY	-2.13	112.55	117.79
5	B	1101	YZY	C27-C28-C29	-2.07	108.82	124.73
5	A	803	YZY	C27-C28-C29	-2.07	108.83	124.73
4	A	802	Y01	CBI-CBE-CBB	-2.07	116.25	119.49
5	C	803	YZY	C27-C28-C29	-2.06	108.89	124.73
5	C	804	YZY	C27-C28-C29	-2.06	108.91	124.73
5	B	1101	YZY	C16-C15-C14	-2.06	103.98	114.42
4	C	802	Y01	OAH-CAX-CAL	2.06	120.64	114.03
4	A	802	Y01	OAH-CAX-CAL	2.06	120.63	114.03
4	D	802	Y01	CBI-CBE-CBB	-2.05	116.28	119.49
5	C	803	YZY	C16-C15-C14	-2.04	104.06	114.42
5	C	804	YZY	C16-C15-C14	-2.04	104.07	114.42
5	A	803	YZY	C16-C15-C14	-2.04	104.07	114.42
4	D	802	Y01	OAH-CAX-CAL	2.04	120.58	114.03
4	D	802	Y01	CAS-CAU-CBI	-2.03	109.30	112.78
4	A	802	Y01	CAS-CAU-CBI	-2.03	109.31	112.78
4	C	802	Y01	CBI-CBE-CBB	-2.01	116.34	119.49

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	803	YZY	C20-C21-C22-C23
5	B	1101	YZY	C20-C21-C22-C23
5	C	803	YZY	C20-C21-C22-C23
5	C	804	YZY	C20-C21-C22-C23
5	B	1101	YZY	C4-C5-C6-C7
5	C	804	YZY	C4-C5-C6-C7
5	A	803	YZY	C4-C5-C6-C7
5	C	803	YZY	C4-C5-C6-C7
5	A	803	YZY	C3-C4-C5-C6
5	B	1101	YZY	C3-C4-C5-C6
5	C	803	YZY	C3-C4-C5-C6
5	C	804	YZY	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
5	A	803	YZY	C21-C22-C23-C24
5	B	1101	YZY	C21-C22-C23-C24
5	C	803	YZY	C21-C22-C23-C24
5	C	804	YZY	C21-C22-C23-C24
5	A	803	YZY	C6-C7-C8-C9
5	B	1101	YZY	C6-C7-C8-C9
5	C	803	YZY	C6-C7-C8-C9
5	C	804	YZY	C6-C7-C8-C9
5	A	803	YZY	C30-C31-C32-C33
5	B	1101	YZY	C30-C31-C32-C33
5	C	803	YZY	C30-C31-C32-C33
5	C	804	YZY	C30-C31-C32-C33
5	A	803	YZY	O4-C19-C2-C1
5	B	1101	YZY	O4-C19-C2-C1
5	C	803	YZY	O4-C19-C2-C1
5	C	804	YZY	O4-C19-C2-C1
5	A	803	YZY	O4-C19-C2-O2
5	B	1101	YZY	O4-C19-C2-O2
5	C	803	YZY	O4-C19-C2-O2
5	C	804	YZY	O4-C19-C2-O2
5	C	803	YZY	C22-C23-C24-C25
5	C	804	YZY	C22-C23-C24-C25
5	A	803	YZY	C22-C23-C24-C25
5	B	1101	YZY	C22-C23-C24-C25
5	B	1101	YZY	C7-C8-C9-C10
5	C	804	YZY	C7-C8-C9-C10
5	A	803	YZY	C7-C8-C9-C10
4	A	802	Y01	CAC-CBB-CBE-CBI
4	C	802	Y01	CAC-CBB-CBE-CBI
4	D	802	Y01	CAC-CBB-CBE-CBI
5	C	803	YZY	C7-C8-C9-C10
5	B	1101	YZY	O2-C3-C4-C5
5	C	803	YZY	O2-C3-C4-C5
5	A	803	YZY	O2-C3-C4-C5
5	C	804	YZY	O2-C3-C4-C5
5	A	803	YZY	C31-C32-C33-C34
4	C	802	Y01	CAO-CBB-CBE-CBI
4	D	802	Y01	CAO-CBB-CBE-CBI
5	C	803	YZY	C31-C32-C33-C34
5	C	804	YZY	C31-C32-C33-C34
5	B	1101	YZY	C24-C25-C26-C27
5	B	1101	YZY	C31-C32-C33-C34

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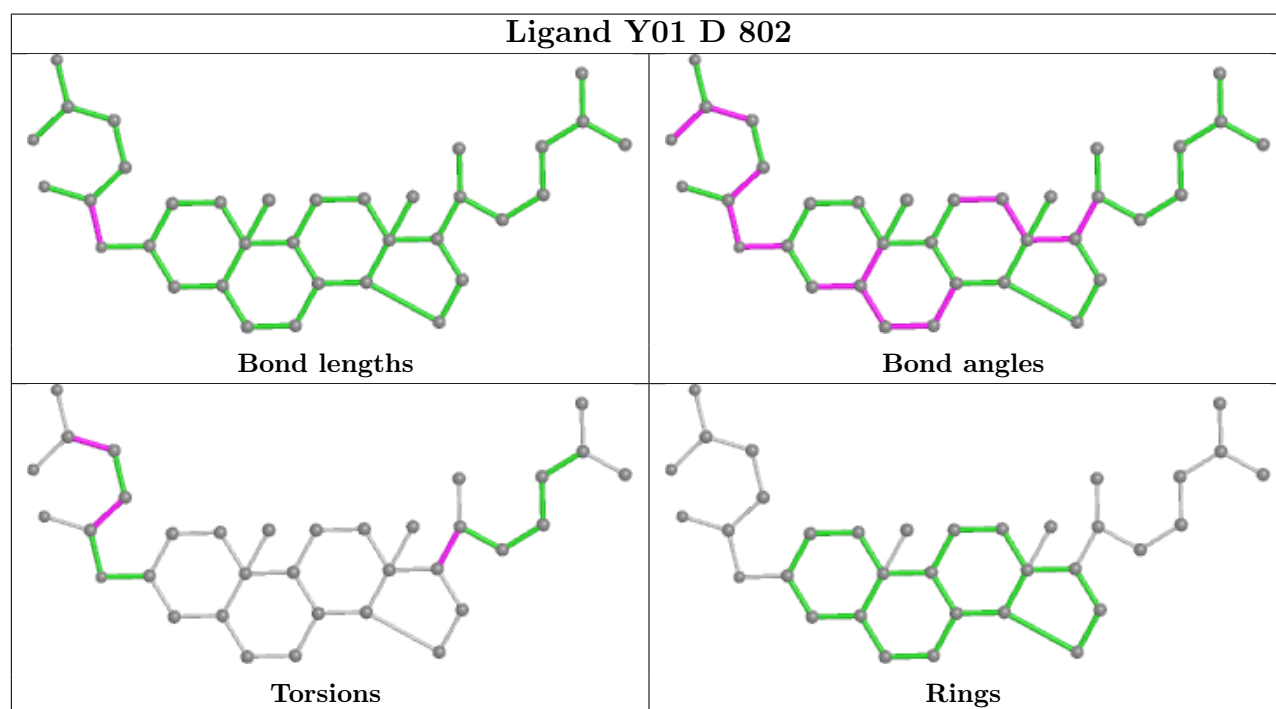
Mol	Chain	Res	Type	Atoms
5	C	803	YZY	C24-C25-C26-C27
5	A	803	YZY	C24-C25-C26-C27
5	C	804	YZY	C24-C25-C26-C27
4	A	802	Y01	CAO-CBB-CBE-CBI
4	A	802	Y01	CAM-CAL-CAX-OAF
4	D	802	Y01	CAM-CAL-CAX-OAF
4	C	802	Y01	CAM-CAL-CAX-OAF
5	A	803	YZY	C10-C11-C12-C13
4	D	802	Y01	CAL-CAM-CAY-OAW
4	A	802	Y01	CAM-CAL-CAX-OAH
4	C	802	Y01	CAM-CAL-CAX-OAH
4	D	802	Y01	CAM-CAL-CAX-OAH
5	B	1101	YZY	C10-C11-C12-C13
4	A	802	Y01	CAL-CAM-CAY-OAW
4	C	802	Y01	CAL-CAM-CAY-OAW
5	C	803	YZY	C10-C11-C12-C13
5	C	804	YZY	C10-C11-C12-C13
5	A	803	YZY	C28-C29-C30-C31
5	B	1101	YZY	C28-C29-C30-C31
5	C	803	YZY	C28-C29-C30-C31
5	C	804	YZY	C28-C29-C30-C31
5	A	803	YZY	O5-C20-O4-C19
5	B	1101	YZY	O5-C20-O4-C19
5	C	804	YZY	C12-C13-C14-C15
5	C	803	YZY	C12-C13-C14-C15
5	C	803	YZY	O5-C20-O4-C19
5	C	804	YZY	O5-C20-O4-C19
5	B	1101	YZY	C12-C13-C14-C15
5	A	803	YZY	C12-C13-C14-C15
4	C	802	Y01	CAO-CBB-CBE-CAP

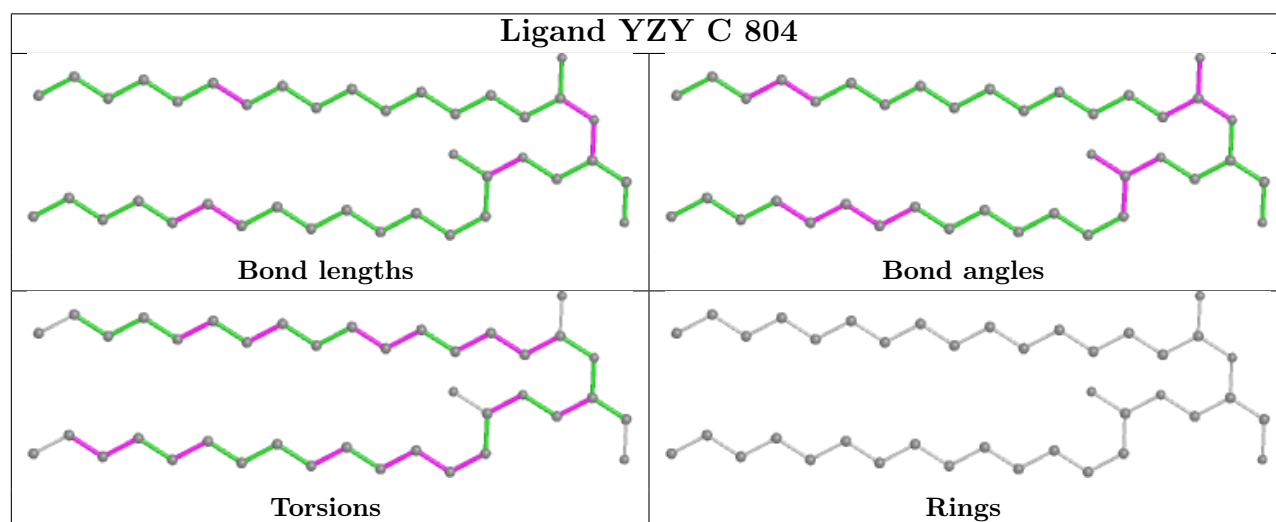
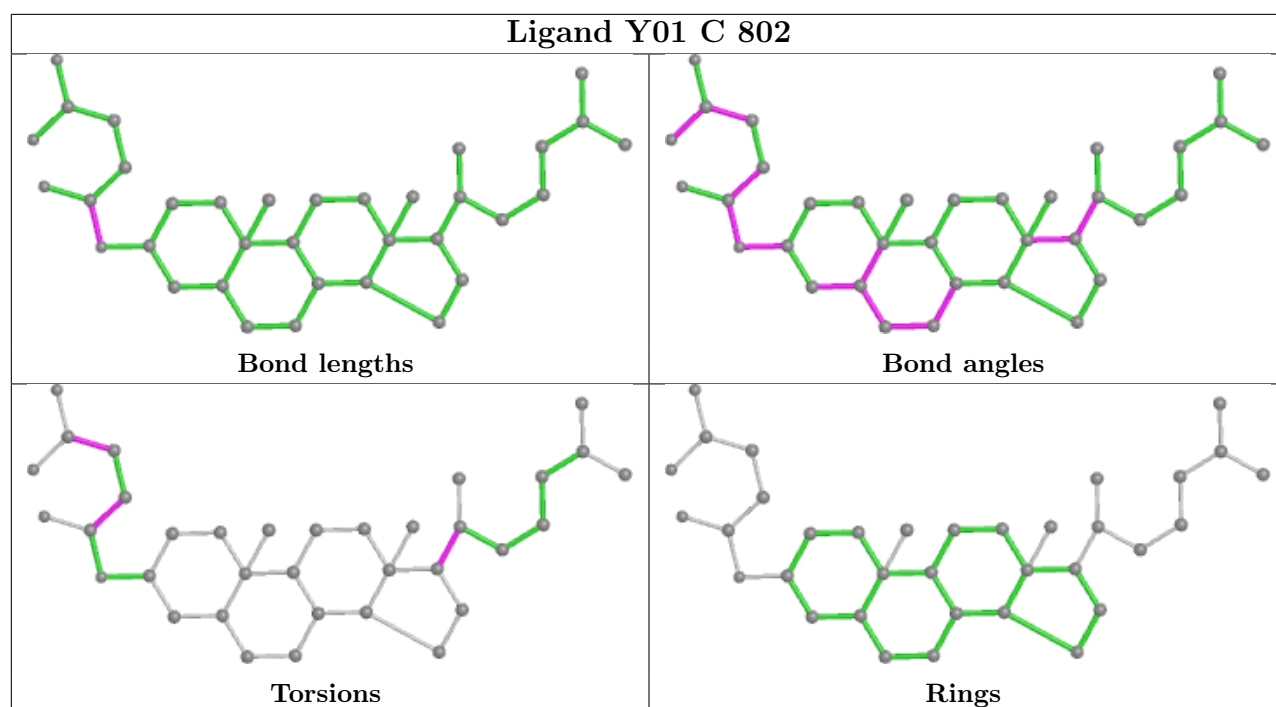
There are no ring outliers.

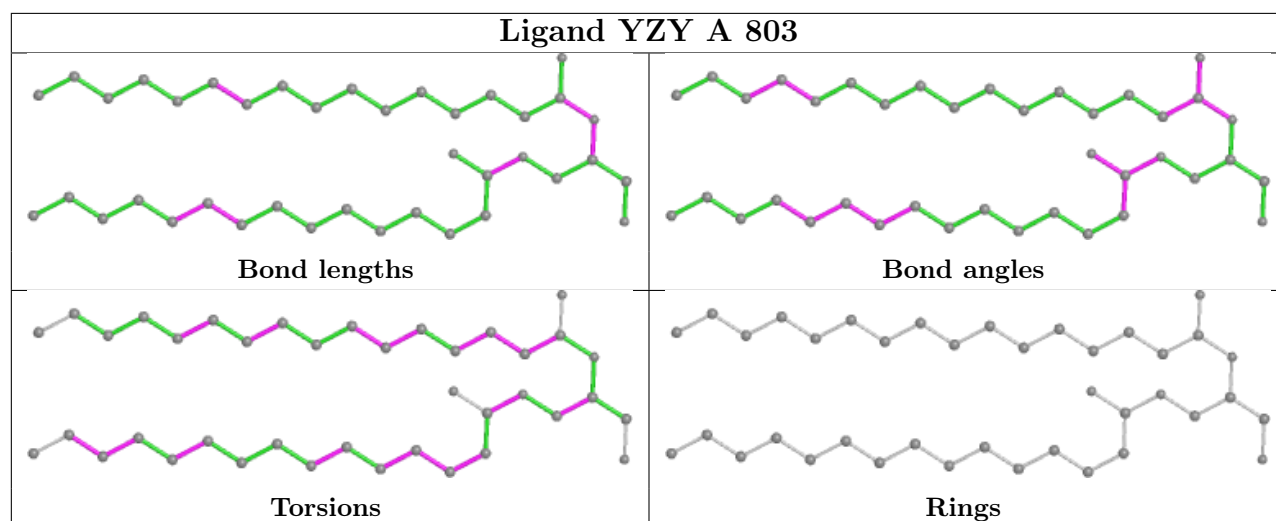
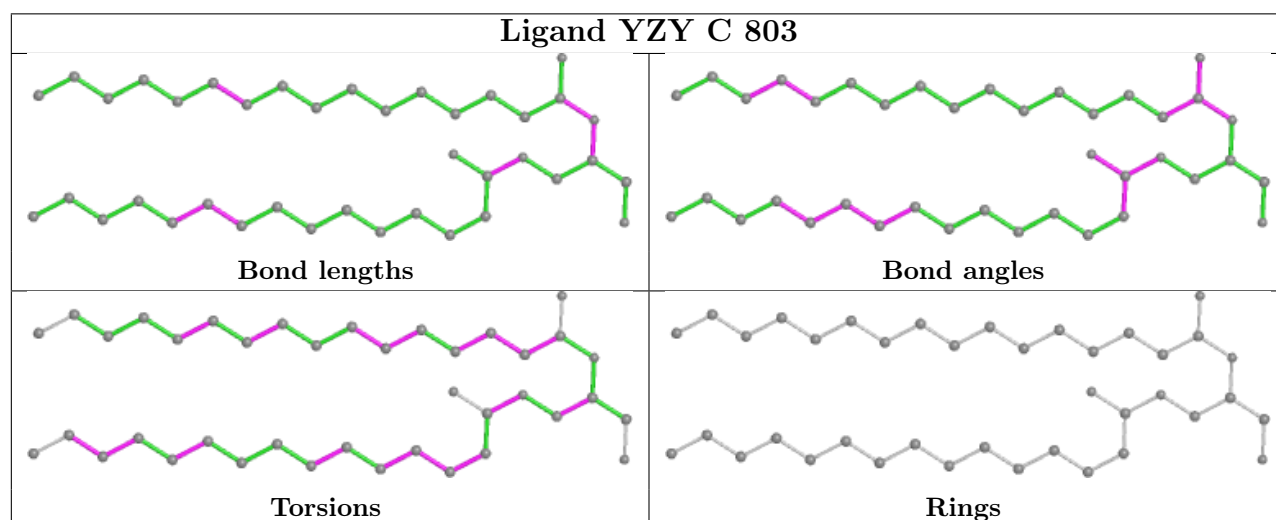
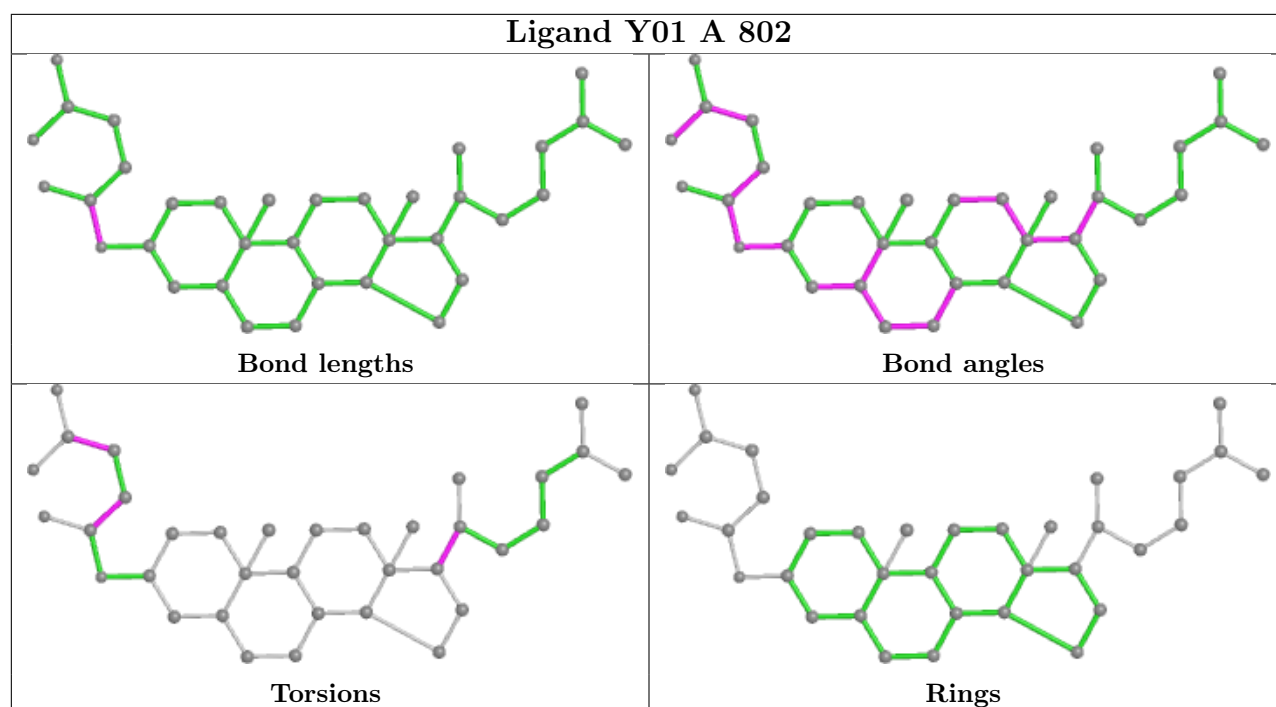
6 monomers are involved in 32 short contacts:

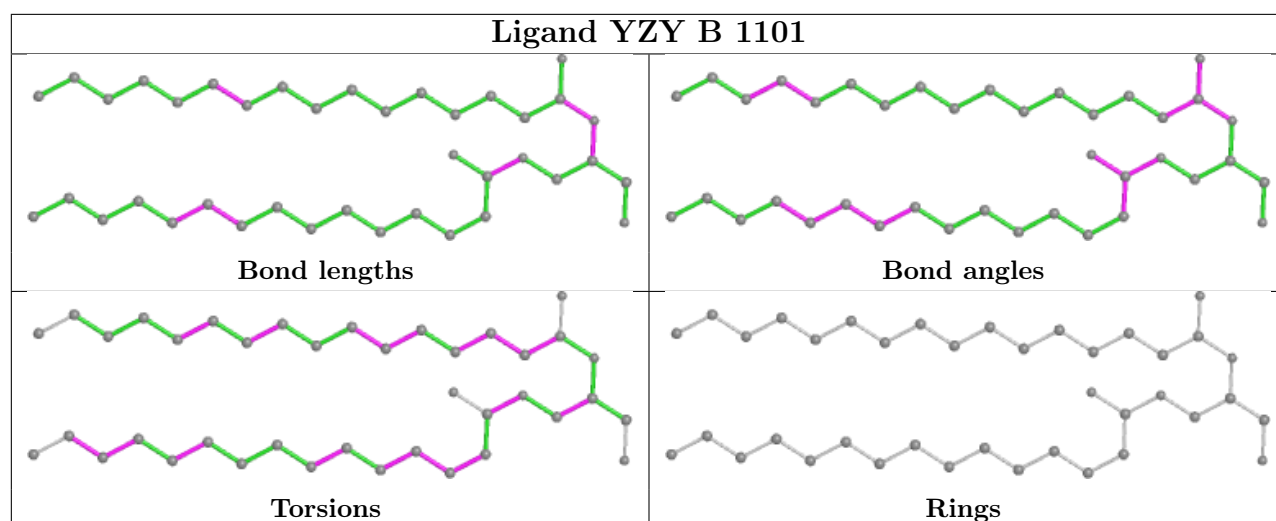
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	802	Y01	2	0
4	C	802	Y01	4	0
5	C	804	YZY	2	0
4	A	802	Y01	4	0
5	A	803	YZY	2	0
5	B	1101	YZY	18	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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.

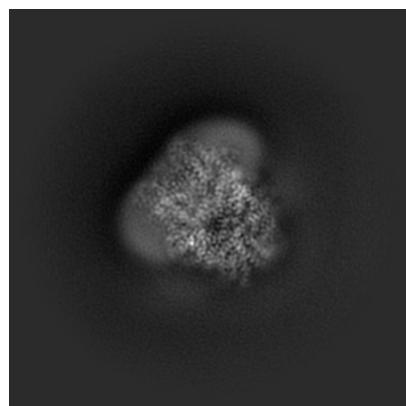
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62060. These allow visual inspection of the internal detail of the map and identification of artifacts.

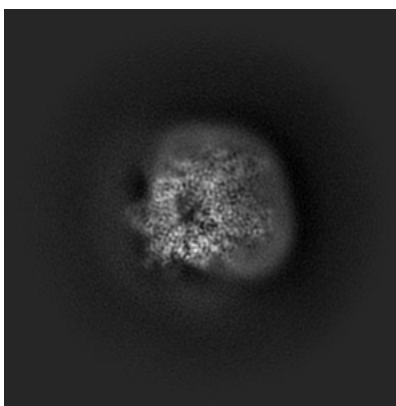
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

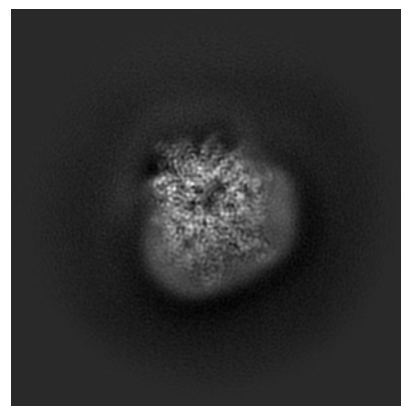
6.1.1 Primary map



X

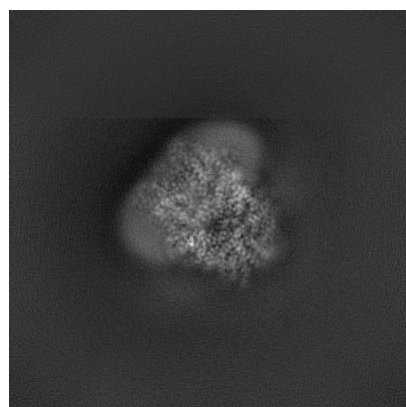


Y

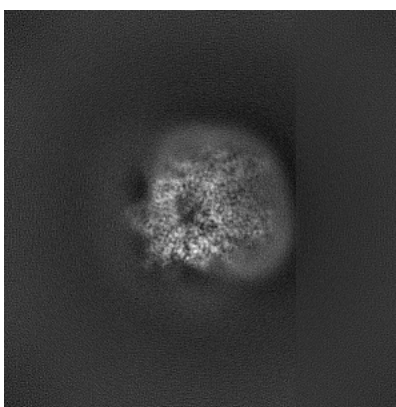


Z

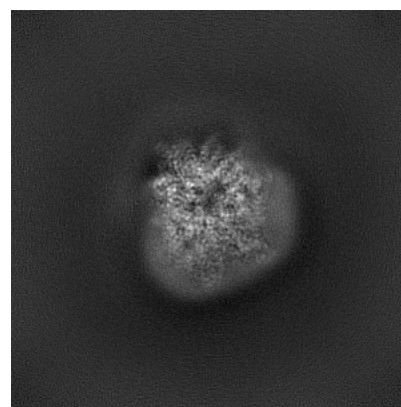
6.1.2 Raw map



X



Y

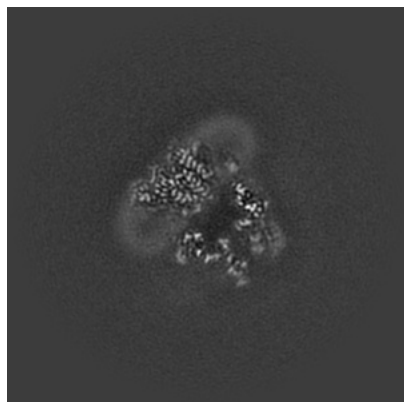


Z

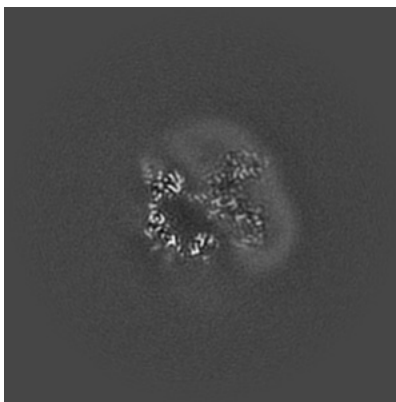
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

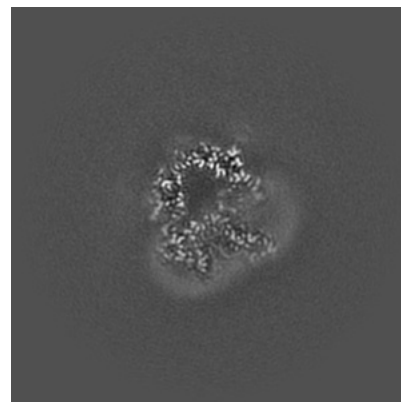
6.2.1 Primary map



X Index: 200

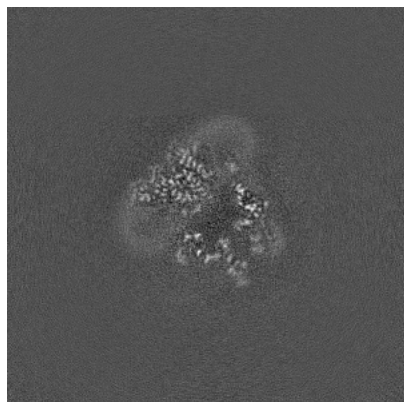


Y Index: 200

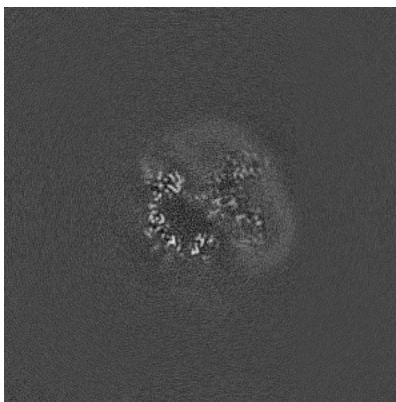


Z Index: 200

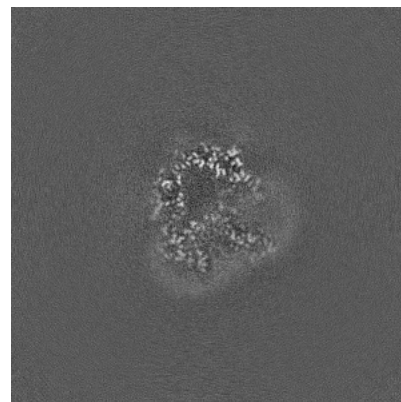
6.2.2 Raw map



X Index: 200



Y Index: 200

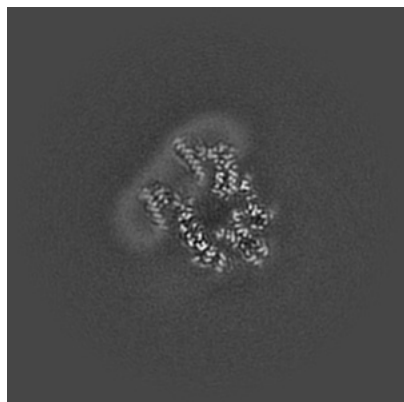


Z Index: 200

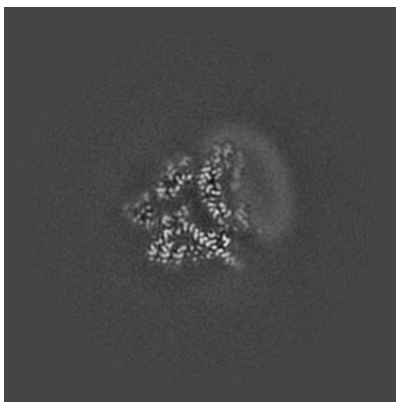
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

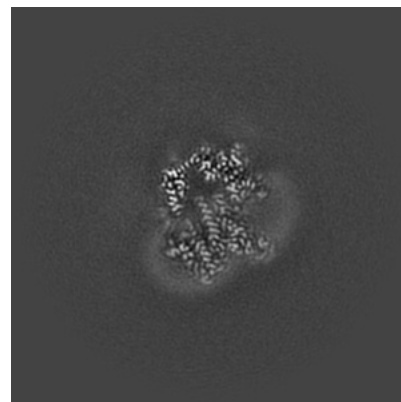
6.3.1 Primary map



X Index: 177

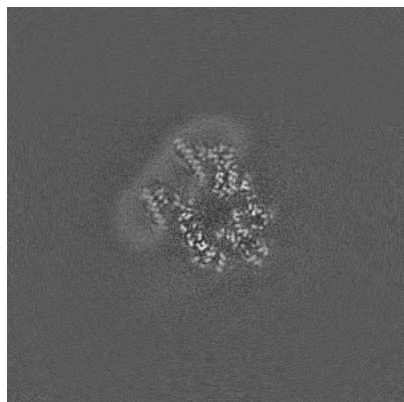


Y Index: 230

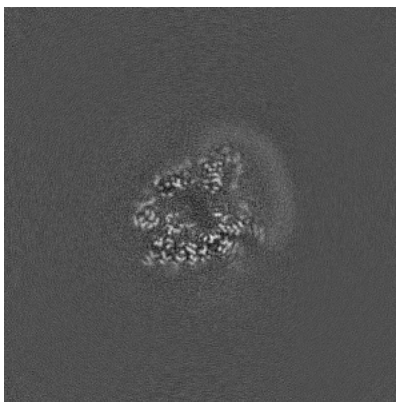


Z Index: 207

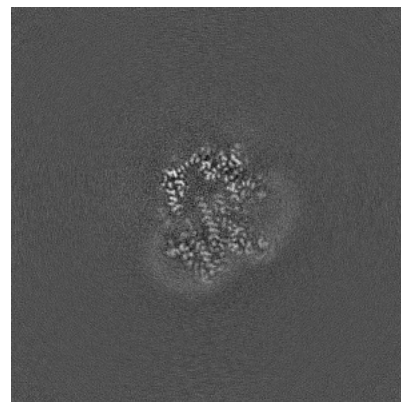
6.3.2 Raw map



X Index: 177



Y Index: 225

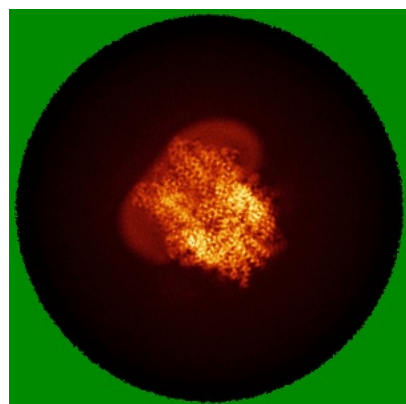


Z Index: 207

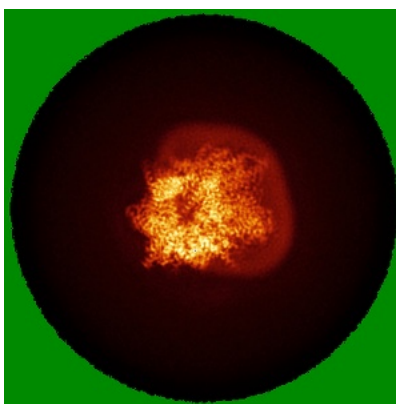
The images above show the largest variance slices of the map in three orthogonal directions.

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

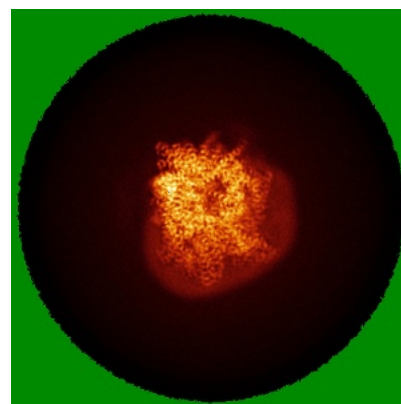
6.4.1 Primary map



X

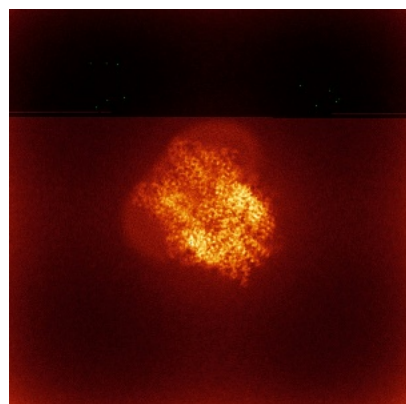


Y

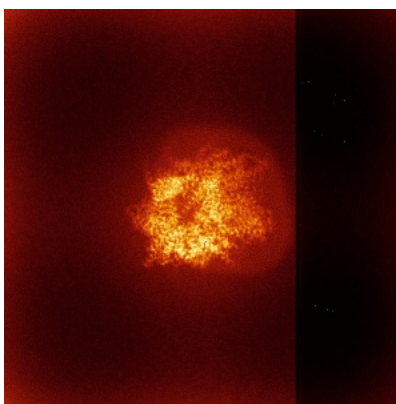


Z

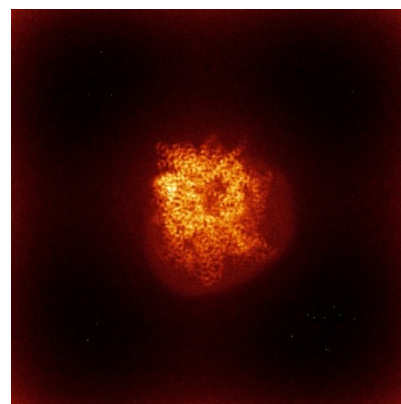
6.4.2 Raw map



X



Y

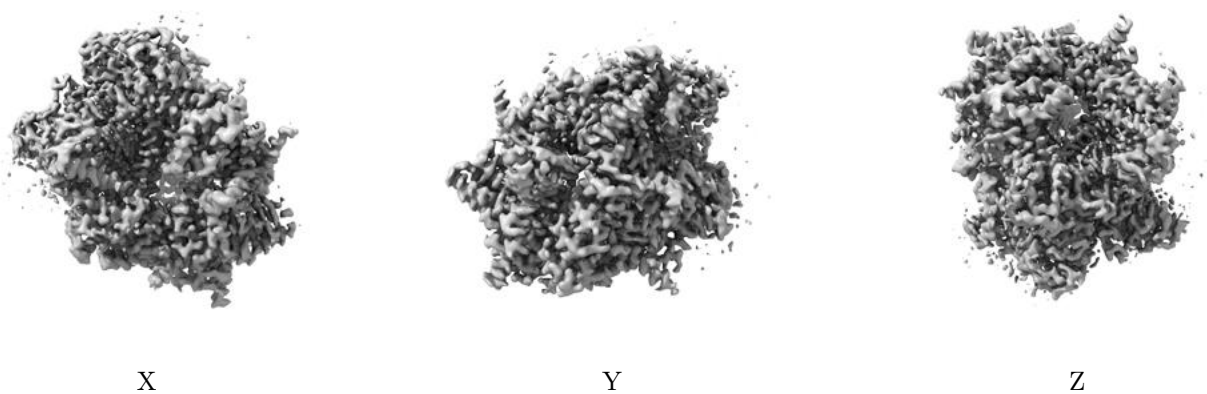


Z

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.

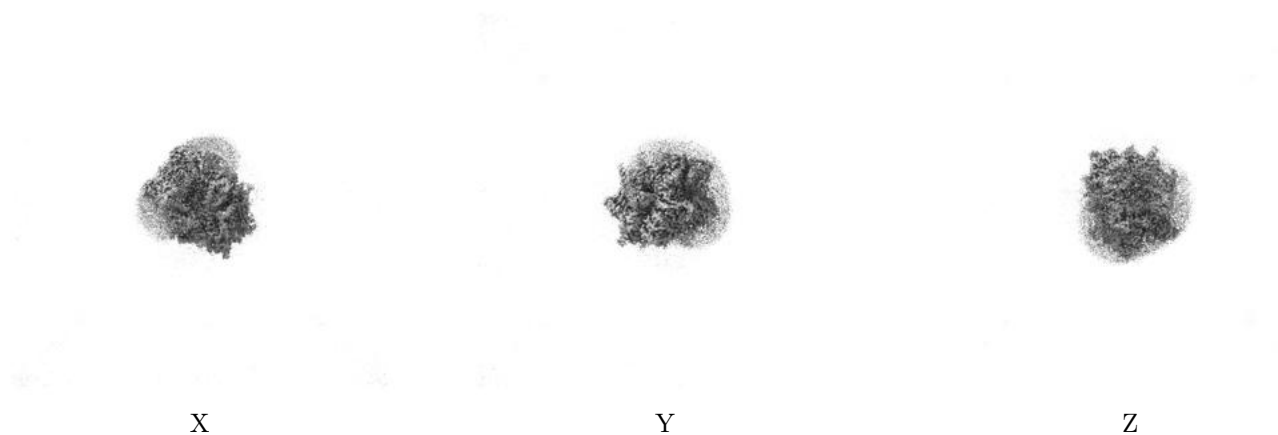
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

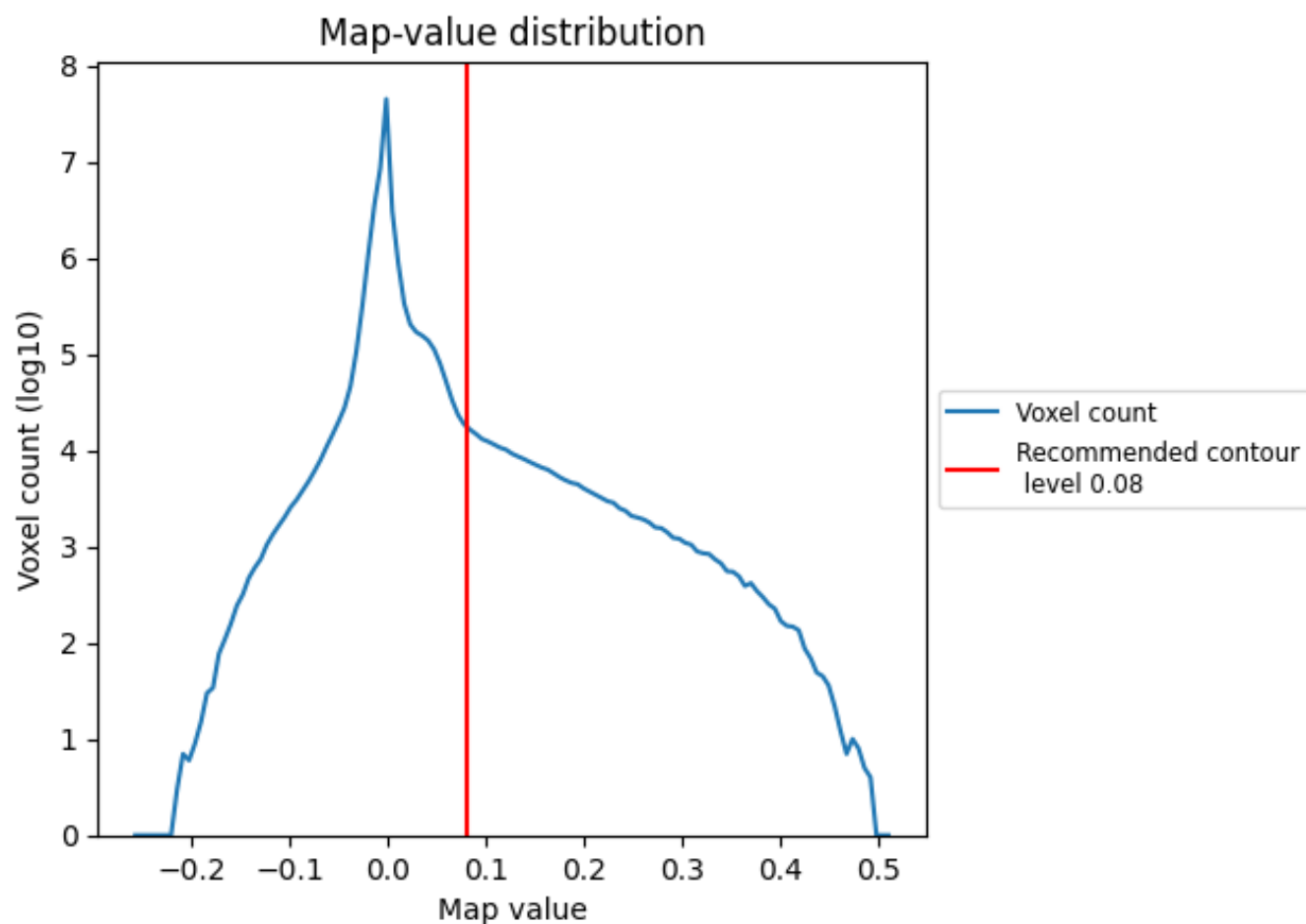
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

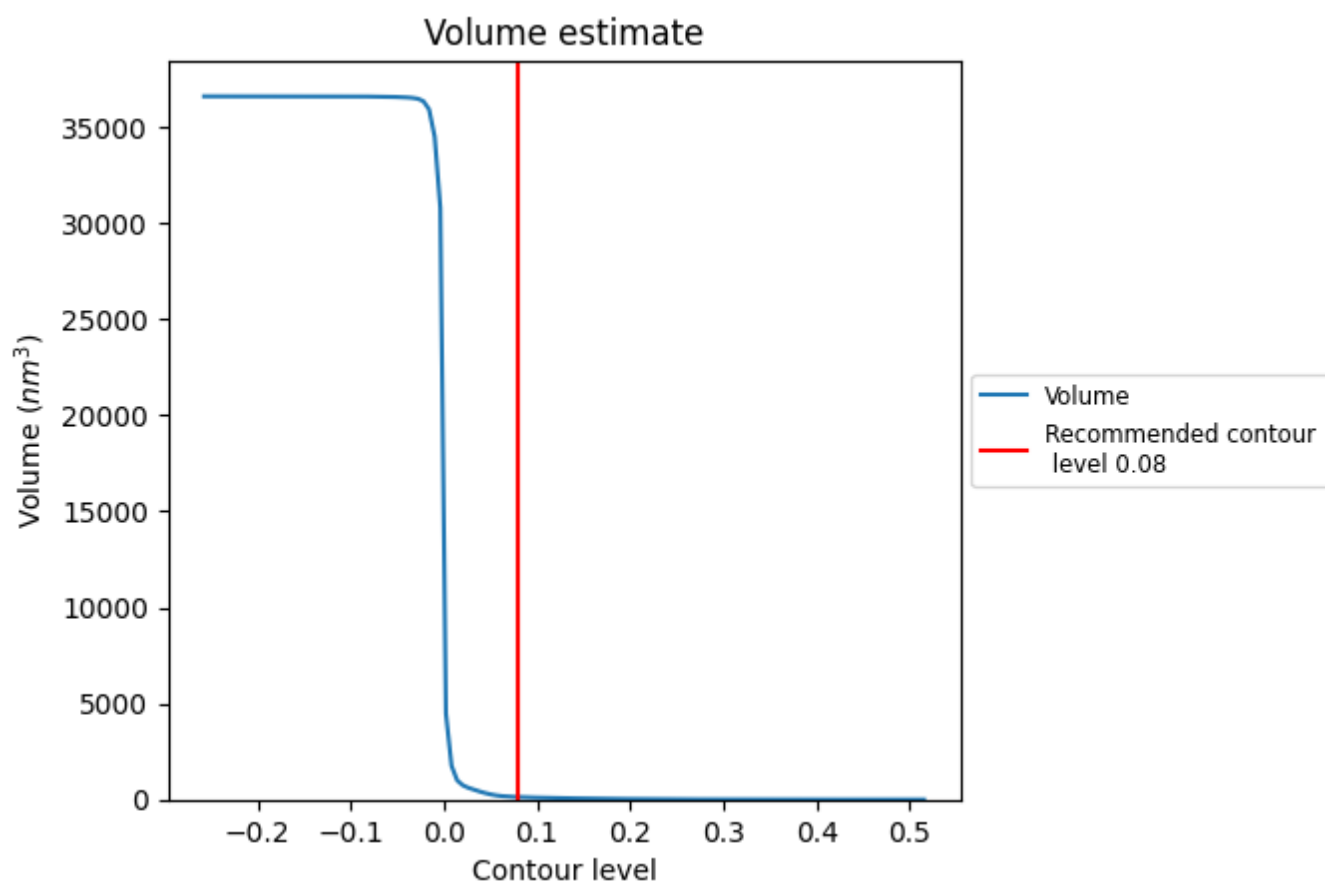
This section contains the results of statistical analysis of the map.

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.

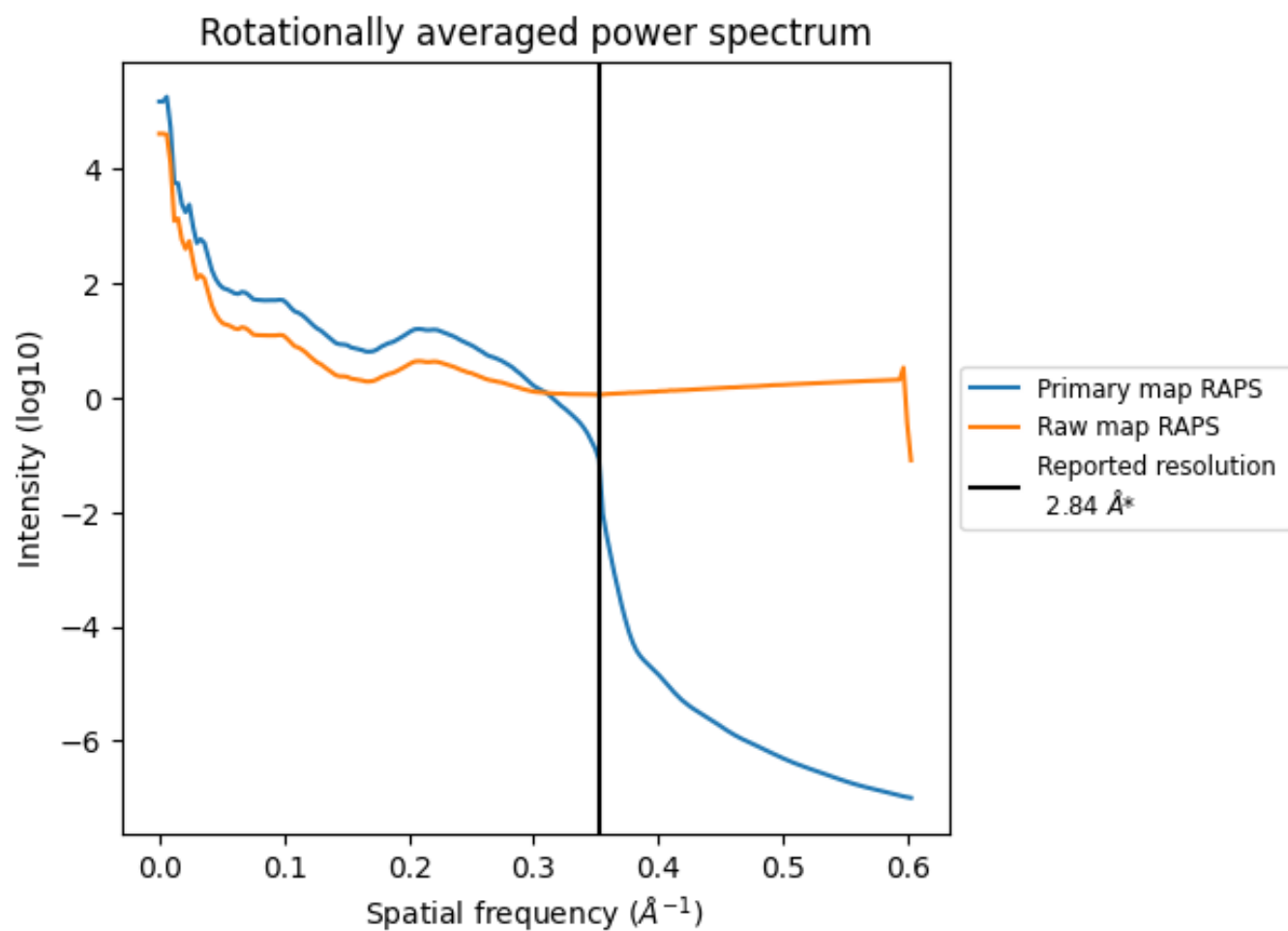
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 131 nm³; this corresponds to an approximate mass of 118 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 ⓘ

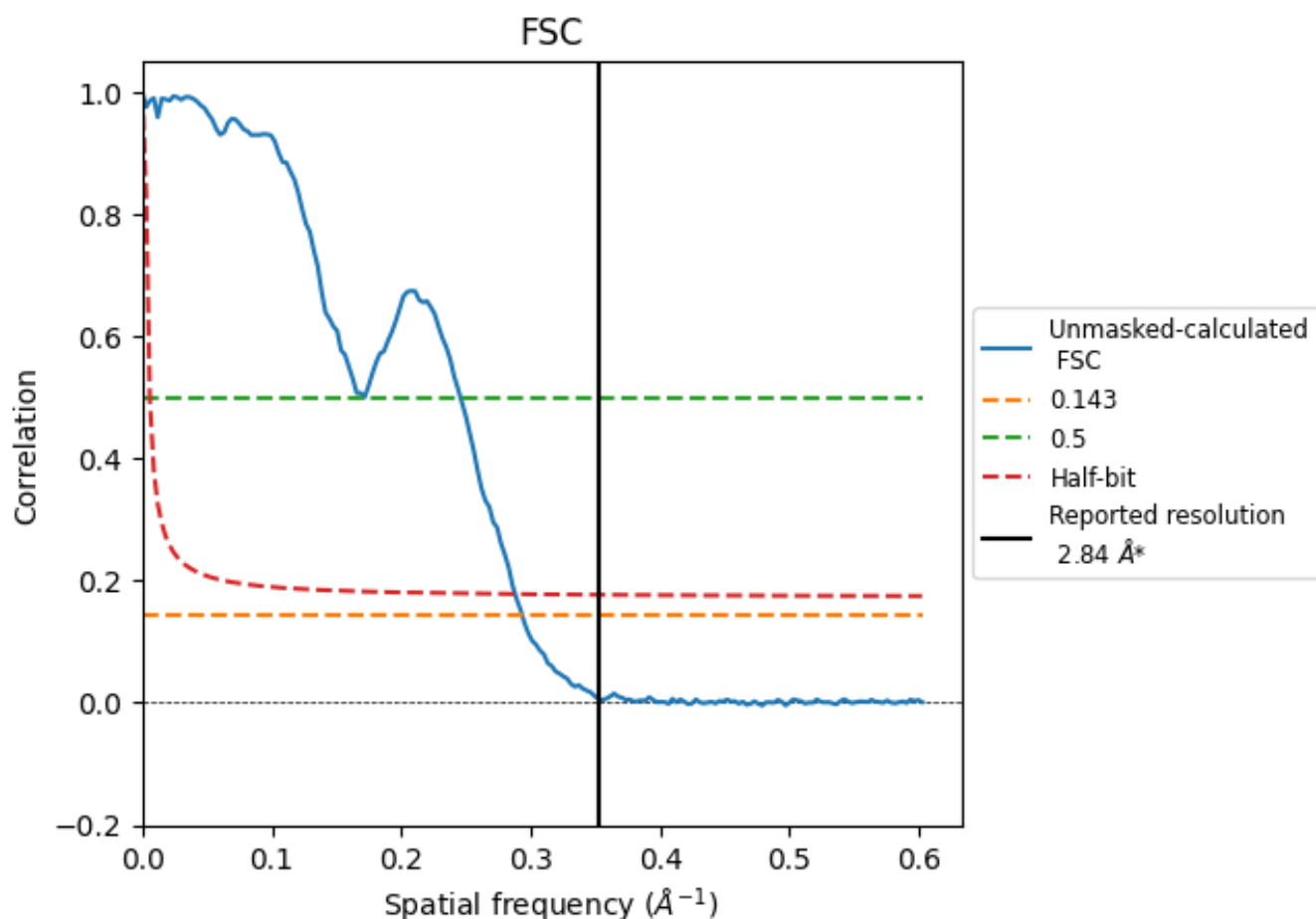


*Reported resolution corresponds to spatial frequency of 0.352 Å⁻¹

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 0.352 \AA^{-1}

8.2 Resolution estimates [i](#)

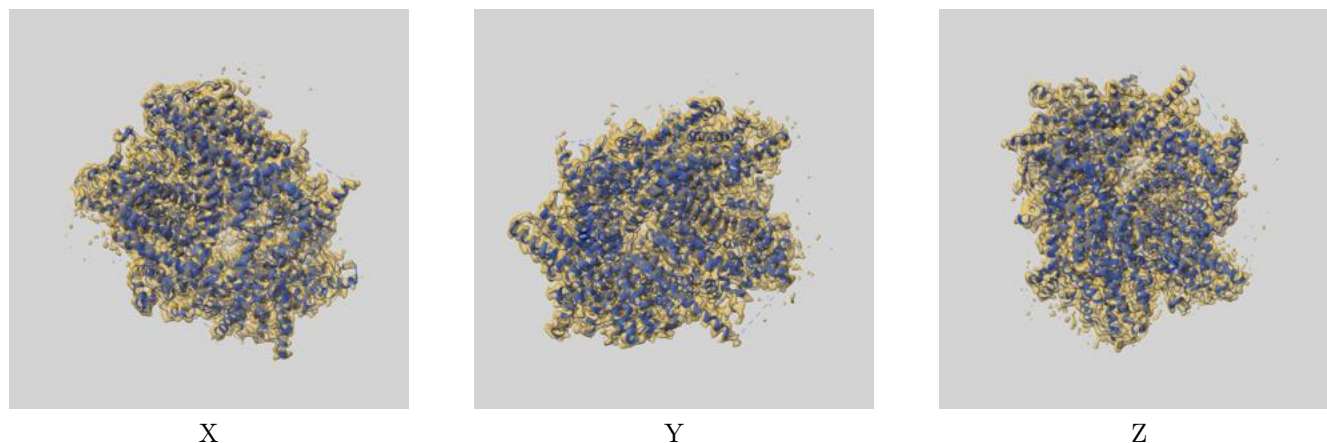
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.41	5.83	3.47

*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 3.41 differs from the reported value 2.84 by more than 10 %

9 Map-model fit [i](#)

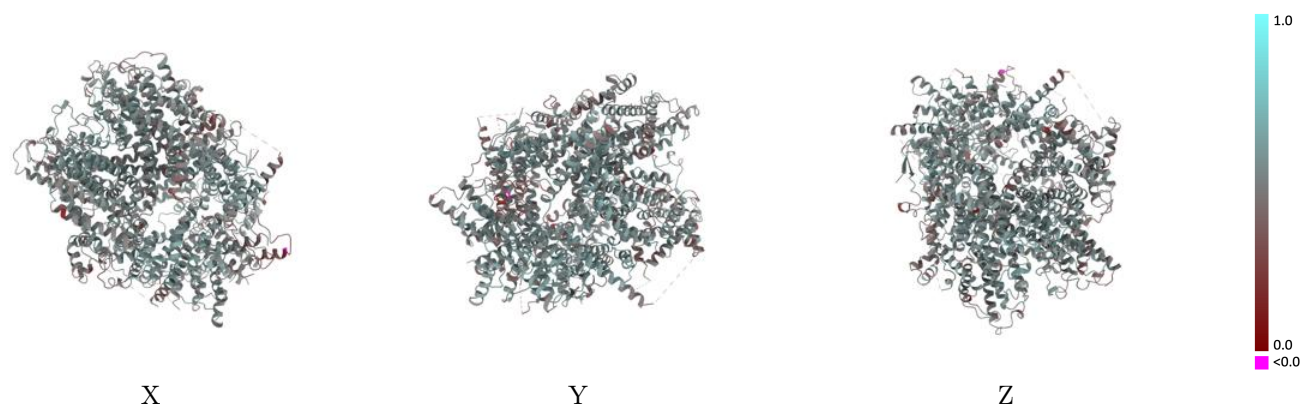
This section contains information regarding the fit between EMDB map EMD-62060 and PDB model 9K4I. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



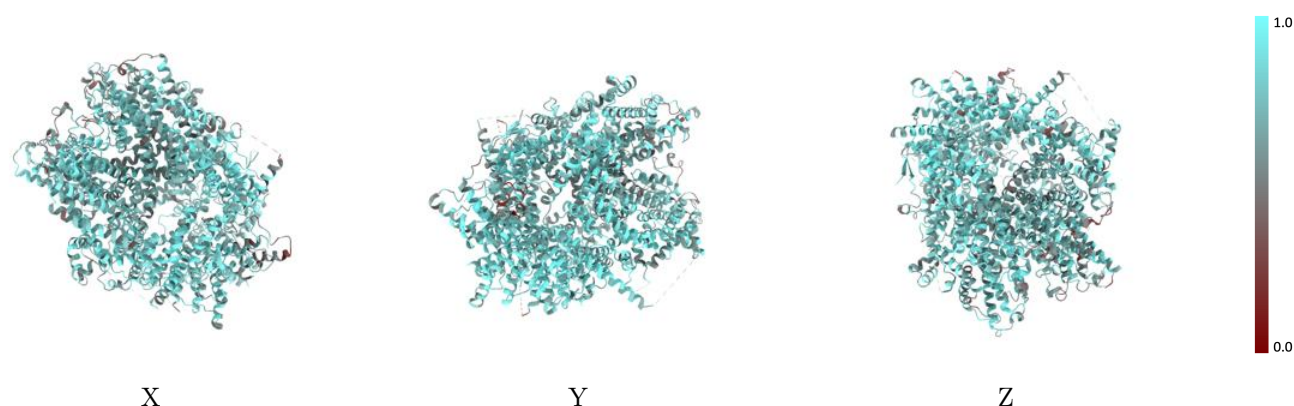
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



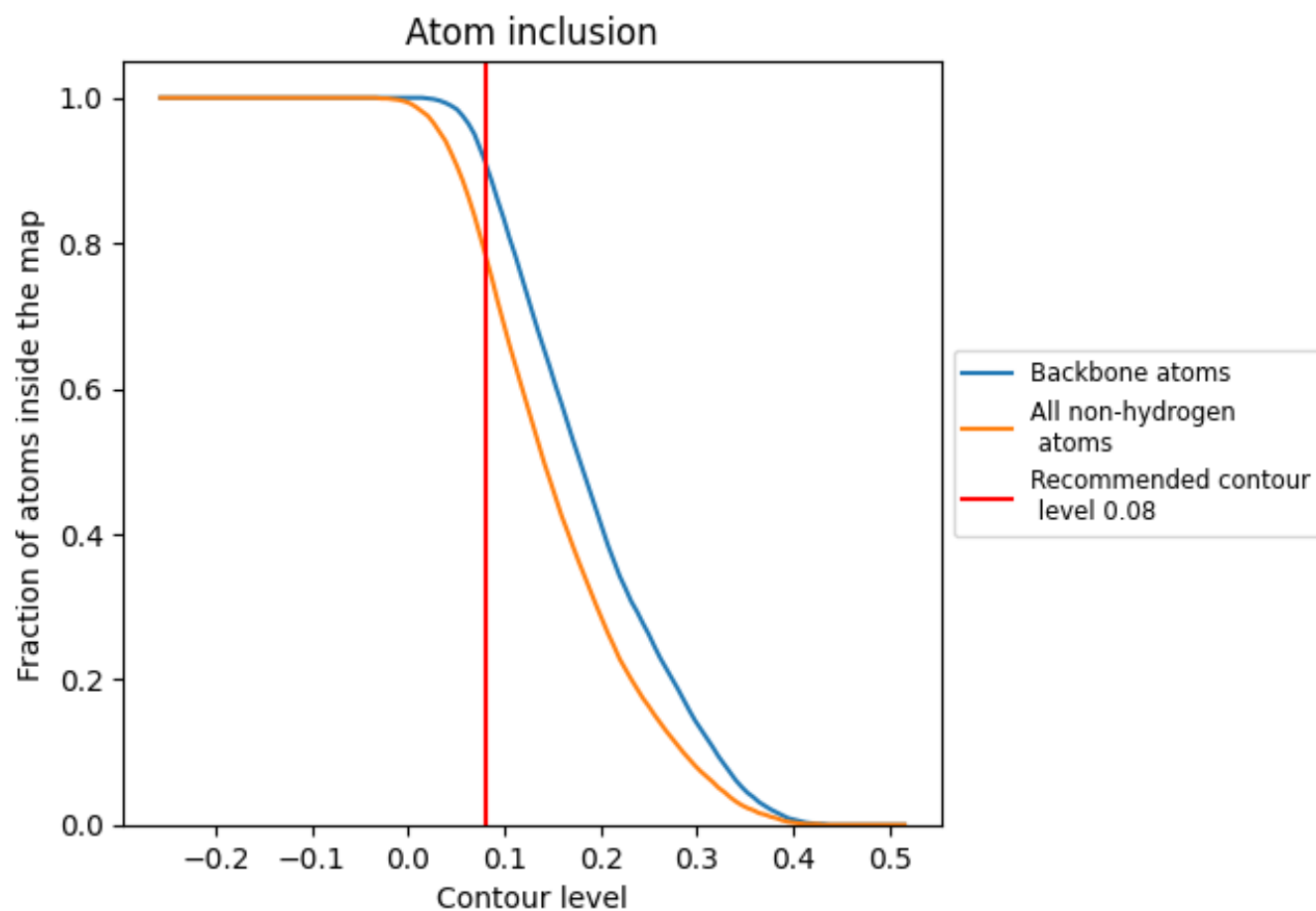
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 79% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7860	<div></div> 0.5160
A	<div></div> 0.7970	<div></div> 0.5220
B	<div></div> 0.7400	<div></div> 0.4960
C	<div></div> 0.7880	<div></div> 0.5190
D	<div></div> 0.8160	<div></div> 0.5270

