



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 02:19 PM UTC

PDB ID : 8QYK / pdb_00008qyk
EMDB ID : EMD-18756
Title : Zorya anti-bacteriophage defense system ZorAB, ZorA delta_359-592, ZorA tail middle deletion.
Authors : Hu, H.; Taylor, N.M.I.
Deposited on : 2023-10-26
Resolution : 2.07 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

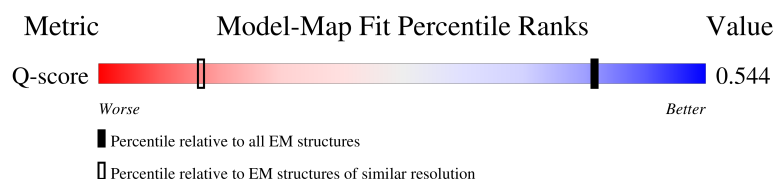
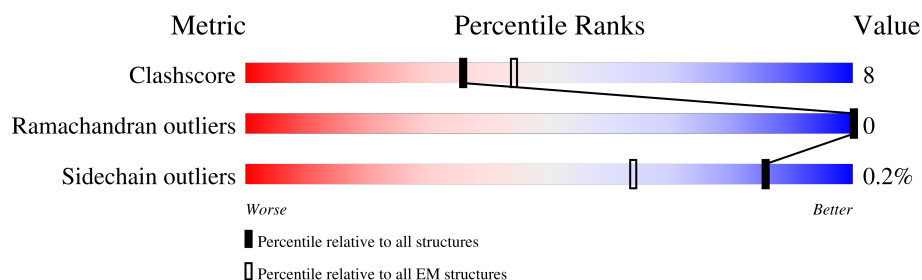
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

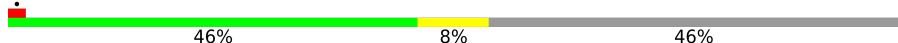
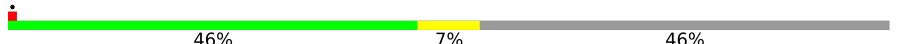
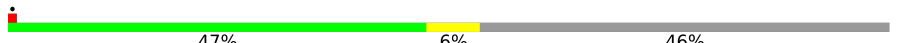
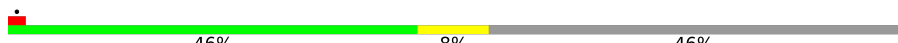
The reported resolution of this entry is 2.07 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1932 (1.58 - 2.57)

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	495	
1	B	495	
1	C	495	
1	D	495	

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Mol	Chain	Length	Quality of chain
1	E	495	44% 9% 46%
2	F	246	50% 82% 18%
2	G	246	50% 77% 23%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16182 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 Anti-phage defense ZorAB system ZorA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	265	Total	C	N	O	S	1	0
			2129	1384	344	396	5		
1	B	265	Total	C	N	O	S	0	0
			2120	1379	340	396	5		
1	C	265	Total	C	N	O	S	0	0
			2120	1379	340	396	5		
1	D	265	Total	C	N	O	S	0	0
			2120	1379	340	396	5		
1	E	265	Total	C	N	O	S	1	0
			2127	1384	342	396	5		

There are 680 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	360	SER	-	expression tag	UNP A0A0V7WZR2
A	361	ALA	-	expression tag	UNP A0A0V7WZR2
A	362	GLY	-	expression tag	UNP A0A0V7WZR2
A	363	SER	-	expression tag	UNP A0A0V7WZR2
A	364	SER	-	expression tag	UNP A0A0V7WZR2
A	365	LEU	-	expression tag	UNP A0A0V7WZR2
A	366	SER	-	expression tag	UNP A0A0V7WZR2
A	367	LEU	-	expression tag	UNP A0A0V7WZR2
A	368	ALA	-	expression tag	UNP A0A0V7WZR2
A	369	THR	-	expression tag	UNP A0A0V7WZR2
A	370	SER	-	expression tag	UNP A0A0V7WZR2
A	371	GLU	-	expression tag	UNP A0A0V7WZR2
A	372	LEU	-	expression tag	UNP A0A0V7WZR2
A	373	THR	-	expression tag	UNP A0A0V7WZR2
A	374	SER	-	expression tag	UNP A0A0V7WZR2
A	375	VAL	-	expression tag	UNP A0A0V7WZR2
A	376	VAL	-	expression tag	UNP A0A0V7WZR2
A	377	ALA	-	expression tag	UNP A0A0V7WZR2
A	378	ASP	-	expression tag	UNP A0A0V7WZR2
A	379	TYR	-	expression tag	UNP A0A0V7WZR2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ARG	-	expression tag	UNP A0A0V7WZR2
A	381	ASN	-	expression tag	UNP A0A0V7WZR2
A	382	ASN	-	expression tag	UNP A0A0V7WZR2
A	383	ARG	-	expression tag	UNP A0A0V7WZR2
A	384	GLU	-	expression tag	UNP A0A0V7WZR2
A	385	ALA	-	expression tag	UNP A0A0V7WZR2
A	386	VAL	-	expression tag	UNP A0A0V7WZR2
A	387	SER	-	expression tag	UNP A0A0V7WZR2
A	388	LYS	-	expression tag	UNP A0A0V7WZR2
A	389	SER	-	expression tag	UNP A0A0V7WZR2
A	390	ILE	-	expression tag	UNP A0A0V7WZR2
A	391	ALA	-	expression tag	UNP A0A0V7WZR2
A	392	MET	-	expression tag	UNP A0A0V7WZR2
A	393	LEU	-	expression tag	UNP A0A0V7WZR2
A	394	GLU	-	expression tag	UNP A0A0V7WZR2
A	395	LEU	-	expression tag	UNP A0A0V7WZR2
A	396	LEU	-	expression tag	UNP A0A0V7WZR2
A	397	ALA	-	expression tag	UNP A0A0V7WZR2
A	398	ALA	-	expression tag	UNP A0A0V7WZR2
A	399	ASN	-	expression tag	UNP A0A0V7WZR2
A	400	THR	-	expression tag	UNP A0A0V7WZR2
A	401	GLN	-	expression tag	UNP A0A0V7WZR2
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A	403	GLU	-	expression tag	UNP A0A0V7WZR2
A	404	GLN	-	expression tag	UNP A0A0V7WZR2
A	405	THR	-	expression tag	UNP A0A0V7WZR2
A	406	THR	-	expression tag	UNP A0A0V7WZR2
A	407	ARG	-	expression tag	UNP A0A0V7WZR2
A	408	ASN	-	expression tag	UNP A0A0V7WZR2
A	409	GLN	-	expression tag	UNP A0A0V7WZR2
A	410	PHE	-	expression tag	UNP A0A0V7WZR2
A	411	ILE	-	expression tag	UNP A0A0V7WZR2
A	412	ALA	-	expression tag	UNP A0A0V7WZR2
A	413	ASP	-	expression tag	UNP A0A0V7WZR2
A	414	LEU	-	expression tag	UNP A0A0V7WZR2
A	415	LYS	-	expression tag	UNP A0A0V7WZR2
A	416	GLN	-	expression tag	UNP A0A0V7WZR2
A	417	HIS	-	expression tag	UNP A0A0V7WZR2
A	418	GLY	-	expression tag	UNP A0A0V7WZR2
A	419	GLU	-	expression tag	UNP A0A0V7WZR2
A	420	ARG	-	expression tag	UNP A0A0V7WZR2
A	421	LEU	-	expression tag	UNP A0A0V7WZR2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	422	GLN	-	expression tag	UNP A0A0V7WZR2
A	423	SER	-	expression tag	UNP A0A0V7WZR2
A	424	TYR	-	expression tag	UNP A0A0V7WZR2
A	425	ASN	-	expression tag	UNP A0A0V7WZR2
A	426	ARG	-	expression tag	UNP A0A0V7WZR2
A	427	GLU	-	expression tag	UNP A0A0V7WZR2
A	428	ALA	-	expression tag	UNP A0A0V7WZR2
A	429	GLN	-	expression tag	UNP A0A0V7WZR2
A	430	VAL	-	expression tag	UNP A0A0V7WZR2
A	431	PHE	-	expression tag	UNP A0A0V7WZR2
A	432	MET	-	expression tag	UNP A0A0V7WZR2
A	433	GLU	-	expression tag	UNP A0A0V7WZR2
A	434	ASN	-	expression tag	UNP A0A0V7WZR2
A	435	VAL	-	expression tag	UNP A0A0V7WZR2
A	436	SER	-	expression tag	UNP A0A0V7WZR2
A	437	ASP	-	expression tag	UNP A0A0V7WZR2
A	438	VAL	-	expression tag	UNP A0A0V7WZR2
A	439	LEU	-	expression tag	UNP A0A0V7WZR2
A	440	GLY	-	expression tag	UNP A0A0V7WZR2
A	441	LYS	-	expression tag	UNP A0A0V7WZR2
A	442	GLY	-	expression tag	UNP A0A0V7WZR2
A	443	PHE	-	expression tag	UNP A0A0V7WZR2
A	444	GLU	-	expression tag	UNP A0A0V7WZR2
A	445	ASP	-	expression tag	UNP A0A0V7WZR2
A	446	PHE	-	expression tag	UNP A0A0V7WZR2
A	447	SER	-	expression tag	UNP A0A0V7WZR2
A	448	GLU	-	expression tag	UNP A0A0V7WZR2
A	449	GLY	-	expression tag	UNP A0A0V7WZR2
A	450	VAL	-	expression tag	UNP A0A0V7WZR2
A	451	SER	-	expression tag	UNP A0A0V7WZR2
A	452	ARG	-	expression tag	UNP A0A0V7WZR2
A	453	SER	-	expression tag	UNP A0A0V7WZR2
A	454	LEU	-	expression tag	UNP A0A0V7WZR2
A	455	ASP	-	expression tag	UNP A0A0V7WZR2
A	456	LYS	-	expression tag	UNP A0A0V7WZR2
A	457	THR	-	expression tag	UNP A0A0V7WZR2
A	458	LEU	-	expression tag	UNP A0A0V7WZR2
A	459	GLY	-	expression tag	UNP A0A0V7WZR2
A	460	LYS	-	expression tag	UNP A0A0V7WZR2
A	461	LEU	-	expression tag	UNP A0A0V7WZR2
A	462	ASP	-	expression tag	UNP A0A0V7WZR2
A	463	VAL	-	expression tag	UNP A0A0V7WZR2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	464	GLU	-	expression tag	UNP A0A0V7WZR2
A	465	MET	-	expression tag	UNP A0A0V7WZR2
A	466	ALA	-	expression tag	UNP A0A0V7WZR2
A	467	LYS	-	expression tag	UNP A0A0V7WZR2
A	468	ALA	-	expression tag	UNP A0A0V7WZR2
A	469	SER	-	expression tag	UNP A0A0V7WZR2
A	470	ASN	-	expression tag	UNP A0A0V7WZR2
A	471	LEU	-	expression tag	UNP A0A0V7WZR2
A	472	LEU	-	expression tag	UNP A0A0V7WZR2
A	473	ALA	-	expression tag	UNP A0A0V7WZR2
A	474	GLY	-	expression tag	UNP A0A0V7WZR2
A	475	SER	-	expression tag	UNP A0A0V7WZR2
A	476	VAL	-	expression tag	UNP A0A0V7WZR2
A	477	GLU	-	expression tag	UNP A0A0V7WZR2
A	478	GLN	-	expression tag	UNP A0A0V7WZR2
A	479	LEU	-	expression tag	UNP A0A0V7WZR2
A	480	GLY	-	expression tag	UNP A0A0V7WZR2
A	481	GLU	-	expression tag	UNP A0A0V7WZR2
A	482	SER	-	expression tag	UNP A0A0V7WZR2
A	483	VAL	-	expression tag	UNP A0A0V7WZR2
A	484	SER	-	expression tag	UNP A0A0V7WZR2
A	485	GLU	-	expression tag	UNP A0A0V7WZR2
A	486	LEU	-	expression tag	UNP A0A0V7WZR2
A	487	ASP	-	expression tag	UNP A0A0V7WZR2
A	488	ASP	-	expression tag	UNP A0A0V7WZR2
A	489	VAL	-	expression tag	UNP A0A0V7WZR2
A	490	LEU	-	expression tag	UNP A0A0V7WZR2
A	491	SER	-	expression tag	UNP A0A0V7WZR2
A	492	ARG	-	expression tag	UNP A0A0V7WZR2
A	493	VAL	-	expression tag	UNP A0A0V7WZR2
A	494	ARG	-	expression tag	UNP A0A0V7WZR2
A	495	THR	-	expression tag	UNP A0A0V7WZR2
B	360	SER	-	expression tag	UNP A0A0V7WZR2
B	361	ALA	-	expression tag	UNP A0A0V7WZR2
B	362	GLY	-	expression tag	UNP A0A0V7WZR2
B	363	SER	-	expression tag	UNP A0A0V7WZR2
B	364	SER	-	expression tag	UNP A0A0V7WZR2
B	365	LEU	-	expression tag	UNP A0A0V7WZR2
B	366	SER	-	expression tag	UNP A0A0V7WZR2
B	367	LEU	-	expression tag	UNP A0A0V7WZR2
B	368	ALA	-	expression tag	UNP A0A0V7WZR2
B	369	THR	-	expression tag	UNP A0A0V7WZR2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	370	SER	-	expression tag	UNP A0A0V7WZR2
B	371	GLU	-	expression tag	UNP A0A0V7WZR2
B	372	LEU	-	expression tag	UNP A0A0V7WZR2
B	373	THR	-	expression tag	UNP A0A0V7WZR2
B	374	SER	-	expression tag	UNP A0A0V7WZR2
B	375	VAL	-	expression tag	UNP A0A0V7WZR2
B	376	VAL	-	expression tag	UNP A0A0V7WZR2
B	377	ALA	-	expression tag	UNP A0A0V7WZR2
B	378	ASP	-	expression tag	UNP A0A0V7WZR2
B	379	TYR	-	expression tag	UNP A0A0V7WZR2
B	380	ARG	-	expression tag	UNP A0A0V7WZR2
B	381	ASN	-	expression tag	UNP A0A0V7WZR2
B	382	ASN	-	expression tag	UNP A0A0V7WZR2
B	383	ARG	-	expression tag	UNP A0A0V7WZR2
B	384	GLU	-	expression tag	UNP A0A0V7WZR2
B	385	ALA	-	expression tag	UNP A0A0V7WZR2
B	386	VAL	-	expression tag	UNP A0A0V7WZR2
B	387	SER	-	expression tag	UNP A0A0V7WZR2
B	388	LYS	-	expression tag	UNP A0A0V7WZR2
B	389	SER	-	expression tag	UNP A0A0V7WZR2
B	390	ILE	-	expression tag	UNP A0A0V7WZR2
B	391	ALA	-	expression tag	UNP A0A0V7WZR2
B	392	MET	-	expression tag	UNP A0A0V7WZR2
B	393	LEU	-	expression tag	UNP A0A0V7WZR2
B	394	GLU	-	expression tag	UNP A0A0V7WZR2
B	395	LEU	-	expression tag	UNP A0A0V7WZR2
B	396	LEU	-	expression tag	UNP A0A0V7WZR2
B	397	ALA	-	expression tag	UNP A0A0V7WZR2
B	398	ALA	-	expression tag	UNP A0A0V7WZR2
B	399	ASN	-	expression tag	UNP A0A0V7WZR2
B	400	THR	-	expression tag	UNP A0A0V7WZR2
B	401	GLN	-	expression tag	UNP A0A0V7WZR2
B	402	SER	-	expression tag	UNP A0A0V7WZR2
B	403	GLU	-	expression tag	UNP A0A0V7WZR2
B	404	GLN	-	expression tag	UNP A0A0V7WZR2
B	405	THR	-	expression tag	UNP A0A0V7WZR2
B	406	THR	-	expression tag	UNP A0A0V7WZR2
B	407	ARG	-	expression tag	UNP A0A0V7WZR2
B	408	ASN	-	expression tag	UNP A0A0V7WZR2
B	409	GLN	-	expression tag	UNP A0A0V7WZR2
B	410	PHE	-	expression tag	UNP A0A0V7WZR2
B	411	ILE	-	expression tag	UNP A0A0V7WZR2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	412	ALA	-	expression tag	UNP A0A0V7WZR2
B	413	ASP	-	expression tag	UNP A0A0V7WZR2
B	414	LEU	-	expression tag	UNP A0A0V7WZR2
B	415	LYS	-	expression tag	UNP A0A0V7WZR2
B	416	GLN	-	expression tag	UNP A0A0V7WZR2
B	417	HIS	-	expression tag	UNP A0A0V7WZR2
B	418	GLY	-	expression tag	UNP A0A0V7WZR2
B	419	GLU	-	expression tag	UNP A0A0V7WZR2
B	420	ARG	-	expression tag	UNP A0A0V7WZR2
B	421	LEU	-	expression tag	UNP A0A0V7WZR2
B	422	GLN	-	expression tag	UNP A0A0V7WZR2
B	423	SER	-	expression tag	UNP A0A0V7WZR2
B	424	TYR	-	expression tag	UNP A0A0V7WZR2
B	425	ASN	-	expression tag	UNP A0A0V7WZR2
B	426	ARG	-	expression tag	UNP A0A0V7WZR2
B	427	GLU	-	expression tag	UNP A0A0V7WZR2
B	428	ALA	-	expression tag	UNP A0A0V7WZR2
B	429	GLN	-	expression tag	UNP A0A0V7WZR2
B	430	VAL	-	expression tag	UNP A0A0V7WZR2
B	431	PHE	-	expression tag	UNP A0A0V7WZR2
B	432	MET	-	expression tag	UNP A0A0V7WZR2
B	433	GLU	-	expression tag	UNP A0A0V7WZR2
B	434	ASN	-	expression tag	UNP A0A0V7WZR2
B	435	VAL	-	expression tag	UNP A0A0V7WZR2
B	436	SER	-	expression tag	UNP A0A0V7WZR2
B	437	ASP	-	expression tag	UNP A0A0V7WZR2
B	438	VAL	-	expression tag	UNP A0A0V7WZR2
B	439	LEU	-	expression tag	UNP A0A0V7WZR2
B	440	GLY	-	expression tag	UNP A0A0V7WZR2
B	441	LYS	-	expression tag	UNP A0A0V7WZR2
B	442	GLY	-	expression tag	UNP A0A0V7WZR2
B	443	PHE	-	expression tag	UNP A0A0V7WZR2
B	444	GLU	-	expression tag	UNP A0A0V7WZR2
B	445	ASP	-	expression tag	UNP A0A0V7WZR2
B	446	PHE	-	expression tag	UNP A0A0V7WZR2
B	447	SER	-	expression tag	UNP A0A0V7WZR2
B	448	GLU	-	expression tag	UNP A0A0V7WZR2
B	449	GLY	-	expression tag	UNP A0A0V7WZR2
B	450	VAL	-	expression tag	UNP A0A0V7WZR2
B	451	SER	-	expression tag	UNP A0A0V7WZR2
B	452	ARG	-	expression tag	UNP A0A0V7WZR2
B	453	SER	-	expression tag	UNP A0A0V7WZR2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	454	LEU	-	expression tag	UNP A0A0V7WZR2
B	455	ASP	-	expression tag	UNP A0A0V7WZR2
B	456	LYS	-	expression tag	UNP A0A0V7WZR2
B	457	THR	-	expression tag	UNP A0A0V7WZR2
B	458	LEU	-	expression tag	UNP A0A0V7WZR2
B	459	GLY	-	expression tag	UNP A0A0V7WZR2
B	460	LYS	-	expression tag	UNP A0A0V7WZR2
B	461	LEU	-	expression tag	UNP A0A0V7WZR2
B	462	ASP	-	expression tag	UNP A0A0V7WZR2
B	463	VAL	-	expression tag	UNP A0A0V7WZR2
B	464	GLU	-	expression tag	UNP A0A0V7WZR2
B	465	MET	-	expression tag	UNP A0A0V7WZR2
B	466	ALA	-	expression tag	UNP A0A0V7WZR2
B	467	LYS	-	expression tag	UNP A0A0V7WZR2
B	468	ALA	-	expression tag	UNP A0A0V7WZR2
B	469	SER	-	expression tag	UNP A0A0V7WZR2
B	470	ASN	-	expression tag	UNP A0A0V7WZR2
B	471	LEU	-	expression tag	UNP A0A0V7WZR2
B	472	LEU	-	expression tag	UNP A0A0V7WZR2
B	473	ALA	-	expression tag	UNP A0A0V7WZR2
B	474	GLY	-	expression tag	UNP A0A0V7WZR2
B	475	SER	-	expression tag	UNP A0A0V7WZR2
B	476	VAL	-	expression tag	UNP A0A0V7WZR2
B	477	GLU	-	expression tag	UNP A0A0V7WZR2
B	478	GLN	-	expression tag	UNP A0A0V7WZR2
B	479	LEU	-	expression tag	UNP A0A0V7WZR2
B	480	GLY	-	expression tag	UNP A0A0V7WZR2
B	481	GLU	-	expression tag	UNP A0A0V7WZR2
B	482	SER	-	expression tag	UNP A0A0V7WZR2
B	483	VAL	-	expression tag	UNP A0A0V7WZR2
B	484	SER	-	expression tag	UNP A0A0V7WZR2
B	485	GLU	-	expression tag	UNP A0A0V7WZR2
B	486	LEU	-	expression tag	UNP A0A0V7WZR2
B	487	ASP	-	expression tag	UNP A0A0V7WZR2
B	488	ASP	-	expression tag	UNP A0A0V7WZR2
B	489	VAL	-	expression tag	UNP A0A0V7WZR2
B	490	LEU	-	expression tag	UNP A0A0V7WZR2
B	491	SER	-	expression tag	UNP A0A0V7WZR2
B	492	ARG	-	expression tag	UNP A0A0V7WZR2
B	493	VAL	-	expression tag	UNP A0A0V7WZR2
B	494	ARG	-	expression tag	UNP A0A0V7WZR2
B	495	THR	-	expression tag	UNP A0A0V7WZR2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	360	SER	-	expression tag	UNP A0A0V7WZR2
C	361	ALA	-	expression tag	UNP A0A0V7WZR2
C	362	GLY	-	expression tag	UNP A0A0V7WZR2
C	363	SER	-	expression tag	UNP A0A0V7WZR2
C	364	SER	-	expression tag	UNP A0A0V7WZR2
C	365	LEU	-	expression tag	UNP A0A0V7WZR2
C	366	SER	-	expression tag	UNP A0A0V7WZR2
C	367	LEU	-	expression tag	UNP A0A0V7WZR2
C	368	ALA	-	expression tag	UNP A0A0V7WZR2
C	369	THR	-	expression tag	UNP A0A0V7WZR2
C	370	SER	-	expression tag	UNP A0A0V7WZR2
C	371	GLU	-	expression tag	UNP A0A0V7WZR2
C	372	LEU	-	expression tag	UNP A0A0V7WZR2
C	373	THR	-	expression tag	UNP A0A0V7WZR2
C	374	SER	-	expression tag	UNP A0A0V7WZR2
C	375	VAL	-	expression tag	UNP A0A0V7WZR2
C	376	VAL	-	expression tag	UNP A0A0V7WZR2
C	377	ALA	-	expression tag	UNP A0A0V7WZR2
C	378	ASP	-	expression tag	UNP A0A0V7WZR2
C	379	TYR	-	expression tag	UNP A0A0V7WZR2
C	380	ARG	-	expression tag	UNP A0A0V7WZR2
C	381	ASN	-	expression tag	UNP A0A0V7WZR2
C	382	ASN	-	expression tag	UNP A0A0V7WZR2
C	383	ARG	-	expression tag	UNP A0A0V7WZR2
C	384	GLU	-	expression tag	UNP A0A0V7WZR2
C	385	ALA	-	expression tag	UNP A0A0V7WZR2
C	386	VAL	-	expression tag	UNP A0A0V7WZR2
C	387	SER	-	expression tag	UNP A0A0V7WZR2
C	388	LYS	-	expression tag	UNP A0A0V7WZR2
C	389	SER	-	expression tag	UNP A0A0V7WZR2
C	390	ILE	-	expression tag	UNP A0A0V7WZR2
C	391	ALA	-	expression tag	UNP A0A0V7WZR2
C	392	MET	-	expression tag	UNP A0A0V7WZR2
C	393	LEU	-	expression tag	UNP A0A0V7WZR2
C	394	GLU	-	expression tag	UNP A0A0V7WZR2
C	395	LEU	-	expression tag	UNP A0A0V7WZR2
C	396	LEU	-	expression tag	UNP A0A0V7WZR2
C	397	ALA	-	expression tag	UNP A0A0V7WZR2
C	398	ALA	-	expression tag	UNP A0A0V7WZR2
C	399	ASN	-	expression tag	UNP A0A0V7WZR2
C	400	THR	-	expression tag	UNP A0A0V7WZR2
C	401	GLN	-	expression tag	UNP A0A0V7WZR2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	402	SER	-	expression tag	UNP A0A0V7WZR2
C	403	GLU	-	expression tag	UNP A0A0V7WZR2
C	404	GLN	-	expression tag	UNP A0A0V7WZR2
C	405	THR	-	expression tag	UNP A0A0V7WZR2
C	406	THR	-	expression tag	UNP A0A0V7WZR2
C	407	ARG	-	expression tag	UNP A0A0V7WZR2
C	408	ASN	-	expression tag	UNP A0A0V7WZR2
C	409	GLN	-	expression tag	UNP A0A0V7WZR2
C	410	PHE	-	expression tag	UNP A0A0V7WZR2
C	411	ILE	-	expression tag	UNP A0A0V7WZR2
C	412	ALA	-	expression tag	UNP A0A0V7WZR2
C	413	ASP	-	expression tag	UNP A0A0V7WZR2
C	414	LEU	-	expression tag	UNP A0A0V7WZR2
C	415	LYS	-	expression tag	UNP A0A0V7WZR2
C	416	GLN	-	expression tag	UNP A0A0V7WZR2
C	417	HIS	-	expression tag	UNP A0A0V7WZR2
C	418	GLY	-	expression tag	UNP A0A0V7WZR2
C	419	GLU	-	expression tag	UNP A0A0V7WZR2
C	420	ARG	-	expression tag	UNP A0A0V7WZR2
C	421	LEU	-	expression tag	UNP A0A0V7WZR2
C	422	GLN	-	expression tag	UNP A0A0V7WZR2
C	423	SER	-	expression tag	UNP A0A0V7WZR2
C	424	TYR	-	expression tag	UNP A0A0V7WZR2
C	425	ASN	-	expression tag	UNP A0A0V7WZR2
C	426	ARG	-	expression tag	UNP A0A0V7WZR2
C	427	GLU	-	expression tag	UNP A0A0V7WZR2
C	428	ALA	-	expression tag	UNP A0A0V7WZR2
C	429	GLN	-	expression tag	UNP A0A0V7WZR2
C	430	VAL	-	expression tag	UNP A0A0V7WZR2
C	431	PHE	-	expression tag	UNP A0A0V7WZR2
C	432	MET	-	expression tag	UNP A0A0V7WZR2
C	433	GLU	-	expression tag	UNP A0A0V7WZR2
C	434	ASN	-	expression tag	UNP A0A0V7WZR2
C	435	VAL	-	expression tag	UNP A0A0V7WZR2
C	436	SER	-	expression tag	UNP A0A0V7WZR2
C	437	ASP	-	expression tag	UNP A0A0V7WZR2
C	438	VAL	-	expression tag	UNP A0A0V7WZR2
C	439	LEU	-	expression tag	UNP A0A0V7WZR2
C	440	GLY	-	expression tag	UNP A0A0V7WZR2
C	441	LYS	-	expression tag	UNP A0A0V7WZR2
C	442	GLY	-	expression tag	UNP A0A0V7WZR2
C	443	PHE	-	expression tag	UNP A0A0V7WZR2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	444	GLU	-	expression tag	UNP A0A0V7WZR2
C	445	ASP	-	expression tag	UNP A0A0V7WZR2
C	446	PHE	-	expression tag	UNP A0A0V7WZR2
C	447	SER	-	expression tag	UNP A0A0V7WZR2
C	448	GLU	-	expression tag	UNP A0A0V7WZR2
C	449	GLY	-	expression tag	UNP A0A0V7WZR2
C	450	VAL	-	expression tag	UNP A0A0V7WZR2
C	451	SER	-	expression tag	UNP A0A0V7WZR2
C	452	ARG	-	expression tag	UNP A0A0V7WZR2
C	453	SER	-	expression tag	UNP A0A0V7WZR2
C	454	LEU	-	expression tag	UNP A0A0V7WZR2
C	455	ASP	-	expression tag	UNP A0A0V7WZR2
C	456	LYS	-	expression tag	UNP A0A0V7WZR2
C	457	THR	-	expression tag	UNP A0A0V7WZR2
C	458	LEU	-	expression tag	UNP A0A0V7WZR2
C	459	GLY	-	expression tag	UNP A0A0V7WZR2
C	460	LYS	-	expression tag	UNP A0A0V7WZR2
C	461	LEU	-	expression tag	UNP A0A0V7WZR2
C	462	ASP	-	expression tag	UNP A0A0V7WZR2
C	463	VAL	-	expression tag	UNP A0A0V7WZR2
C	464	GLU	-	expression tag	UNP A0A0V7WZR2
C	465	MET	-	expression tag	UNP A0A0V7WZR2
C	466	ALA	-	expression tag	UNP A0A0V7WZR2
C	467	LYS	-	expression tag	UNP A0A0V7WZR2
C	468	ALA	-	expression tag	UNP A0A0V7WZR2
C	469	SER	-	expression tag	UNP A0A0V7WZR2
C	470	ASN	-	expression tag	UNP A0A0V7WZR2
C	471	LEU	-	expression tag	UNP A0A0V7WZR2
C	472	LEU	-	expression tag	UNP A0A0V7WZR2
C	473	ALA	-	expression tag	UNP A0A0V7WZR2
C	474	GLY	-	expression tag	UNP A0A0V7WZR2
C	475	SER	-	expression tag	UNP A0A0V7WZR2
C	476	VAL	-	expression tag	UNP A0A0V7WZR2
C	477	GLU	-	expression tag	UNP A0A0V7WZR2
C	478	GLN	-	expression tag	UNP A0A0V7WZR2
C	479	LEU	-	expression tag	UNP A0A0V7WZR2
C	480	GLY	-	expression tag	UNP A0A0V7WZR2
C	481	GLU	-	expression tag	UNP A0A0V7WZR2
C	482	SER	-	expression tag	UNP A0A0V7WZR2
C	483	VAL	-	expression tag	UNP A0A0V7WZR2
C	484	SER	-	expression tag	UNP A0A0V7WZR2
C	485	GLU	-	expression tag	UNP A0A0V7WZR2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	486	LEU	-	expression tag	UNP A0A0V7WZR2
C	487	ASP	-	expression tag	UNP A0A0V7WZR2
C	488	ASP	-	expression tag	UNP A0A0V7WZR2
C	489	VAL	-	expression tag	UNP A0A0V7WZR2
C	490	LEU	-	expression tag	UNP A0A0V7WZR2
C	491	SER	-	expression tag	UNP A0A0V7WZR2
C	492	ARG	-	expression tag	UNP A0A0V7WZR2
C	493	VAL	-	expression tag	UNP A0A0V7WZR2
C	494	ARG	-	expression tag	UNP A0A0V7WZR2
C	495	THR	-	expression tag	UNP A0A0V7WZR2
D	360	SER	-	expression tag	UNP A0A0V7WZR2
D	361	ALA	-	expression tag	UNP A0A0V7WZR2
D	362	GLY	-	expression tag	UNP A0A0V7WZR2
D	363	SER	-	expression tag	UNP A0A0V7WZR2
D	364	SER	-	expression tag	UNP A0A0V7WZR2
D	365	LEU	-	expression tag	UNP A0A0V7WZR2
D	366	SER	-	expression tag	UNP A0A0V7WZR2
D	367	LEU	-	expression tag	UNP A0A0V7WZR2
D	368	ALA	-	expression tag	UNP A0A0V7WZR2
D	369	THR	-	expression tag	UNP A0A0V7WZR2
D	370	SER	-	expression tag	UNP A0A0V7WZR2
D	371	GLU	-	expression tag	UNP A0A0V7WZR2
D	372	LEU	-	expression tag	UNP A0A0V7WZR2
D	373	THR	-	expression tag	UNP A0A0V7WZR2
D	374	SER	-	expression tag	UNP A0A0V7WZR2
D	375	VAL	-	expression tag	UNP A0A0V7WZR2
D	376	VAL	-	expression tag	UNP A0A0V7WZR2
D	377	ALA	-	expression tag	UNP A0A0V7WZR2
D	378	ASP	-	expression tag	UNP A0A0V7WZR2
D	379	TYR	-	expression tag	UNP A0A0V7WZR2
D	380	ARG	-	expression tag	UNP A0A0V7WZR2
D	381	ASN	-	expression tag	UNP A0A0V7WZR2
D	382	ASN	-	expression tag	UNP A0A0V7WZR2
D	383	ARG	-	expression tag	UNP A0A0V7WZR2
D	384	GLU	-	expression tag	UNP A0A0V7WZR2
D	385	ALA	-	expression tag	UNP A0A0V7WZR2
D	386	VAL	-	expression tag	UNP A0A0V7WZR2
D	387	SER	-	expression tag	UNP A0A0V7WZR2
D	388	LYS	-	expression tag	UNP A0A0V7WZR2
D	389	SER	-	expression tag	UNP A0A0V7WZR2
D	390	ILE	-	expression tag	UNP A0A0V7WZR2
D	391	ALA	-	expression tag	UNP A0A0V7WZR2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	392	MET	-	expression tag	UNP A0A0V7WZR2
D	393	LEU	-	expression tag	UNP A0A0V7WZR2
D	394	GLU	-	expression tag	UNP A0A0V7WZR2
D	395	LEU	-	expression tag	UNP A0A0V7WZR2
D	396	LEU	-	expression tag	UNP A0A0V7WZR2
D	397	ALA	-	expression tag	UNP A0A0V7WZR2
D	398	ALA	-	expression tag	UNP A0A0V7WZR2
D	399	ASN	-	expression tag	UNP A0A0V7WZR2
D	400	THR	-	expression tag	UNP A0A0V7WZR2
D	401	GLN	-	expression tag	UNP A0A0V7WZR2
D	402	SER	-	expression tag	UNP A0A0V7WZR2
D	403	GLU	-	expression tag	UNP A0A0V7WZR2
D	404	GLN	-	expression tag	UNP A0A0V7WZR2
D	405	THR	-	expression tag	UNP A0A0V7WZR2
D	406	THR	-	expression tag	UNP A0A0V7WZR2
D	407	ARG	-	expression tag	UNP A0A0V7WZR2
D	408	ASN	-	expression tag	UNP A0A0V7WZR2
D	409	GLN	-	expression tag	UNP A0A0V7WZR2
D	410	PHE	-	expression tag	UNP A0A0V7WZR2
D	411	ILE	-	expression tag	UNP A0A0V7WZR2
D	412	ALA	-	expression tag	UNP A0A0V7WZR2
D	413	ASP	-	expression tag	UNP A0A0V7WZR2
D	414	LEU	-	expression tag	UNP A0A0V7WZR2
D	415	LYS	-	expression tag	UNP A0A0V7WZR2
D	416	GLN	-	expression tag	UNP A0A0V7WZR2
D	417	HIS	-	expression tag	UNP A0A0V7WZR2
D	418	GLY	-	expression tag	UNP A0A0V7WZR2
D	419	GLU	-	expression tag	UNP A0A0V7WZR2
D	420	ARG	-	expression tag	UNP A0A0V7WZR2
D	421	LEU	-	expression tag	UNP A0A0V7WZR2
D	422	GLN	-	expression tag	UNP A0A0V7WZR2
D	423	SER	-	expression tag	UNP A0A0V7WZR2
D	424	TYR	-	expression tag	UNP A0A0V7WZR2
D	425	ASN	-	expression tag	UNP A0A0V7WZR2
D	426	ARG	-	expression tag	UNP A0A0V7WZR2
D	427	GLU	-	expression tag	UNP A0A0V7WZR2
D	428	ALA	-	expression tag	UNP A0A0V7WZR2
D	429	GLN	-	expression tag	UNP A0A0V7WZR2
D	430	VAL	-	expression tag	UNP A0A0V7WZR2
D	431	PHE	-	expression tag	UNP A0A0V7WZR2
D	432	MET	-	expression tag	UNP A0A0V7WZR2
D	433	GLU	-	expression tag	UNP A0A0V7WZR2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	434	ASN	-	expression tag	UNP A0A0V7WZR2
D	435	VAL	-	expression tag	UNP A0A0V7WZR2
D	436	SER	-	expression tag	UNP A0A0V7WZR2
D	437	ASP	-	expression tag	UNP A0A0V7WZR2
D	438	VAL	-	expression tag	UNP A0A0V7WZR2
D	439	LEU	-	expression tag	UNP A0A0V7WZR2
D	440	GLY	-	expression tag	UNP A0A0V7WZR2
D	441	LYS	-	expression tag	UNP A0A0V7WZR2
D	442	GLY	-	expression tag	UNP A0A0V7WZR2
D	443	PHE	-	expression tag	UNP A0A0V7WZR2
D	444	GLU	-	expression tag	UNP A0A0V7WZR2
D	445	ASP	-	expression tag	UNP A0A0V7WZR2
D	446	PHE	-	expression tag	UNP A0A0V7WZR2
D	447	SER	-	expression tag	UNP A0A0V7WZR2
D	448	GLU	-	expression tag	UNP A0A0V7WZR2
D	449	GLY	-	expression tag	UNP A0A0V7WZR2
D	450	VAL	-	expression tag	UNP A0A0V7WZR2
D	451	SER	-	expression tag	UNP A0A0V7WZR2
D	452	ARG	-	expression tag	UNP A0A0V7WZR2
D	453	SER	-	expression tag	UNP A0A0V7WZR2
D	454	LEU	-	expression tag	UNP A0A0V7WZR2
D	455	ASP	-	expression tag	UNP A0A0V7WZR2
D	456	LYS	-	expression tag	UNP A0A0V7WZR2
D	457	THR	-	expression tag	UNP A0A0V7WZR2
D	458	LEU	-	expression tag	UNP A0A0V7WZR2
D	459	GLY	-	expression tag	UNP A0A0V7WZR2
D	460	LYS	-	expression tag	UNP A0A0V7WZR2
D	461	LEU	-	expression tag	UNP A0A0V7WZR2
D	462	ASP	-	expression tag	UNP A0A0V7WZR2
D	463	VAL	-	expression tag	UNP A0A0V7WZR2
D	464	GLU	-	expression tag	UNP A0A0V7WZR2
D	465	MET	-	expression tag	UNP A0A0V7WZR2
D	466	ALA	-	expression tag	UNP A0A0V7WZR2
D	467	LYS	-	expression tag	UNP A0A0V7WZR2
D	468	ALA	-	expression tag	UNP A0A0V7WZR2
D	469	SER	-	expression tag	UNP A0A0V7WZR2
D	470	ASN	-	expression tag	UNP A0A0V7WZR2
D	471	LEU	-	expression tag	UNP A0A0V7WZR2
D	472	LEU	-	expression tag	UNP A0A0V7WZR2
D	473	ALA	-	expression tag	UNP A0A0V7WZR2
D	474	GLY	-	expression tag	UNP A0A0V7WZR2
D	475	SER	-	expression tag	UNP A0A0V7WZR2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	476	VAL	-	expression tag	UNP A0A0V7WZR2
D	477	GLU	-	expression tag	UNP A0A0V7WZR2
D	478	GLN	-	expression tag	UNP A0A0V7WZR2
D	479	LEU	-	expression tag	UNP A0A0V7WZR2
D	480	GLY	-	expression tag	UNP A0A0V7WZR2
D	481	GLU	-	expression tag	UNP A0A0V7WZR2
D	482	SER	-	expression tag	UNP A0A0V7WZR2
D	483	VAL	-	expression tag	UNP A0A0V7WZR2
D	484	SER	-	expression tag	UNP A0A0V7WZR2
D	485	GLU	-	expression tag	UNP A0A0V7WZR2
D	486	LEU	-	expression tag	UNP A0A0V7WZR2
D	487	ASP	-	expression tag	UNP A0A0V7WZR2
D	488	ASP	-	expression tag	UNP A0A0V7WZR2
D	489	VAL	-	expression tag	UNP A0A0V7WZR2
D	490	LEU	-	expression tag	UNP A0A0V7WZR2
D	491	SER	-	expression tag	UNP A0A0V7WZR2
D	492	ARG	-	expression tag	UNP A0A0V7WZR2
D	493	VAL	-	expression tag	UNP A0A0V7WZR2
D	494	ARG	-	expression tag	UNP A0A0V7WZR2
D	495	THR	-	expression tag	UNP A0A0V7WZR2
E	360	SER	-	expression tag	UNP A0A0V7WZR2
E	361	ALA	-	expression tag	UNP A0A0V7WZR2
E	362	GLY	-	expression tag	UNP A0A0V7WZR2
E	363	SER	-	expression tag	UNP A0A0V7WZR2
E	364	SER	-	expression tag	UNP A0A0V7WZR2
E	365	LEU	-	expression tag	UNP A0A0V7WZR2
E	366	SER	-	expression tag	UNP A0A0V7WZR2
E	367	LEU	-	expression tag	UNP A0A0V7WZR2
E	368	ALA	-	expression tag	UNP A0A0V7WZR2
E	369	THR	-	expression tag	UNP A0A0V7WZR2
E	370	SER	-	expression tag	UNP A0A0V7WZR2
E	371	GLU	-	expression tag	UNP A0A0V7WZR2
E	372	LEU	-	expression tag	UNP A0A0V7WZR2
E	373	THR	-	expression tag	UNP A0A0V7WZR2
E	374	SER	-	expression tag	UNP A0A0V7WZR2
E	375	VAL	-	expression tag	UNP A0A0V7WZR2
E	376	VAL	-	expression tag	UNP A0A0V7WZR2
E	377	ALA	-	expression tag	UNP A0A0V7WZR2
E	378	ASP	-	expression tag	UNP A0A0V7WZR2
E	379	TYR	-	expression tag	UNP A0A0V7WZR2
E	380	ARG	-	expression tag	UNP A0A0V7WZR2
E	381	ASN	-	expression tag	UNP A0A0V7WZR2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	382	ASN	-	expression tag	UNP A0A0V7WZR2
E	383	ARG	-	expression tag	UNP A0A0V7WZR2
E	384	GLU	-	expression tag	UNP A0A0V7WZR2
E	385	ALA	-	expression tag	UNP A0A0V7WZR2
E	386	VAL	-	expression tag	UNP A0A0V7WZR2
E	387	SER	-	expression tag	UNP A0A0V7WZR2
E	388	LYS	-	expression tag	UNP A0A0V7WZR2
E	389	SER	-	expression tag	UNP A0A0V7WZR2
E	390	ILE	-	expression tag	UNP A0A0V7WZR2
E	391	ALA	-	expression tag	UNP A0A0V7WZR2
E	392	MET	-	expression tag	UNP A0A0V7WZR2
E	393	LEU	-	expression tag	UNP A0A0V7WZR2
E	394	GLU	-	expression tag	UNP A0A0V7WZR2
E	395	LEU	-	expression tag	UNP A0A0V7WZR2
E	396	LEU	-	expression tag	UNP A0A0V7WZR2
E	397	ALA	-	expression tag	UNP A0A0V7WZR2
E	398	ALA	-	expression tag	UNP A0A0V7WZR2
E	399	ASN	-	expression tag	UNP A0A0V7WZR2
E	400	THR	-	expression tag	UNP A0A0V7WZR2
E	401	GLN	-	expression tag	UNP A0A0V7WZR2
E	402	SER	-	expression tag	UNP A0A0V7WZR2
E	403	GLU	-	expression tag	UNP A0A0V7WZR2
E	404	GLN	-	expression tag	UNP A0A0V7WZR2
E	405	THR	-	expression tag	UNP A0A0V7WZR2
E	406	THR	-	expression tag	UNP A0A0V7WZR2
E	407	ARG	-	expression tag	UNP A0A0V7WZR2
E	408	ASN	-	expression tag	UNP A0A0V7WZR2
E	409	GLN	-	expression tag	UNP A0A0V7WZR2
E	410	PHE	-	expression tag	UNP A0A0V7WZR2
E	411	ILE	-	expression tag	UNP A0A0V7WZR2
E	412	ALA	-	expression tag	UNP A0A0V7WZR2
E	413	ASP	-	expression tag	UNP A0A0V7WZR2
E	414	LEU	-	expression tag	UNP A0A0V7WZR2
E	415	LYS	-	expression tag	UNP A0A0V7WZR2
E	416	GLN	-	expression tag	UNP A0A0V7WZR2
E	417	HIS	-	expression tag	UNP A0A0V7WZR2
E	418	GLY	-	expression tag	UNP A0A0V7WZR2
E	419	GLU	-	expression tag	UNP A0A0V7WZR2
E	420	ARG	-	expression tag	UNP A0A0V7WZR2
E	421	LEU	-	expression tag	UNP A0A0V7WZR2
E	422	GLN	-	expression tag	UNP A0A0V7WZR2
E	423	SER	-	expression tag	UNP A0A0V7WZR2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	424	TYR	-	expression tag	UNP A0A0V7WZR2
E	425	ASN	-	expression tag	UNP A0A0V7WZR2
E	426	ARG	-	expression tag	UNP A0A0V7WZR2
E	427	GLU	-	expression tag	UNP A0A0V7WZR2
E	428	ALA	-	expression tag	UNP A0A0V7WZR2
E	429	GLN	-	expression tag	UNP A0A0V7WZR2
E	430	VAL	-	expression tag	UNP A0A0V7WZR2
E	431	PHE	-	expression tag	UNP A0A0V7WZR2
E	432	MET	-	expression tag	UNP A0A0V7WZR2
E	433	GLU	-	expression tag	UNP A0A0V7WZR2
E	434	ASN	-	expression tag	UNP A0A0V7WZR2
E	435	VAL	-	expression tag	UNP A0A0V7WZR2
E	436	SER	-	expression tag	UNP A0A0V7WZR2
E	437	ASP	-	expression tag	UNP A0A0V7WZR2
E	438	VAL	-	expression tag	UNP A0A0V7WZR2
E	439	LEU	-	expression tag	UNP A0A0V7WZR2
E	440	GLY	-	expression tag	UNP A0A0V7WZR2
E	441	LYS	-	expression tag	UNP A0A0V7WZR2
E	442	GLY	-	expression tag	UNP A0A0V7WZR2
E	443	PHE	-	expression tag	UNP A0A0V7WZR2
E	444	GLU	-	expression tag	UNP A0A0V7WZR2
E	445	ASP	-	expression tag	UNP A0A0V7WZR2
E	446	PHE	-	expression tag	UNP A0A0V7WZR2
E	447	SER	-	expression tag	UNP A0A0V7WZR2
E	448	GLU	-	expression tag	UNP A0A0V7WZR2
E	449	GLY	-	expression tag	UNP A0A0V7WZR2
E	450	VAL	-	expression tag	UNP A0A0V7WZR2
E	451	SER	-	expression tag	UNP A0A0V7WZR2
E	452	ARG	-	expression tag	UNP A0A0V7WZR2
E	453	SER	-	expression tag	UNP A0A0V7WZR2
E	454	LEU	-	expression tag	UNP A0A0V7WZR2
E	455	ASP	-	expression tag	UNP A0A0V7WZR2
E	456	LYS	-	expression tag	UNP A0A0V7WZR2
E	457	THR	-	expression tag	UNP A0A0V7WZR2
E	458	LEU	-	expression tag	UNP A0A0V7WZR2
E	459	GLY	-	expression tag	UNP A0A0V7WZR2
E	460	LYS	-	expression tag	UNP A0A0V7WZR2
E	461	LEU	-	expression tag	UNP A0A0V7WZR2
E	462	ASP	-	expression tag	UNP A0A0V7WZR2
E	463	VAL	-	expression tag	UNP A0A0V7WZR2
E	464	GLU	-	expression tag	UNP A0A0V7WZR2
E	465	MET	-	expression tag	UNP A0A0V7WZR2

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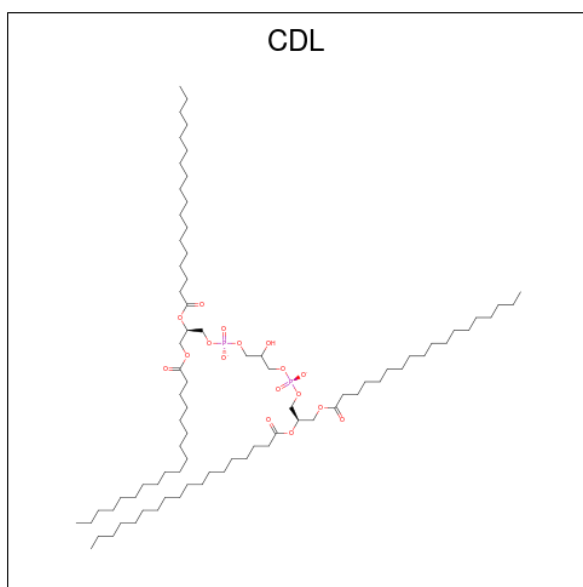
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Chain	Residue	Modelled	Actual	Comment	Reference
E	466	ALA	-	expression tag	UNP A0A0V7WZR2
E	467	LYS	-	expression tag	UNP A0A0V7WZR2
E	468	ALA	-	expression tag	UNP A0A0V7WZR2
E	469	SER	-	expression tag	UNP A0A0V7WZR2
E	470	ASN	-	expression tag	UNP A0A0V7WZR2
E	471	LEU	-	expression tag	UNP A0A0V7WZR2
E	472	LEU	-	expression tag	UNP A0A0V7WZR2
E	473	ALA	-	expression tag	UNP A0A0V7WZR2
E	474	GLY	-	expression tag	UNP A0A0V7WZR2
E	475	SER	-	expression tag	UNP A0A0V7WZR2
E	476	VAL	-	expression tag	UNP A0A0V7WZR2
E	477	GLU	-	expression tag	UNP A0A0V7WZR2
E	478	GLN	-	expression tag	UNP A0A0V7WZR2
E	479	LEU	-	expression tag	UNP A0A0V7WZR2
E	480	GLY	-	expression tag	UNP A0A0V7WZR2
E	481	GLU	-	expression tag	UNP A0A0V7WZR2
E	482	SER	-	expression tag	UNP A0A0V7WZR2
E	483	VAL	-	expression tag	UNP A0A0V7WZR2
E	484	SER	-	expression tag	UNP A0A0V7WZR2
E	485	GLU	-	expression tag	UNP A0A0V7WZR2
E	486	LEU	-	expression tag	UNP A0A0V7WZR2
E	487	ASP	-	expression tag	UNP A0A0V7WZR2
E	488	ASP	-	expression tag	UNP A0A0V7WZR2
E	489	VAL	-	expression tag	UNP A0A0V7WZR2
E	490	LEU	-	expression tag	UNP A0A0V7WZR2
E	491	SER	-	expression tag	UNP A0A0V7WZR2
E	492	ARG	-	expression tag	UNP A0A0V7WZR2
E	493	VAL	-	expression tag	UNP A0A0V7WZR2
E	494	ARG	-	expression tag	UNP A0A0V7WZR2
E	495	THR	-	expression tag	UNP A0A0V7WZR2

- Molecule 2 is a protein called Membrane protein.

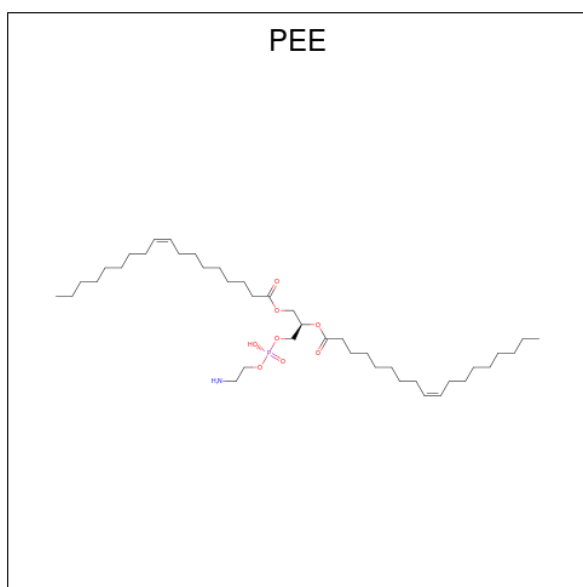
Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	246	Total	C	N	O	S	0	0
			1970	1241	353	364	12		
2	G	246	Total	C	N	O	S	0	0
			1970	1241	353	364	12		

- Molecule 3 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			100	81	17	2	
3	B	1	Total	C	O	P	0
			100	81	17	2	
3	C	1	Total	C	O	P	0
			100	81	17	2	
3	D	1	Total	C	O	P	0
			100	81	17	2	
3	E	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 4 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



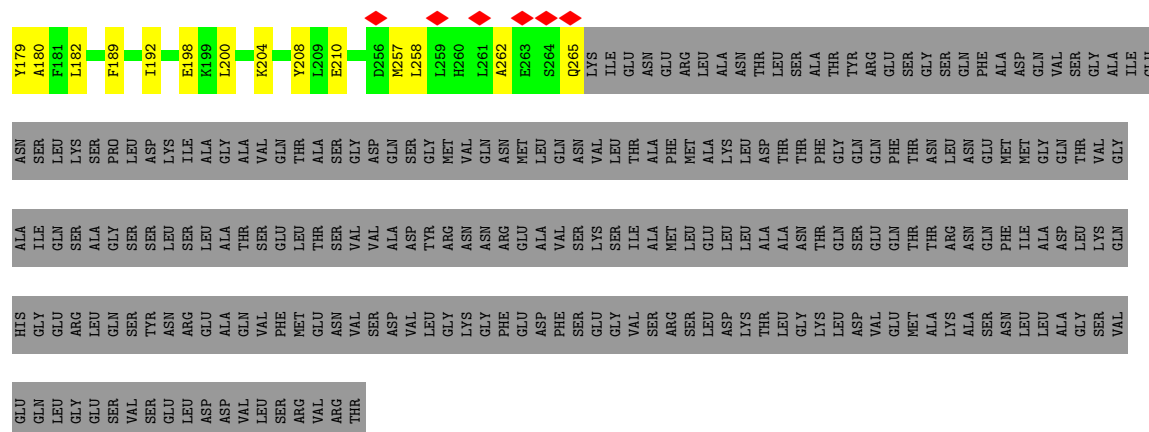
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	D	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	E	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

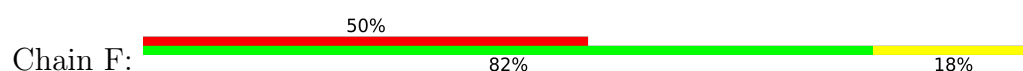
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	B	1	Total	Ca	0
			1	1	
5	C	1	Total	Ca	0
			1	1	
5	D	1	Total	Ca	0
			1	1	
5	E	1	Total	Ca	0
			1	1	

- Molecule 6 is water.

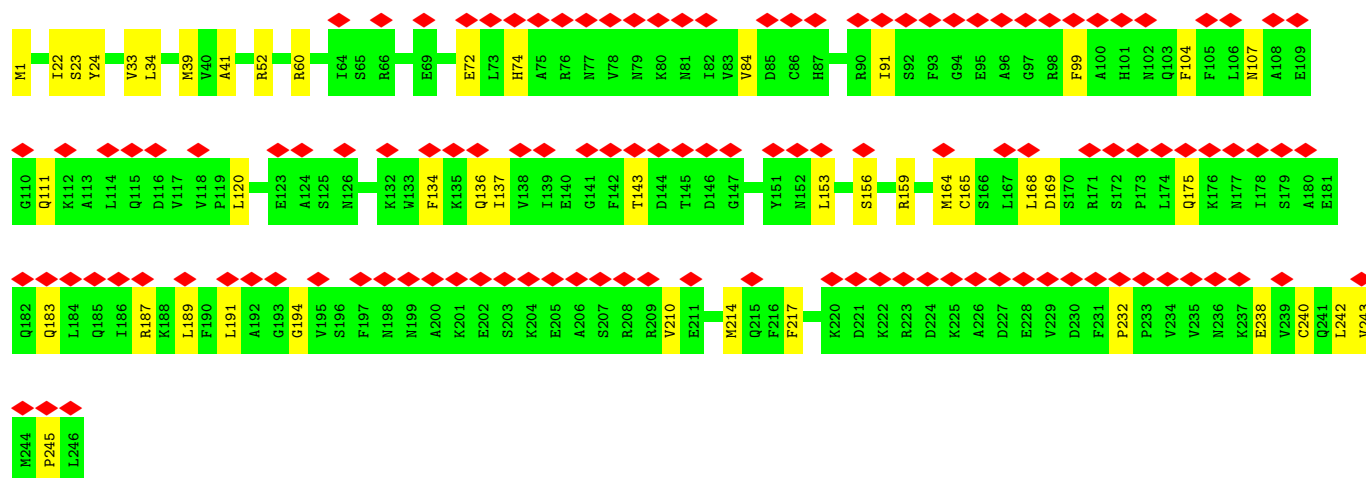
Mol	Chain	Residues	Atoms		AltConf
6	A	160	Total 160	O 160	0
6	B	167	Total 167	O 167	0
6	C	173	Total 173	O 173	0
6	D	163	Total 163	O 163	0
6	E	170	Total 170	O 170	0
6	F	17	Total 17	O 17	0
6	G	16	Total 16	O 16	0



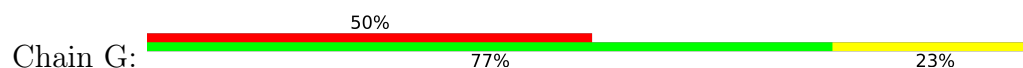
- Molecule 2: Membrane protein



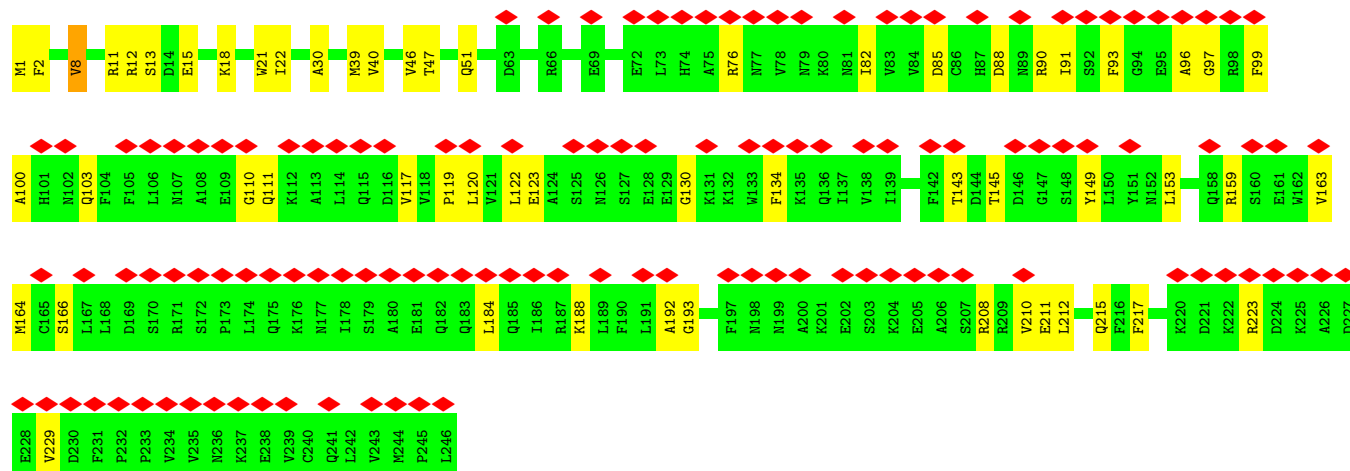
Chain F:



- Molecule 2: Membrane protein



Chain G:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	278186	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	7.515	Depositor
Minimum map value	-3.383	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.095	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	416.0, 416.0, 416.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.832, 0.832, 0.832	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.16	0/2179	0.31	0/2953
1	B	0.16	0/2168	0.30	0/2939
1	C	0.16	0/2168	0.31	0/2939
1	D	0.29	1/2168 (0.0%)	0.40	0/2939
1	E	0.16	0/2177	0.30	0/2950
2	F	0.16	0/2003	0.31	0/2690
2	G	0.24	0/2003	0.47	1/2690 (0.0%)
All	All	0.20	1/14866 (0.0%)	0.35	1/20100 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1
2	G	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	114	ALA	C-O	-7.20	1.14	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	15	GLU	CB-CA-C	5.96	119.49	109.48

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	52	ARG	Sidechain
2	G	12	ARG	Sidechain

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	2129	0	2149	43	0
1	B	2120	0	2136	32	0
1	C	2120	0	2136	30	0
1	D	2120	0	2136	39	0
1	E	2127	0	2149	39	0
2	F	1970	0	1973	36	0
2	G	1970	0	1973	45	0
3	A	100	0	156	8	0
3	B	100	0	156	11	0
3	C	100	0	156	7	0
3	D	100	0	156	12	0
3	E	100	0	156	9	0
4	A	51	0	78	6	0
4	B	51	0	78	2	0
4	C	51	0	78	2	0
4	D	51	0	78	7	0
4	E	51	0	78	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	A	160	0	0	8	0
6	B	167	0	0	2	0
6	C	173	0	0	4	0
6	D	163	0	0	3	0
6	E	170	0	0	4	0
6	F	17	0	0	0	0
6	G	16	0	0	3	0
All	All	16182	0	15822	242	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 8.

All (242) 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:20:PRO:HG3	1:C:179:TYR:HB3	1.64	0.78
1:B:5:ASN:OD1	1:C:175:ARG:NH2	2.16	0.78
1:A:181:PHE:HE2	2:F:33:VAL:HG21	1.52	0.74
1:C:133:LYS:NZ	2:G:13:SER:OG	2.21	0.72
1:D:11:LEU:HD13	4:D:502:PEE:H47	1.73	0.71
1:D:39:LEU:HD21	3:D:501:CDL:H401	1.73	0.70
1:B:79:GLU:HG3	1:B:80:LEU:HD12	1.74	0.70
1:B:149:TYR:HA	1:B:152:MET:HE3	1.74	0.70
1:A:54:ARG:NH2	6:A:605:HOH:O	2.22	0.68
1:D:138:ILE:HG22	1:D:142:MET:HE3	1.74	0.68
2:F:84:VAL:HG13	2:F:91:ILE:HG12	1.76	0.67
2:G:159:ARG:HH12	2:G:208:ARG:HE	1.42	0.67
1:A:257:MET:HE2	1:B:258:LEU:HD12	1.77	0.67
2:F:165:CYS:O	2:F:169:ASP:N	2.28	0.66
1:B:225:GLY:HA3	2:G:1:MET:HG2	1.78	0.66
1:D:196:TRP:HE1	3:D:501:CDL:H762	1.60	0.66
2:G:111:GLN:HE22	2:G:166:SER:HB2	1.60	0.65
2:F:60:ARG:NH1	2:F:217:PHE:O	2.29	0.65
1:E:177:VAL:HG11	2:F:34:LEU:HD11	1.79	0.65
1:A:181:PHE:CE2	2:F:33:VAL:HG21	2.33	0.64
4:A:502:PEE:H78	3:B:501:CDL:H272	1.78	0.64
1:B:200:LEU:HD21	3:B:501:CDL:H122	1.79	0.63
1:C:237:ASN:ND2	6:C:609:HOH:O	2.31	0.63
1:A:44:ARG:NH1	6:A:610:HOH:O	2.31	0.63
1:D:119:GLU:HG2	1:D:209:LEU:HD23	1.79	0.63
3:D:501:CDL:H581	3:D:501:CDL:H201	1.80	0.63
1:D:144:ILE:HB	2:F:24:TYR:CD1	2.35	0.62
1:D:26:THR:HG21	4:D:502:PEE:H76	1.81	0.62
2:F:175:GLN:NE2	2:F:183:GLN:OE1	2.30	0.62
2:G:18:LYS:O	6:G:301:HOH:O	2.15	0.62
2:F:187:ARG:NH2	2:F:238:GLU:OE2	2.32	0.62
1:A:1:MET:N	6:A:612:HOH:O	2.33	0.62
1:E:79:GLU:HG3	1:E:80:LEU:HD12	1.82	0.61
2:F:194:GLY:HA2	2:G:193:GLY:HA3	1.83	0.61
1:E:59:ILE:HD12	1:E:67:GLN:HB2	1.81	0.61
1:D:118:SER:OG	1:D:121:GLN:NE2	2.34	0.61
1:E:208:TYR:OH	3:E:501:CDL:OA4	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:PHE:CE1	1:A:198:GLU:HB3	2.36	0.60
1:B:147:THR:OG1	1:B:184:SER:HB2	2.02	0.60
1:B:120:GLN:HA	1:B:124:ASP:HB2	1.82	0.59
1:C:193:LEU:HD13	3:C:501:CDL:H671	1.84	0.59
1:E:44:ARG:NH2	6:E:604:HOH:O	2.30	0.59
1:C:152:MET:HE2	1:D:182:LEU:HA	1.85	0.58
2:G:163:VAL:HG21	2:G:210:VAL:HG21	1.85	0.58
1:E:175:ARG:NH1	6:E:617:HOH:O	2.36	0.58
1:E:37:PHE:O	1:E:41:ARG:HD2	2.04	0.58
2:G:93:PHE:O	2:G:97:GLY:N	2.36	0.58
1:C:19:VAL:HG13	4:C:502:PEE:H60	1.86	0.58
1:D:11:LEU:O	1:D:149:TYR:OH	2.20	0.58
1:D:147:THR:OG1	1:D:184:SER:HB2	2.04	0.58
1:E:144:ILE:HD11	2:F:23:SER:HA	1.86	0.58
3:C:501:CDL:H791	3:C:501:CDL:H631	1.86	0.57
1:C:41:ARG:NH1	6:C:616:HOH:O	2.36	0.57
3:D:501:CDL:H131	3:D:501:CDL:H312	1.87	0.57
1:D:8:LEU:HD22	1:E:179:TYR:CZ	2.39	0.57
1:A:257:MET:HE1	1:B:254:LEU:HB3	1.86	0.56
1:A:8:LEU:HD21	1:B:182:LEU:HD22	1.87	0.56
3:B:501:CDL:HA22	3:B:501:CDL:HB31	1.86	0.56
1:B:147:THR:HA	1:B:180:ALA:HB1	1.88	0.56
1:E:189:PHE:HB3	3:E:501:CDL:H652	1.88	0.56
2:F:134:PHE:HE2	2:F:189:LEU:HG	1.71	0.56
1:A:147:THR:HA	1:A:180:ALA:HB1	1.87	0.55
1:A:186:PHE:CD1	4:E:502:PEE:H41	2.42	0.55
1:D:72:LYS:O	1:D:76:GLN:HB3	2.07	0.55
1:D:50:LYS:NZ	3:D:501:CDL:OA9	2.25	0.55
2:G:22:ILE:N	6:G:301:HOH:O	2.32	0.54
1:B:29:PHE:HD2	3:C:501:CDL:H801	1.73	0.54
1:E:147:THR:HA	1:E:180:ALA:HB1	1.88	0.54
2:G:100:ALA:HB3	2:G:103:GLN:HG2	1.90	0.54
1:D:11:LEU:HD22	4:D:502:PEE:H42	1.88	0.54
2:F:143:THR:OG1	2:F:156:SER:OG	2.25	0.54
1:A:79:GLU:HG3	1:A:80:LEU:HD12	1.90	0.53
4:A:502:PEE:H40	1:B:186:PHE:HD1	1.73	0.53
1:C:39:LEU:HD21	3:C:501:CDL:H421	1.91	0.53
2:G:76:ARG:NH2	2:G:82:ILE:O	2.41	0.53
1:E:38:TYR:CZ	1:E:198:GLU:HG3	2.43	0.53
2:G:159:ARG:HH12	2:G:208:ARG:HA	1.74	0.52
2:F:136:GLN:HB2	2:F:191:LEU:HD23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:LYS:HA	1:E:21:VAL:HG22	1.92	0.52
1:E:79:GLU:OE2	6:E:601:HOH:O	2.19	0.52
2:F:153:LEU:HD22	2:G:164:MET:SD	2.49	0.52
1:A:234:LYS:O	1:A:238:GLU:HG3	2.09	0.52
4:C:502:PEE:H77	3:D:501:CDL:H642	1.92	0.52
1:E:120:GLN:HA	1:E:124:ASP:HB2	1.90	0.52
1:C:181:PHE:CE1	2:G:30:ALA:HB1	2.44	0.52
2:G:51:GLN:OE1	6:G:302:HOH:O	2.18	0.52
1:D:198:GLU:OE2	1:D:199:LYS:HE2	2.10	0.52
1:D:138:ILE:HD12	1:E:192:ILE:HG23	1.91	0.51
1:C:88:GLU:OE1	6:C:601:HOH:O	2.18	0.51
1:A:23:VAL:HG22	4:A:502:PEE:H66	1.91	0.51
2:F:153:LEU:HD21	2:G:192:ALA:HB3	1.92	0.51
4:A:502:PEE:H77	3:B:501:CDL:H251	1.93	0.51
1:A:34:PHE:HE1	1:A:198:GLU:HB3	1.75	0.51
1:A:199:LYS:NZ	6:A:625:HOH:O	2.44	0.51
1:B:193:LEU:HD21	3:B:501:CDL:H451	1.93	0.50
4:B:502:PEE:H57	4:B:502:PEE:H20	1.93	0.50
1:C:130:GLU:HG3	1:D:206:TYR:HD2	1.75	0.50
1:A:208:TYR:OH	3:A:501:CDL:OA4	2.26	0.50
3:E:501:CDL:H782	3:E:501:CDL:H601	1.94	0.50
4:D:502:PEE:H34	1:E:189:PHE:HE2	1.76	0.50
1:E:77:ARG:NH1	6:E:624:HOH:O	2.43	0.50
2:G:99:PHE:HB2	2:G:208:ARG:HB3	1.93	0.50
2:G:164:MET:HE3	2:G:192:ALA:HB2	1.93	0.50
1:C:148:PHE:HB3	1:D:185:ALA:HB2	1.94	0.50
1:D:159:ASP:O	6:D:601:HOH:O	2.20	0.50
2:F:187:ARG:HH12	2:G:149:TYR:HB2	1.77	0.50
1:B:140:THR:O	1:B:144:ILE:HG12	2.12	0.49
2:G:119:PRO:HA	2:G:122:LEU:HD12	1.94	0.49
1:E:204:LYS:HG3	3:E:501:CDL:HA4	1.94	0.49
2:F:72:GLU:HG3	2:F:84:VAL:HB	1.95	0.49
2:F:243:VAL:HG22	2:F:245:PRO:HD2	1.95	0.49
4:A:502:PEE:H75	3:B:501:CDL:H652	1.94	0.49
2:F:74:HIS:HB3	2:F:120:LEU:HD22	1.95	0.49
1:E:138:ILE:O	1:E:142:MET:HG3	2.13	0.49
2:F:243:VAL:HG13	2:F:245:PRO:HD2	1.94	0.49
1:A:204:LYS:HG3	3:A:501:CDL:H312	1.95	0.48
1:A:257:MET:HE3	1:B:255:ARG:HA	1.95	0.48
1:E:4:LEU:HD12	1:E:7:ILE:HD11	1.95	0.48
1:B:30:ALA:HB2	3:C:501:CDL:H781	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:PHE:HE1	2:G:30:ALA:HB1	1.78	0.48
1:D:174:LEU:HD21	2:G:40:VAL:HG21	1.94	0.48
2:F:137:ILE:HD11	2:F:214:MET:HE2	1.95	0.48
2:G:46:VAL:HG23	2:G:47:THR:HG23	1.96	0.48
1:A:186:PHE:HD1	4:E:502:PEE:H41	1.78	0.48
1:C:173:LEU:O	1:C:177:VAL:HG23	2.14	0.47
3:C:501:CDL:H582	3:C:501:CDL:H611	1.52	0.47
1:B:19:VAL:HB	1:B:20:PRO:HD3	1.96	0.47
1:C:17:TYR:C	1:C:20:PRO:HD2	2.39	0.47
3:D:501:CDL:H182	3:D:501:CDL:H152	1.68	0.47
1:D:194:VAL:O	1:D:198:GLU:HG3	2.14	0.47
1:A:198:GLU:OE2	1:A:199:LYS:HE2	2.14	0.47
1:A:227:GLU:OE1	6:A:601:HOH:O	2.21	0.47
2:F:84:VAL:HG22	2:F:91:ILE:HG23	1.97	0.47
1:A:258:LEU:HD12	1:E:257:MET:HG2	1.96	0.47
1:D:43:ILE:HG12	3:D:501:CDL:H352	1.97	0.47
1:A:194:VAL:O	1:A:198:GLU:HG3	2.15	0.47
1:B:138:ILE:O	1:B:142:MET:HG3	2.15	0.46
1:D:120:GLN:HA	1:D:124:ASP:HB2	1.97	0.46
1:C:152:MET:CE	1:D:182:LEU:HA	2.46	0.46
2:F:99:PHE:HE2	2:F:210:VAL:HG12	1.81	0.46
3:A:501:CDL:H792	1:E:30:ALA:HB2	1.97	0.46
2:G:96:ALA:HB1	2:G:110:GLY:HA2	1.98	0.46
2:G:100:ALA:H	2:G:103:GLN:HE21	1.62	0.46
4:D:502:PEE:H72	4:D:502:PEE:H79	1.68	0.46
1:C:86:GLU:O	1:C:89:GLU:HG2	2.16	0.46
3:E:501:CDL:H761	3:E:501:CDL:H791	1.53	0.46
3:A:501:CDL:PB2	1:E:41:ARG:HH22	2.38	0.45
1:C:98:GLU:HA	1:C:99:ASN:HA	1.75	0.45
2:G:188:LYS:NZ	2:G:229:VAL:O	2.43	0.45
1:A:11:LEU:O	1:A:149:TYR:OH	2.22	0.45
1:C:238:GLU:OE1	6:C:602:HOH:O	2.21	0.45
3:E:501:CDL:H311	3:E:501:CDL:H341	1.73	0.45
2:G:91:ILE:HB	2:G:212:LEU:HB2	1.98	0.45
1:C:17:TYR:O	1:C:20:PRO:HD2	2.15	0.45
1:E:148:PHE:O	1:E:152:MET:HG3	2.17	0.45
1:A:11:LEU:HB3	1:A:149:TYR:HE1	1.81	0.45
2:F:164:MET:HE3	2:F:168:LEU:HD23	1.99	0.45
1:D:34:PHE:CE1	1:D:198:GLU:HB3	2.52	0.45
2:F:164:MET:HG2	2:G:153:LEU:HD22	1.98	0.45
1:A:258:LEU:HD12	1:E:257:MET:SD	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:501:CDL:H381	3:A:501:CDL:H351	1.82	0.45
1:A:90:SER:O	1:A:110:THR:OG1	2.31	0.44
1:E:200:LEU:HD21	3:E:501:CDL:H132	1.99	0.44
2:F:104:PHE:HA	2:F:159:ARG:HG2	1.99	0.44
1:C:121:GLN:HE22	1:D:210:GLU:CD	2.24	0.44
2:G:184:LEU:O	2:G:188:LYS:HG2	2.17	0.44
3:D:501:CDL:H771	3:D:501:CDL:H801	1.83	0.44
1:A:227:GLU:OE2	6:A:602:HOH:O	2.21	0.44
1:A:244:ARG:O	1:A:248:GLU:HG2	2.18	0.44
3:E:501:CDL:H572	3:E:501:CDL:H442	2.00	0.44
2:G:143:THR:HA	2:G:208:ARG:HH22	1.83	0.44
1:A:144:ILE:HD11	2:G:21:TRP:CH2	2.52	0.44
1:A:156:ASN:HB2	1:B:178:LEU:HD11	2.00	0.44
3:A:501:CDL:H252	4:E:502:PEE:H75	1.99	0.44
1:B:134:HIS:CD2	1:C:199:LYS:HD2	2.53	0.44
1:D:88:GLU:OE2	6:D:602:HOH:O	2.21	0.44
3:E:501:CDL:H162	3:E:501:CDL:H191	1.59	0.44
1:E:125:ILE:HB	1:E:126:PRO:HD3	2.00	0.43
1:E:258:LEU:HD23	1:E:258:LEU:HA	1.87	0.43
1:B:77:ARG:NH2	6:B:629:HOH:O	2.52	0.43
1:A:155:LEU:O	6:A:603:HOH:O	2.21	0.43
1:A:162:THR:HG22	1:A:164:GLU:H	1.84	0.43
3:B:501:CDL:H422	3:B:501:CDL:H452	1.57	0.43
1:C:115:SER:HA	2:G:8:VAL:HG22	2.00	0.43
1:A:4:LEU:HD11	1:B:182:LEU:HD21	1.99	0.43
3:B:501:CDL:H742	3:B:501:CDL:H711	1.60	0.43
3:D:501:CDL:H462	3:D:501:CDL:H622	2.00	0.43
2:G:90:ARG:HE	2:G:211:GLU:CD	2.27	0.43
2:F:1:MET:HE2	2:G:2:PHE:HE1	1.83	0.43
1:B:11:LEU:O	1:B:149:TYR:OH	2.19	0.43
1:C:120:GLN:HA	1:C:124:ASP:HB2	2.01	0.43
1:C:201:SER:OG	3:C:501:CDL:H361	2.18	0.43
1:B:196:TRP:HE1	3:B:501:CDL:H572	1.83	0.43
1:C:134:HIS:CE1	1:D:199:LYS:HE3	2.53	0.43
4:B:502:PEE:H58	4:B:502:PEE:H24	2.00	0.42
1:C:1:MET:HE3	1:D:17:TYR:HE2	1.84	0.42
1:D:198:GLU:HG2	6:D:606:HOH:O	2.19	0.42
1:A:56:ILE:HD13	1:A:216:LEU:HG	2.00	0.42
2:G:143:THR:HA	2:G:208:ARG:NH2	2.35	0.42
2:G:93:PHE:HZ	2:G:117:VAL:HG11	1.84	0.42
2:G:120:LEU:O	2:G:123:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:22:ILE:HG12	2:G:21:TRP:CG	2.55	0.42
1:B:147:THR:O	1:B:151:LEU:HG	2.19	0.42
2:F:39:MET:HG3	2:G:39:MET:HB2	2.02	0.42
1:C:199:LYS:HA	1:C:199:LYS:HD3	1.78	0.42
1:A:86:GLU:OE2	6:A:604:HOH:O	2.22	0.42
1:B:216:LEU:HD23	1:B:216:LEU:HA	1.93	0.42
1:E:166:VAL:HG13	2:F:41:ALA:HB1	2.01	0.42
1:A:29:PHE:HE2	3:B:501:CDL:H791	1.85	0.42
1:E:20:PRO:HB3	1:E:179:TYR:O	2.20	0.42
1:E:96:GLU:HB2	1:E:105:VAL:HG11	2.02	0.42
1:D:144:ILE:HG12	2:F:24:TYR:HA	2.02	0.41
2:F:232:PRO:HD3	2:G:145:THR:HB	2.02	0.41
1:D:34:PHE:HE1	1:D:198:GLU:HB3	1.85	0.41
1:B:226:GLU:OE2	6:B:601:HOH:O	2.22	0.41
1:E:262:ALA:HA	1:E:265:GLN:HG2	2.03	0.41
2:G:88:ASP:OD1	2:G:88:ASP:N	2.52	0.41
2:G:130:GLY:HA2	2:G:134:PHE:HB2	2.02	0.41
1:E:177:VAL:HG21	2:F:34:LEU:HD21	2.03	0.41
2:F:240:CYS:SG	2:F:242:LEU:HD23	2.60	0.41
1:B:147:THR:HG23	1:B:180:ALA:HB1	2.02	0.41
2:G:85:ASP:HB3	2:G:90:ARG:HB2	2.03	0.41
2:G:217:PHE:CZ	2:G:223:ARG:HG2	2.56	0.41
1:C:31:PHE:O	1:C:35:ILE:HG12	2.21	0.41
1:D:170:VAL:O	1:D:174:LEU:HG	2.21	0.41
1:A:257:MET:HB3	1:B:258:LEU:HD12	2.03	0.41
1:A:258:LEU:HD23	1:A:258:LEU:HA	1.76	0.41
3:A:501:CDL:H831	1:E:26:THR:HG23	2.03	0.41
4:D:502:PEE:H43	1:E:182:LEU:HA	2.02	0.41
4:A:502:PEE:H75	3:B:501:CDL:H671	2.03	0.41
1:D:197:LEU:HD22	3:D:501:CDL:H392	2.03	0.41
2:G:159:ARG:NH1	2:G:208:ARG:HA	2.36	0.41
3:A:501:CDL:H271	3:A:501:CDL:H242	1.87	0.40
2:F:107:ASN:O	2:F:111:GLN:HG3	2.21	0.40
1:A:255:ARG:HG2	1:E:257:MET:HE2	2.03	0.40
1:B:30:ALA:HB3	1:B:139:LEU:HD21	2.03	0.40
1:D:149:TYR:CE1	4:D:502:PEE:H41	2.56	0.40
1:D:196:TRP:CH2	3:D:501:CDL:H601	2.56	0.40
1:A:4:LEU:HD23	1:B:17:TYR:HB2	2.02	0.40
1:A:199:LYS:HE3	1:E:134:HIS:CE1	2.57	0.40
1:D:95:TYR:HB3	1:D:102:GLU:HG3	2.02	0.40
1:D:121:GLN:CG	1:E:210:GLU:HG3	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	264/495 (53%)	261 (99%)	3 (1%)	0	100	100
1	B	263/495 (53%)	260 (99%)	3 (1%)	0	100	100
1	C	263/495 (53%)	262 (100%)	1 (0%)	0	100	100
1	D	263/495 (53%)	260 (99%)	3 (1%)	0	100	100
1	E	264/495 (53%)	259 (98%)	5 (2%)	0	100	100
2	F	244/246 (99%)	240 (98%)	4 (2%)	0	100	100
2	G	244/246 (99%)	237 (97%)	7 (3%)	0	100	100
All	All	1805/2967 (61%)	1779 (99%)	26 (1%)	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	238/429 (56%)	238 (100%)	0	100	100
1	B	237/429 (55%)	237 (100%)	0	100	100
1	C	237/429 (55%)	237 (100%)	0	100	100
1	D	237/429 (55%)	237 (100%)	0	100	100
1	E	238/429 (56%)	238 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	215/215 (100%)	215 (100%)	0	100	100
2	G	215/215 (100%)	212 (99%)	3 (1%)	59	60
All	All	1617/2575 (63%)	1614 (100%)	3 (0%)	85	91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	8	VAL
2	G	11	ARG
2	G	215	GLN

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	121	GLN
1	A	128	ASN
1	A	265	GLN
1	B	134	HIS
1	C	121	GLN
1	D	82	HIS
1	D	121	GLN
1	E	94	GLN
1	E	134	HIS
1	E	156	ASN
2	F	74	HIS
2	F	152	ASN
2	G	111	GLN
2	G	152	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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
3	CDL	C	501	-	99,99,99	0.30	0	105,111,111	0.21	0
4	PEE	B	502	-	50,50,50	1.49	7 (14%)	53,55,55	1.63	7 (13%)
3	CDL	B	501	-	99,99,99	0.30	0	105,111,111	0.21	0
3	CDL	E	501	-	99,99,99	0.32	0	105,111,111	0.20	0
4	PEE	D	502	-	50,50,50	1.51	9 (18%)	53,55,55	1.65	6 (11%)
4	PEE	C	502	-	50,50,50	1.52	9 (18%)	53,55,55	1.65	6 (11%)
3	CDL	D	501	-	99,99,99	0.30	0	105,111,111	0.20	0
4	PEE	A	502	-	50,50,50	1.52	9 (18%)	53,55,55	1.65	6 (11%)
3	CDL	A	501	-	99,99,99	0.30	0	105,111,111	0.21	0
4	PEE	E	502	-	50,50,50	1.48	9 (18%)	53,55,55	1.64	7 (13%)

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
3	CDL	C	501	-	-	68/110/110/110	-
4	PEE	B	502	-	-	23/54/54/54	-
3	CDL	B	501	-	-	66/110/110/110	-
3	CDL	E	501	-	-	66/110/110/110	-
4	PEE	D	502	-	-	27/54/54/54	-
4	PEE	C	502	-	-	27/54/54/54	-
3	CDL	D	501	-	-	65/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEE	A	502	-	-	31/54/54/54	-
3	CDL	A	501	-	-	64/110/110/110	-
4	PEE	E	502	-	-	24/54/54/54	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	502	PEE	C3-C2	4.01	1.63	1.50
4	A	502	PEE	C3-C2	3.98	1.63	1.50
4	B	502	PEE	C3-C2	3.88	1.62	1.50
4	D	502	PEE	C3-C2	3.88	1.62	1.50
4	E	502	PEE	C3-C2	3.65	1.62	1.50
4	D	502	PEE	P-O3P	3.33	1.72	1.59
4	C	502	PEE	P-O4P	3.30	1.72	1.59
4	B	502	PEE	P-O4P	3.26	1.72	1.59
4	E	502	PEE	P-O4P	3.26	1.72	1.59
4	A	502	PEE	P-O4P	3.26	1.72	1.59
4	D	502	PEE	P-O4P	3.25	1.72	1.59
4	C	502	PEE	P-O3P	3.23	1.72	1.59
4	A	502	PEE	P-O3P	3.22	1.72	1.59
4	E	502	PEE	P-O3P	3.20	1.71	1.59
4	B	502	PEE	P-O3P	3.17	1.71	1.59
4	C	502	PEE	C11-C10	2.47	1.57	1.50
4	A	502	PEE	C31-C30	2.38	1.57	1.50
4	C	502	PEE	C12-C11	2.29	1.60	1.52
4	C	502	PEE	C31-C30	2.25	1.57	1.50
4	B	502	PEE	O3-C30	2.22	1.39	1.33
4	C	502	PEE	O3-C30	2.21	1.39	1.33
4	D	502	PEE	C31-C30	2.21	1.57	1.50
4	D	502	PEE	C11-C10	2.20	1.57	1.50
4	E	502	PEE	C12-C11	2.18	1.60	1.52
4	D	502	PEE	C12-C11	2.18	1.60	1.52
4	D	502	PEE	C5-C4	2.17	1.58	1.49
4	D	502	PEE	O3-C30	2.16	1.39	1.33
4	D	502	PEE	O2-C10	2.16	1.40	1.34
4	A	502	PEE	C12-C11	2.15	1.60	1.52
4	A	502	PEE	C11-C10	2.14	1.56	1.50
4	C	502	PEE	C5-C4	2.14	1.58	1.49
4	A	502	PEE	O3-C30	2.13	1.39	1.33
4	A	502	PEE	O2-C10	2.13	1.40	1.34
4	E	502	PEE	O3-C30	2.12	1.39	1.33
4	B	502	PEE	C5-C4	2.11	1.58	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	502	PEE	O2-C10	2.10	1.40	1.34
4	A	502	PEE	C5-C4	2.10	1.58	1.49
4	E	502	PEE	C31-C30	2.09	1.56	1.50
4	E	502	PEE	C5-C4	2.06	1.58	1.49
4	B	502	PEE	C12-C11	2.05	1.59	1.52
4	E	502	PEE	C11-C10	2.04	1.56	1.50
4	B	502	PEE	C31-C30	2.03	1.56	1.50
4	E	502	PEE	O2-C10	2.02	1.40	1.34

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	502	PEE	O2-C10-C11	6.14	124.77	111.48
4	A	502	PEE	O2-C10-C11	5.98	124.41	111.48
4	D	502	PEE	O2-C10-C11	5.97	124.39	111.48
4	E	502	PEE	O2-C10-C11	5.78	123.98	111.48
4	B	502	PEE	O2-C10-C11	5.64	123.69	111.48
4	D	502	PEE	C40-C39-C38	5.30	164.53	124.83
4	A	502	PEE	C40-C39-C38	5.26	164.23	124.83
4	D	502	PEE	C37-C38-C39	5.24	164.12	124.83
4	E	502	PEE	C40-C39-C38	5.23	164.05	124.83
4	B	502	PEE	C40-C39-C38	5.21	163.83	124.83
4	A	502	PEE	C37-C38-C39	5.19	163.74	124.83
4	C	502	PEE	C40-C39-C38	5.17	163.55	124.83
4	E	502	PEE	C37-C38-C39	5.17	163.53	124.83
4	B	502	PEE	C37-C38-C39	5.15	163.43	124.83
4	C	502	PEE	C37-C38-C39	5.13	163.24	124.83
4	B	502	PEE	O3-C30-C31	3.97	123.94	111.83
4	C	502	PEE	O3-C30-C31	3.87	123.63	111.83
4	A	502	PEE	O3-C30-C31	3.84	123.55	111.83
4	D	502	PEE	O3-C30-C31	3.82	123.48	111.83
4	E	502	PEE	O3-C30-C31	3.82	123.47	111.83
4	C	502	PEE	O2-C10-O4	-2.71	117.37	123.70
4	A	502	PEE	O3-C30-O5	-2.61	117.10	123.63
4	A	502	PEE	O2-C10-O4	-2.61	117.60	123.70
4	B	502	PEE	O3-C30-O5	-2.61	117.10	123.63
4	D	502	PEE	O2-C10-O4	-2.57	117.69	123.70
4	E	502	PEE	O3-C30-O5	-2.57	117.20	123.63
4	C	502	PEE	O3-C30-O5	-2.56	117.23	123.63
4	D	502	PEE	O3-C30-O5	-2.56	117.23	123.63
4	E	502	PEE	O2-C10-O4	-2.51	117.85	123.70
4	B	502	PEE	O2-C10-O4	-2.50	117.87	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	502	PEE	C3-C2-C1	-2.16	106.74	111.78
4	B	502	PEE	C3-C2-C1	-2.07	106.97	111.78

There are no chirality outliers.

All (461) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	CDL	CA2-OA2-PA1-OA3
3	A	501	CDL	CA2-OA2-PA1-OA4
3	A	501	CDL	CA2-OA2-PA1-OA5
3	A	501	CDL	CB3-OB5-PB2-OB2
3	A	501	CDL	CB3-OB5-PB2-OB3
3	B	501	CDL	CA2-OA2-PA1-OA3
3	B	501	CDL	CA2-OA2-PA1-OA4
3	B	501	CDL	CA2-OA2-PA1-OA5
3	B	501	CDL	CB2-OB2-PB2-OB3
3	B	501	CDL	CB2-OB2-PB2-OB4
3	B	501	CDL	CB2-OB2-PB2-OB5
3	C	501	CDL	CB2-C1-CA2-OA2
3	C	501	CDL	CA3-OA5-PA1-OA3
3	C	501	CDL	CB2-OB2-PB2-OB3
3	C	501	CDL	CB2-OB2-PB2-OB5
3	C	501	CDL	CB3-OB5-PB2-OB2
3	C	501	CDL	CB3-OB5-PB2-OB3
3	C	501	CDL	CB3-OB5-PB2-OB4
3	D	501	CDL	CA2-OA2-PA1-OA3
3	D	501	CDL	CA3-OA5-PA1-OA3
3	D	501	CDL	C11-CA5-OA6-CA4
3	D	501	CDL	CB2-OB2-PB2-OB3
3	D	501	CDL	CB2-OB2-PB2-OB4
3	D	501	CDL	CB2-OB2-PB2-OB5
3	E	501	CDL	CA2-C1-CB2-OB2
3	E	501	CDL	CA3-OA5-PA1-OA2
3	E	501	CDL	CB2-OB2-PB2-OB3
4	A	502	PEE	C11-C10-O2-C2
4	A	502	PEE	O4-C10-O2-C2
4	A	502	PEE	O3P-C1-C2-O2
4	B	502	PEE	O2-C2-C3-O3
4	C	502	PEE	O4-C10-O2-C2
4	C	502	PEE	C1-O3P-P-O2P
4	C	502	PEE	C1-O3P-P-O1P
4	C	502	PEE	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
4	C	502	PEE	C4-O4P-P-O1P
4	D	502	PEE	C11-C10-O2-C2
4	D	502	PEE	O4-C10-O2-C2
4	D	502	PEE	C1-O3P-P-O2P
4	D	502	PEE	C1-O3P-P-O4P
4	D	502	PEE	C4-O4P-P-O3P
4	D	502	PEE	C4-O4P-P-O1P
4	E	502	PEE	C11-C10-O2-C2
4	E	502	PEE	C4-O4P-P-O2P
4	E	502	PEE	C4-O4P-P-O1P
3	A	501	CDL	OA9-CA7-OA8-CA6
3	D	501	CDL	OB9-CB7-OB8-CB6
4	D	502	PEE	O5-C30-O3-C3
3	A	501	CDL	C31-CA7-OA8-CA6
3	D	501	CDL	C71-CB7-OB8-CB6
4	D	502	PEE	C31-C30-O3-C3
3	B	501	CDL	OB9-CB7-OB8-CB6
3	E	501	CDL	OA9-CA7-OA8-CA6
3	E	501	CDL	OB9-CB7-OB8-CB6
3	A	501	CDL	OB9-CB7-OB8-CB6
3	B	501	CDL	OA7-CA5-OA6-CA4
4	E	502	PEE	O4-C10-O2-C2
3	B	501	CDL	C71-CB7-OB8-CB6
3	E	501	CDL	C71-CB7-OB8-CB6
4	B	502	PEE	C31-C30-O3-C3
3	B	501	CDL	C11-CA5-OA6-CA4
4	C	502	PEE	C11-C10-O2-C2
3	A	501	CDL	C71-CB7-OB8-CB6
3	E	501	CDL	C31-CA7-OA8-CA6
3	D	501	CDL	OA7-CA5-OA6-CA4
3	E	501	CDL	C40-C41-C42-C43
3	E	501	CDL	O1-C1-CB2-OB2
4	B	502	PEE	O5-C30-O3-C3
3	A	501	CDL	C51-CB5-OB6-CB4
4	D	502	PEE	C2-C1-O3P-P
4	B	502	PEE	C43-C44-C45-C46
4	A	502	PEE	C43-C44-C45-C46
3	A	501	CDL	C37-C38-C39-C40
4	C	502	PEE	C43-C44-C45-C46
3	B	501	CDL	C59-C60-C61-C62
4	E	502	PEE	C43-C44-C45-C46
3	E	501	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
3	D	501	CDL	C77-C78-C79-C80
4	D	502	PEE	C43-C44-C45-C46
4	A	502	PEE	C31-C30-O3-C3
3	B	501	CDL	C42-C43-C44-C45
3	C	501	CDL	C58-C59-C60-C61
3	E	501	CDL	C76-C77-C78-C79
3	D	501	CDL	C37-C38-C39-C40
3	D	501	CDL	C39-C40-C41-C42
3	C	501	CDL	CB7-C71-C72-C73
3	B	501	CDL	C80-C81-C82-C83
3	A	501	CDL	OB7-CB5-OB6-CB4
4	B	502	PEE	C11-C10-O2-C2
3	B	501	CDL	C71-C72-C73-C74
3	D	501	CDL	C11-C12-C13-C14
3	C	501	CDL	C62-C63-C64-C65
3	D	501	CDL	C82-C83-C84-C85
3	E	501	CDL	CB5-C51-C52-C53
3	E	501	CDL	C16-C17-C18-C19
3	A	501	CDL	CB7-C71-C72-C73
4	A	502	PEE	O5-C30-O3-C3
3	E	501	CDL	CA5-C11-C12-C13
3	C	501	CDL	C13-C14-C15-C16
3	E	501	CDL	OB7-CB5-OB6-CB4
4	B	502	PEE	C31-C32-C33-C34
3	A	501	CDL	C35-C36-C37-C38
4	B	502	PEE	O4-C10-O2-C2
3	C	501	CDL	C31-CA7-OA8-CA6
3	B	501	CDL	CB7-C71-C72-C73
3	C	501	CDL	O1-C1-CA2-OA2
3	A	501	CDL	CB4-CB3-OB5-PB2
3	E	501	CDL	C52-C53-C54-C55
3	C	501	CDL	C19-C20-C21-C22
3	C	501	CDL	OA9-CA7-OA8-CA6
3	B	501	CDL	C54-C55-C56-C57
4	B	502	PEE	C20-C21-C22-C23
3	A	501	CDL	C17-C18-C19-C20
3	B	501	CDL	C11-C12-C13-C14
3	C	501	CDL	C37-C38-C39-C40
3	E	501	CDL	C19-C20-C21-C22
3	C	501	CDL	C11-C12-C13-C14
3	D	501	CDL	C54-C55-C56-C57
3	E	501	CDL	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
4	B	502	PEE	C40-C41-C42-C43
4	D	502	PEE	C34-C35-C36-C37
3	B	501	CDL	C12-C13-C14-C15
3	B	501	CDL	C61-C62-C63-C64
3	B	501	CDL	C72-C73-C74-C75
3	C	501	CDL	C42-C43-C44-C45
3	C	501	CDL	C57-C58-C59-C60
3	D	501	CDL	C16-C17-C18-C19
3	D	501	CDL	C19-C20-C21-C22
3	E	501	CDL	C12-C13-C14-C15
3	B	501	CDL	C33-C34-C35-C36
3	D	501	CDL	C38-C39-C40-C41
3	E	501	CDL	C14-C15-C16-C17
3	E	501	CDL	C57-C58-C59-C60
4	E	502	PEE	C33-C34-C35-C36
3	E	501	CDL	C17-C18-C19-C20
3	C	501	CDL	C17-C18-C19-C20
3	C	501	CDL	C75-C76-C77-C78
3	D	501	CDL	C15-C16-C17-C18
3	D	501	CDL	C40-C41-C42-C43
3	D	501	CDL	C73-C74-C75-C76
3	E	501	CDL	C20-C21-C22-C23
4	A	502	PEE	C40-C41-C42-C43
4	E	502	PEE	C31-C32-C33-C34
4	B	502	PEE	C34-C35-C36-C37
3	A	501	CDL	C62-C63-C64-C65
3	B	501	CDL	C75-C76-C77-C78
3	D	501	CDL	C13-C14-C15-C16
4	A	502	PEE	C13-C14-C15-C16
3	A	501	CDL	C55-C56-C57-C58
3	E	501	CDL	C31-C32-C33-C34
3	E	501	CDL	C74-C75-C76-C77
3	B	501	CDL	C56-C57-C58-C59
3	B	501	CDL	C78-C79-C80-C81
3	C	501	CDL	C60-C61-C62-C63
3	D	501	CDL	C53-C54-C55-C56
3	D	501	CDL	C78-C79-C80-C81
3	A	501	CDL	C72-C73-C74-C75
4	E	502	PEE	C12-C13-C14-C15
3	E	501	CDL	C58-C59-C60-C61
4	A	502	PEE	C31-C32-C33-C34
3	A	501	CDL	C56-C57-C58-C59

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Mol	Chain	Res	Type	Atoms
4	D	502	PEE	C39-C40-C41-C42
3	B	501	CDL	C63-C64-C65-C66
3	D	501	CDL	C61-C62-C63-C64
4	D	502	PEE	C21-C22-C23-C24
3	B	501	CDL	C37-C38-C39-C40
3	D	501	CDL	CB5-C51-C52-C53
3	A	501	CDL	C20-C21-C22-C23
3	B	501	CDL	C13-C14-C15-C16
3	D	501	CDL	C33-C34-C35-C36
3	E	501	CDL	C51-C52-C53-C54
4	D	502	PEE	C31-C32-C33-C34
3	A	501	CDL	C32-C33-C34-C35
3	E	501	CDL	C11-C12-C13-C14
4	B	502	PEE	C32-C33-C34-C35
4	E	502	PEE	C30-C31-C32-C33
3	C	501	CDL	C33-C34-C35-C36
3	D	501	CDL	C42-C43-C44-C45
3	E	501	CDL	C71-C72-C73-C74
3	A	501	CDL	C52-C53-C54-C55
3	C	501	CDL	C63-C64-C65-C66
3	D	501	CDL	C17-C18-C19-C20
4	B	502	PEE	C11-C12-C13-C14
3	E	501	CDL	C75-C76-C77-C78
4	A	502	PEE	C32-C33-C34-C35
3	A	501	CDL	C57-C58-C59-C60
3	B	501	CDL	C41-C42-C43-C44
3	A	501	CDL	C61-C62-C63-C64
3	A	501	CDL	C11-CA5-OA6-CA4
3	D	501	CDL	C51-CB5-OB6-CB4
3	E	501	CDL	C11-CA5-OA6-CA4
3	C	501	CDL	C44-C45-C46-C47
3	B	501	CDL	C82-C83-C84-C85
3	E	501	CDL	OA7-CA5-OA6-CA4
3	A	501	CDL	C12-C13-C14-C15
4	E	502	PEE	C39-C40-C41-C42
4	E	502	PEE	C10-C11-C12-C13
4	C	502	PEE	C13-C14-C15-C16
3	D	501	CDL	C57-C58-C59-C60
3	C	501	CDL	C72-C73-C74-C75
4	C	502	PEE	C34-C35-C36-C37
4	A	502	PEE	C41-C42-C43-C44
3	E	501	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
3	E	501	CDL	C63-C64-C65-C66
4	E	502	PEE	C21-C22-C23-C24
3	B	501	CDL	C81-C82-C83-C84
4	A	502	PEE	C19-C20-C21-C22
4	B	502	PEE	C19-C20-C21-C22
3	B	501	CDL	C34-C35-C36-C37
4	A	502	PEE	C22-C23-C24-C25
4	D	502	PEE	C33-C34-C35-C36
3	C	501	CDL	C32-C33-C34-C35
3	B	501	CDL	C40-C41-C42-C43
3	D	501	CDL	C81-C82-C83-C84
3	A	501	CDL	OA7-CA5-OA6-CA4
3	C	501	CDL	C38-C39-C40-C41
4	A	502	PEE	C20-C21-C22-C23
3	B	501	CDL	C31-C32-C33-C34
3	C	501	CDL	C82-C83-C84-C85
3	B	501	CDL	C20-C21-C22-C23
3	B	501	CDL	C55-C56-C57-C58
3	B	501	CDL	C77-C78-C79-C80
3	A	501	CDL	OB5-CB3-CB4-CB6
3	C	501	CDL	C24-C25-C26-C27
3	D	501	CDL	OB7-CB5-OB6-CB4
3	D	501	CDL	C22-C23-C24-C25
3	B	501	CDL	C52-C53-C54-C55
4	A	502	PEE	C34-C35-C36-C37
3	A	501	CDL	CB3-CB4-CB6-OB8
3	E	501	CDL	CA3-CA4-CA6-OA8
4	B	502	PEE	C1-C2-C3-O3
4	E	502	PEE	C1-C2-C3-O3
4	A	502	PEE	C39-C40-C41-C42
4	E	502	PEE	C19-C20-C21-C22
3	D	501	CDL	C56-C57-C58-C59
3	D	501	CDL	C74-C75-C76-C77
4	A	502	PEE	C11-C12-C13-C14
3	B	501	CDL	C16-C17-C18-C19
3	B	501	CDL	C74-C75-C76-C77
3	B	501	CDL	C17-C18-C19-C20
3	C	501	CDL	C59-C60-C61-C62
3	D	501	CDL	C59-C60-C61-C62
4	C	502	PEE	C11-C12-C13-C14
3	C	501	CDL	C40-C41-C42-C43
3	C	501	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
3	D	501	CDL	C62-C63-C64-C65
3	B	501	CDL	C32-C33-C34-C35
4	A	502	PEE	C3-C2-O2-C10
4	D	502	PEE	C3-C2-O2-C10
3	B	501	CDL	C14-C15-C16-C17
4	C	502	PEE	C15-C16-C17-C18
4	C	502	PEE	C39-C40-C41-C42
4	D	502	PEE	C15-C16-C17-C18
3	D	501	CDL	C51-C52-C53-C54
3	B	501	CDL	C24-C25-C26-C27
3	B	501	CDL	C62-C63-C64-C65
4	A	502	PEE	C21-C22-C23-C24
3	C	501	CDL	C20-C21-C22-C23
3	D	501	CDL	C60-C61-C62-C63
3	A	501	CDL	C36-C37-C38-C39
3	A	501	CDL	C16-C17-C18-C19
3	A	501	CDL	C59-C60-C61-C62
4	B	502	PEE	C44-C45-C46-C47
3	C	501	CDL	C80-C81-C82-C83
3	E	501	CDL	C59-C60-C61-C62
4	E	502	PEE	C32-C33-C34-C35
3	E	501	CDL	OA6-CA4-CA6-OA8
3	B	501	CDL	C84-C85-C86-C87
3	A	501	CDL	C22-C23-C24-C25
3	C	501	CDL	C56-C57-C58-C59
4	C	502	PEE	C14-C15-C16-C17
4	C	502	PEE	C22-C23-C24-C25
3	C	501	CDL	C34-C35-C36-C37
4	A	502	PEE	C24-C25-C26-C27
4	A	502	PEE	C12-C13-C14-C15
3	C	501	CDL	C55-C56-C57-C58
3	A	501	CDL	C84-C85-C86-C87
3	A	501	CDL	C15-C16-C17-C18
3	B	501	CDL	C36-C37-C38-C39
3	D	501	CDL	C12-C13-C14-C15
3	E	501	CDL	C18-C19-C20-C21
3	D	501	CDL	CA4-CA3-OA5-PA1
3	C	501	CDL	C77-C78-C79-C80
3	E	501	CDL	C81-C82-C83-C84
4	B	502	PEE	O3P-C1-C2-C3
4	D	502	PEE	O3P-C1-C2-C3
3	D	501	CDL	C80-C81-C82-C83

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Mol	Chain	Res	Type	Atoms
4	A	502	PEE	C44-C45-C46-C47
3	E	501	CDL	C44-C45-C46-C47
4	C	502	PEE	C44-C45-C46-C47
4	D	502	PEE	C44-C45-C46-C47
4	C	502	PEE	C40-C41-C42-C43
3	D	501	CDL	C20-C21-C22-C23
3	D	501	CDL	C44-C45-C46-C47
3	A	501	CDL	C23-C24-C25-C26
3	E	501	CDL	C22-C23-C24-C25
4	C	502	PEE	C1-C2-C3-O3
3	B	501	CDL	C73-C74-C75-C76
3	C	501	CDL	C78-C79-C80-C81
3	D	501	CDL	C43-C44-C45-C46
3	E	501	CDL	C62-C63-C64-C65
3	E	501	CDL	C84-C85-C86-C87
4	B	502	PEE	O3P-C1-C2-O2
3	E	501	CDL	O1-C1-CA2-OA2
3	D	501	CDL	C1-CA2-OA2-PA1
4	C	502	PEE	C31-C32-C33-C34
3	A	501	CDL	OB6-CB4-CB6-OB8
4	E	502	PEE	O2-C2-C3-O3
4	B	502	PEE	C12-C13-C14-C15
4	A	502	PEE	C38-C39-C40-C41
4	B	502	PEE	C10-C11-C12-C13
3	A	501	CDL	C24-C25-C26-C27
4	E	502	PEE	C34-C35-C36-C37
3	A	501	CDL	C44-C45-C46-C47
4	D	502	PEE	C11-C12-C13-C14
3	E	501	CDL	C13-C14-C15-C16
3	E	501	CDL	C72-C73-C74-C75
3	D	501	CDL	C36-C37-C38-C39
3	E	501	CDL	C78-C79-C80-C81
3	C	501	CDL	OA5-CA3-CA4-CA6
4	C	502	PEE	C36-C37-C38-C39
3	E	501	CDL	C21-C22-C23-C24
4	C	502	PEE	C3-C2-O2-C10
3	A	501	CDL	C74-C75-C76-C77
4	A	502	PEE	O2-C10-C11-C12
3	A	501	CDL	OB5-CB3-CB4-OB6
4	D	502	PEE	O3P-C1-C2-O2
3	A	501	CDL	C53-C54-C55-C56
4	C	502	PEE	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	D	501	CDL	C84-C85-C86-C87
3	B	501	CDL	O1-C1-CA2-OA2
4	C	502	PEE	C20-C21-C22-C23
3	A	501	CDL	C13-C14-C15-C16
3	C	501	CDL	OB5-CB3-CB4-CB6
4	A	502	PEE	O3P-C1-C2-C3
3	E	501	CDL	C37-C38-C39-C40
3	E	501	CDL	C15-C16-C17-C18
3	E	501	CDL	C32-C33-C34-C35
3	E	501	CDL	C23-C24-C25-C26
3	C	501	CDL	OA5-CA3-CA4-OA6
3	C	501	CDL	OB5-CB3-CB4-OB6
3	B	501	CDL	C79-C80-C81-C82
4	D	502	PEE	C40-C41-C42-C43
3	D	501	CDL	CA2-C1-CB2-OB2
3	C	501	CDL	C76-C77-C78-C79
4	E	502	PEE	C31-C30-O3-C3
4	E	502	PEE	O5-C30-O3-C3
3	B	501	CDL	C38-C39-C40-C41
4	A	502	PEE	C33-C34-C35-C36
3	A	501	CDL	CB2-OB2-PB2-OB3
3	A	501	CDL	CB3-OB5-PB2-OB4
3	B	501	CDL	CB3-OB5-PB2-OB2
3	B	501	CDL	CB3-OB5-PB2-OB3
3	B	501	CDL	CB3-OB5-PB2-OB4
3	C	501	CDL	CA3-OA5-PA1-OA2
3	C	501	CDL	CA3-OA5-PA1-OA4
3	C	501	CDL	CB2-OB2-PB2-OB4
3	D	501	CDL	CA2-OA2-PA1-OA4
3	D	501	CDL	CA2-OA2-PA1-OA5
3	D	501	CDL	CB3-OB5-PB2-OB2
3	D	501	CDL	CB3-OB5-PB2-OB3
3	D	501	CDL	CB3-OB5-PB2-OB4
3	E	501	CDL	CA2-OA2-PA1-OA5
3	E	501	CDL	CA3-OA5-PA1-OA3
3	E	501	CDL	CB3-OB5-PB2-OB2
3	E	501	CDL	CB3-OB5-PB2-OB3
3	E	501	CDL	CB3-OB5-PB2-OB4
4	A	502	PEE	C1-O3P-P-O1P
4	B	502	PEE	C1-O3P-P-O1P
4	D	502	PEE	O4P-C4-C5-N
4	E	502	PEE	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
3	B	501	CDL	C1-CA2-OA2-PA1
3	C	501	CDL	C1-CA2-OA2-PA1
3	C	501	CDL	CA4-CA3-OA5-PA1
3	C	501	CDL	C1-CB2-OB2-PB2
3	E	501	CDL	CB4-CB3-OB5-PB2
4	D	502	PEE	C10-C11-C12-C13
3	A	501	CDL	CA7-C31-C32-C33
3	D	501	CDL	C23-C24-C25-C26
4	D	502	PEE	C42-C43-C44-C45
3	C	501	CDL	C36-C37-C38-C39
3	C	501	CDL	C14-C15-C16-C17
3	B	501	CDL	C60-C61-C62-C63
4	E	502	PEE	C15-C16-C17-C18
3	C	501	CDL	C39-C40-C41-C42
4	D	502	PEE	O2-C10-C11-C12
3	D	501	CDL	C18-C19-C20-C21
3	E	501	CDL	CB2-C1-CA2-OA2
3	A	501	CDL	C43-C44-C45-C46
3	C	501	CDL	C84-C85-C86-C87
3	A	501	CDL	C58-C59-C60-C61
3	B	501	CDL	OB5-CB3-CB4-OB6
4	A	502	PEE	C42-C43-C44-C45
3	D	501	CDL	C63-C64-C65-C66
3	B	501	CDL	OB6-CB4-CB6-OB8
3	A	501	CDL	C11-C12-C13-C14
3	A	501	CDL	C34-C35-C36-C37
4	B	502	PEE	C41-C42-C43-C44
4	C	502	PEE	C23-C24-C25-C26
3	C	501	CDL	C12-C13-C14-C15
4	C	502	PEE	C18-C19-C20-C21
4	E	502	PEE	C36-C37-C38-C39
3	C	501	CDL	C64-C65-C66-C67
3	C	501	CDL	C52-C53-C54-C55
3	A	501	CDL	C75-C76-C77-C78
3	A	501	CDL	C63-C64-C65-C66
3	D	501	CDL	C32-C33-C34-C35
3	B	501	CDL	CA2-C1-CB2-OB2
4	E	502	PEE	C44-C45-C46-C47
4	C	502	PEE	C33-C34-C35-C36
3	A	501	CDL	C80-C81-C82-C83
3	B	501	CDL	C57-C58-C59-C60
3	A	501	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
3	B	501	CDL	C19-C20-C21-C22
4	C	502	PEE	C21-C22-C23-C24
3	C	501	CDL	CB3-CB4-CB6-OB8
3	C	501	CDL	C16-C17-C18-C19
3	B	501	CDL	OB5-CB3-CB4-CB6
4	A	502	PEE	O3-C30-C31-C32
4	D	502	PEE	C16-C17-C18-C19
4	C	502	PEE	O2-C10-C11-C12
3	B	501	CDL	O1-C1-CB2-OB2
3	E	501	CDL	C1-CA2-OA2-PA1
3	A	501	CDL	C64-C65-C66-C67
4	B	502	PEE	C16-C17-C18-C19
3	D	501	CDL	C75-C76-C77-C78
3	E	501	CDL	C77-C78-C79-C80
3	B	501	CDL	C15-C16-C17-C18
3	A	501	CDL	C81-C82-C83-C84
3	C	501	CDL	C54-C55-C56-C57
3	A	501	CDL	C19-C20-C21-C22
3	A	501	CDL	C21-C22-C23-C24
3	E	501	CDL	C24-C25-C26-C27
3	D	501	CDL	C52-C51-CB5-OB6
3	C	501	CDL	C31-C32-C33-C34
3	A	501	CDL	C52-C51-CB5-OB6
3	C	501	CDL	C12-C11-CA5-OA6
3	C	501	CDL	C32-C31-CA7-OA8
3	D	501	CDL	C72-C71-CB7-OB8
3	C	501	CDL	C41-C42-C43-C44
3	B	501	CDL	C39-C40-C41-C42
3	E	501	CDL	C60-C61-C62-C63
4	B	502	PEE	C21-C22-C23-C24
3	E	501	CDL	C38-C39-C40-C41
3	E	501	CDL	C73-C74-C75-C76
3	D	501	CDL	C72-C73-C74-C75
3	A	501	CDL	C72-C71-CB7-OB8
3	B	501	CDL	C23-C24-C25-C26
3	A	501	CDL	C52-C51-CB5-OB7
3	A	501	CDL	CA5-C11-C12-C13
3	B	501	CDL	C43-C44-C45-C46
3	C	501	CDL	C12-C11-CA5-OA7
4	E	502	PEE	C40-C41-C42-C43
4	A	502	PEE	C18-C19-C20-C21
3	D	501	CDL	C52-C51-CB5-OB7

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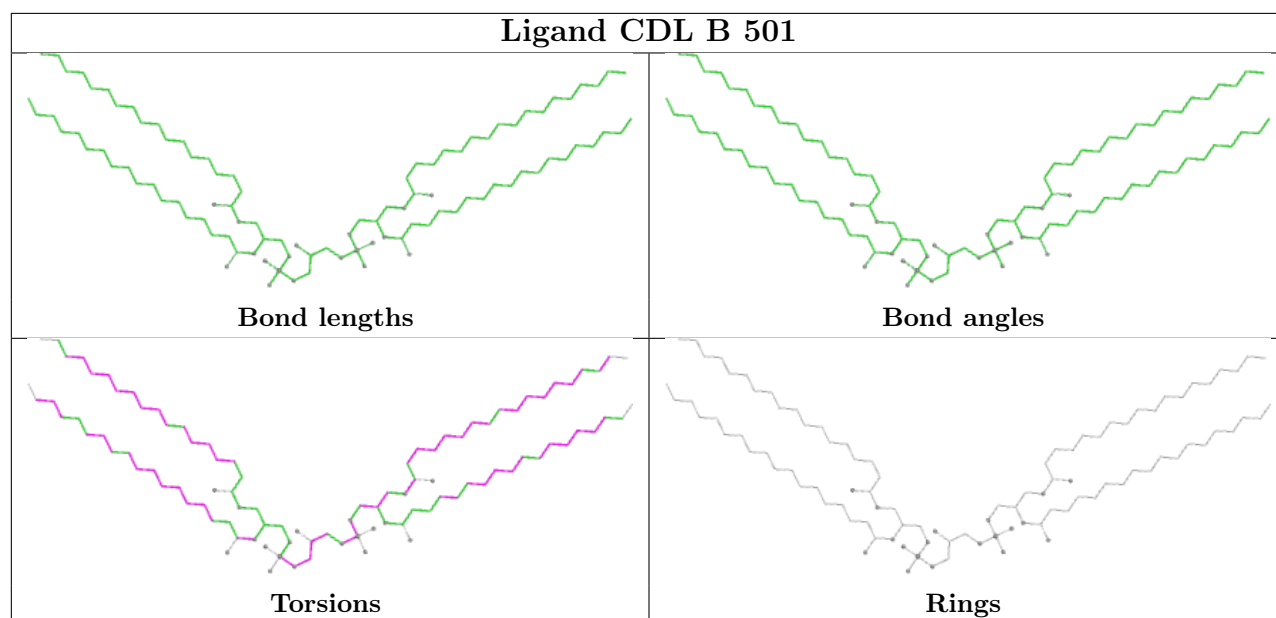
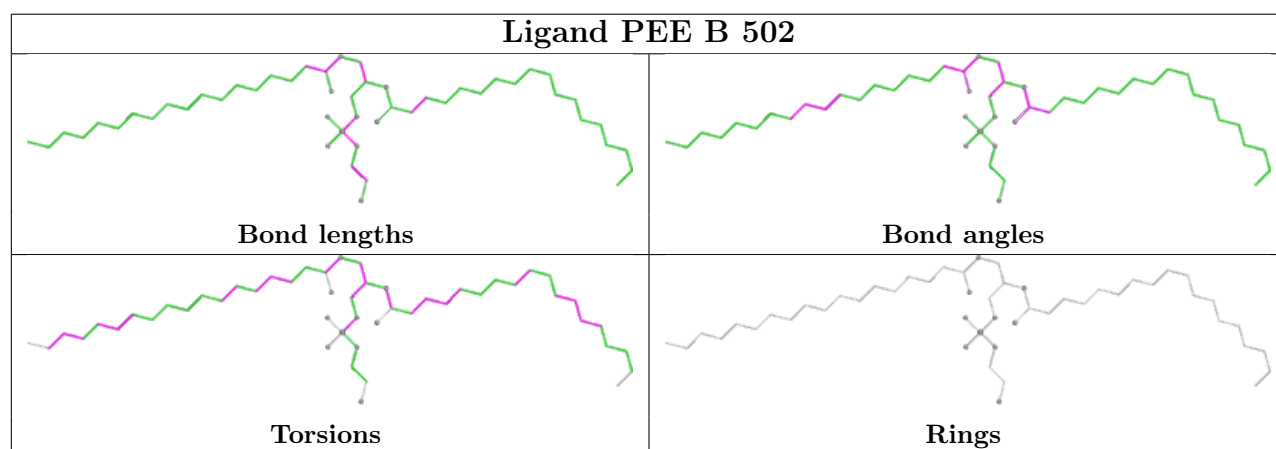
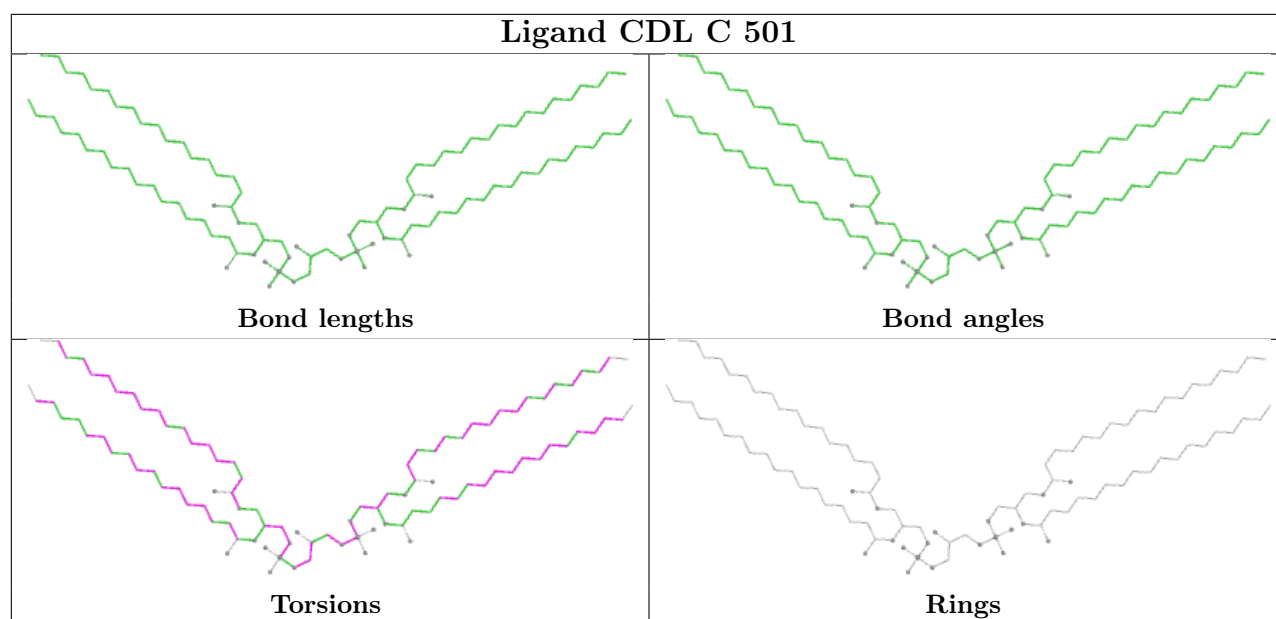
Mol	Chain	Res	Type	Atoms
4	A	502	PEE	O4-C10-C11-C12
3	C	501	CDL	C72-C71-CB7-OB8
3	D	501	CDL	C72-C71-CB7-OB9
3	A	501	CDL	C72-C71-CB7-OB9
3	E	501	CDL	C56-C57-C58-C59
3	C	501	CDL	C32-C31-CA7-OA9

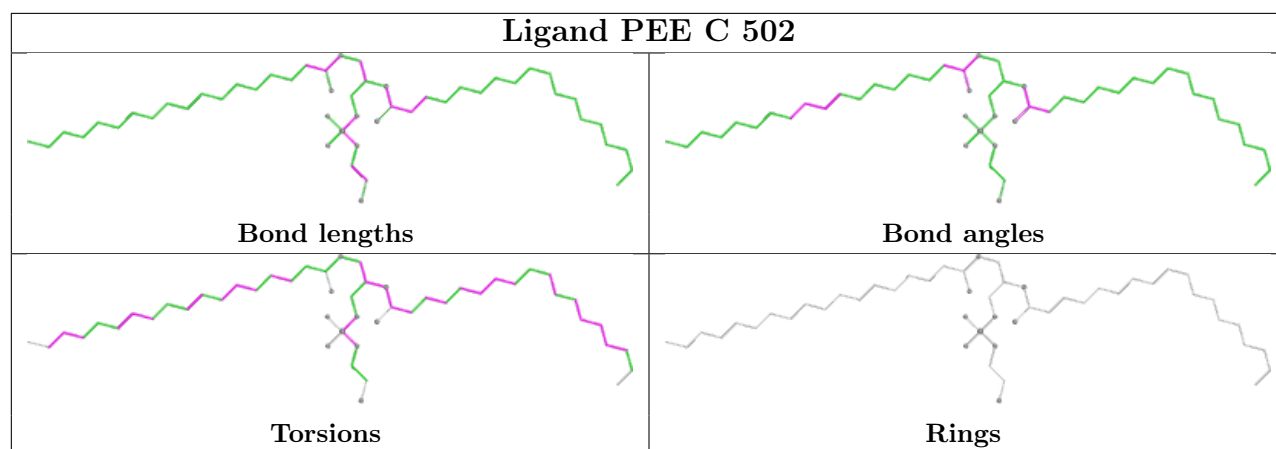
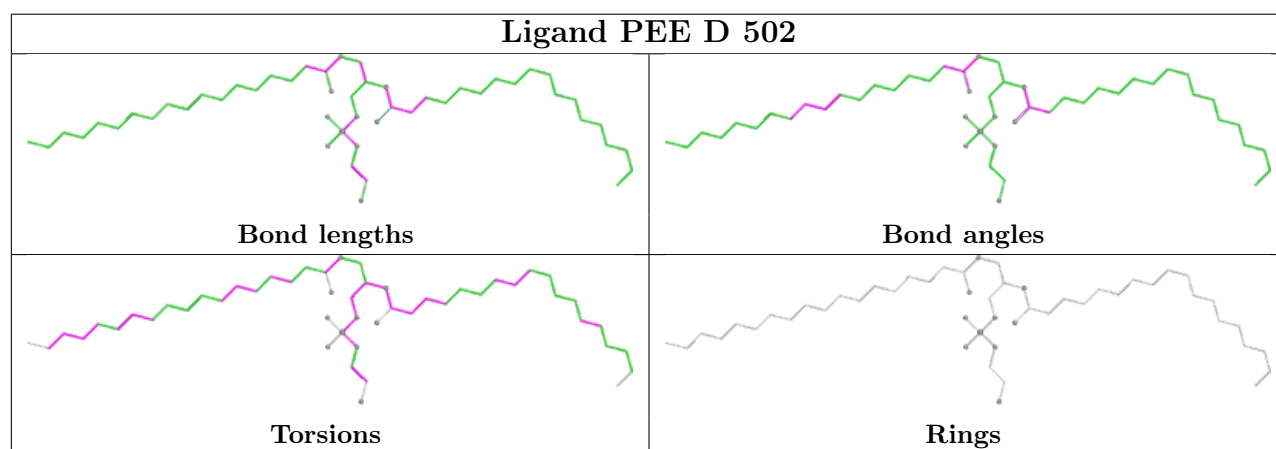
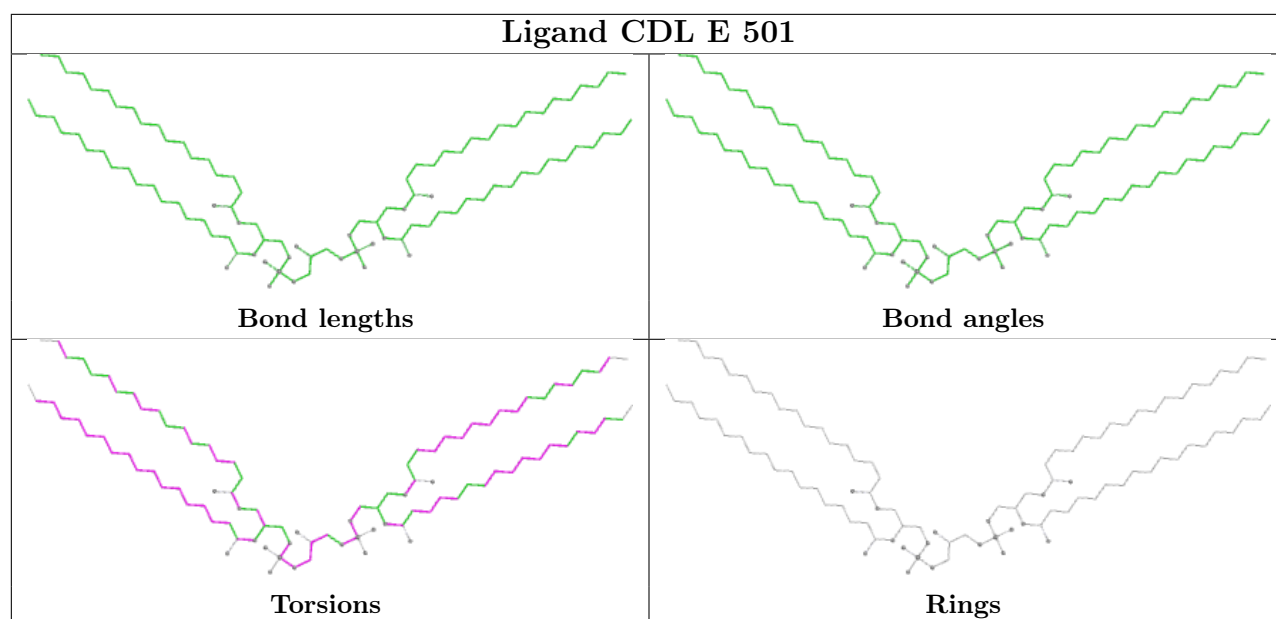
There are no ring outliers.

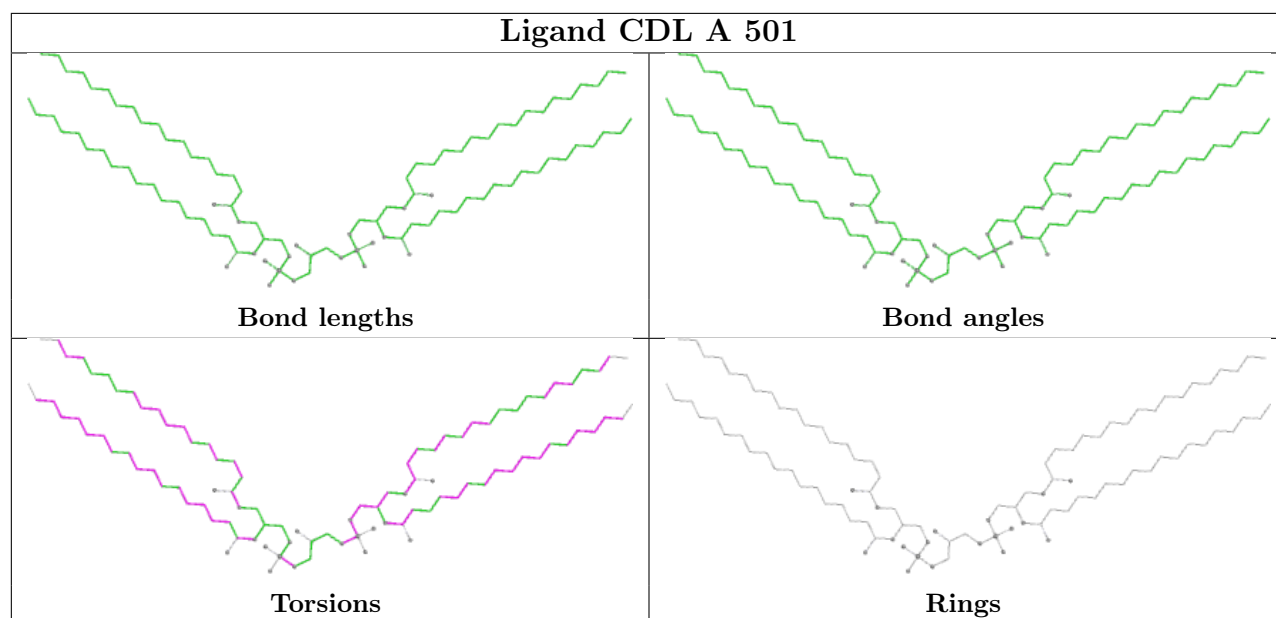
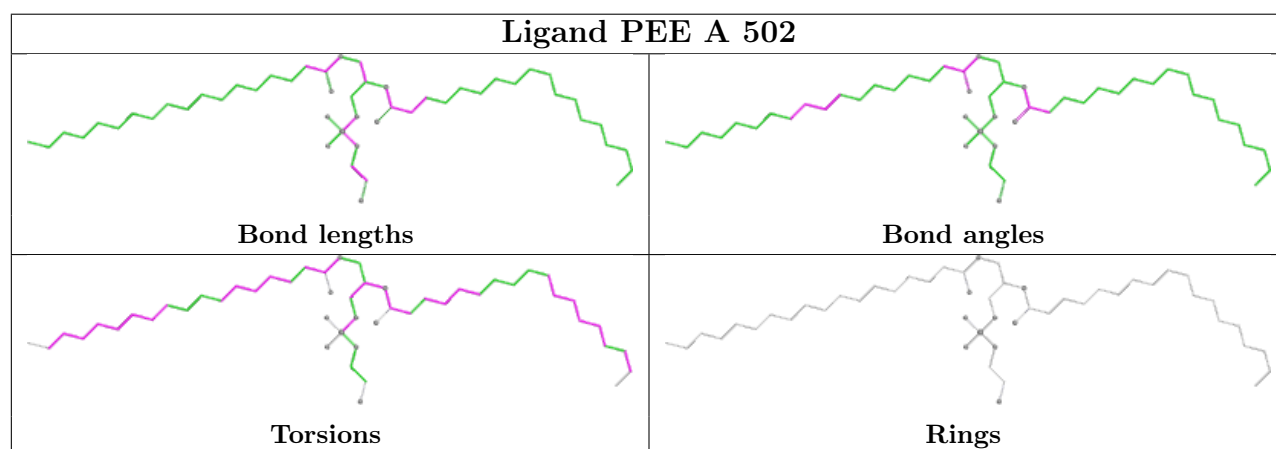
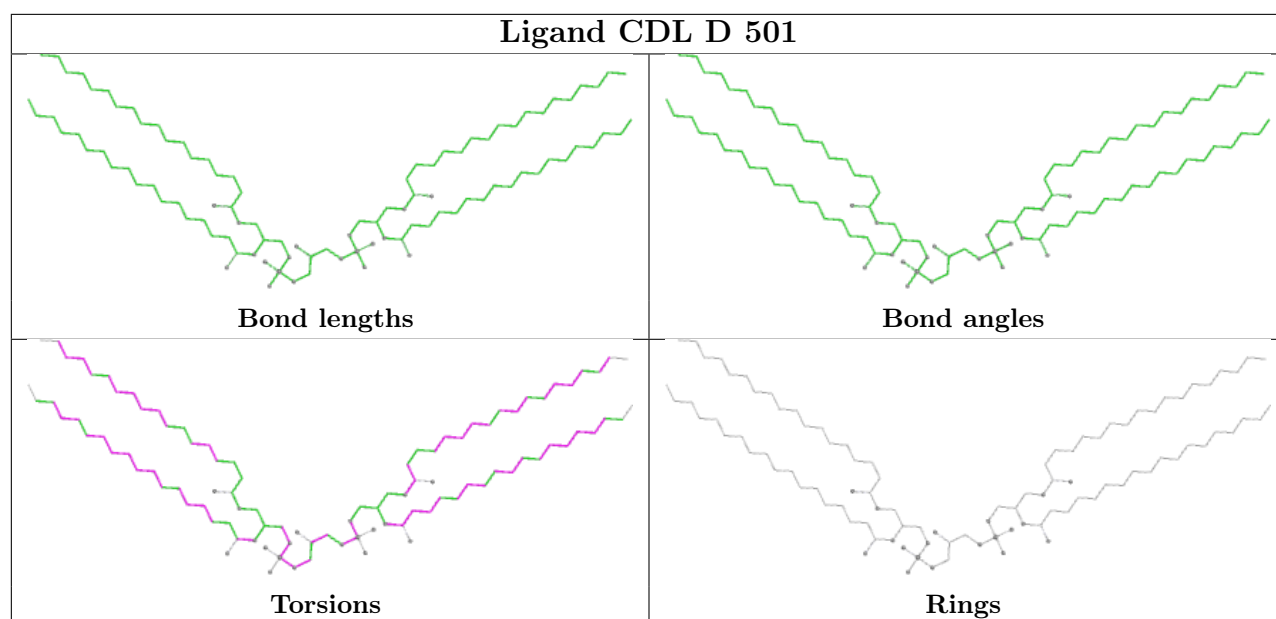
10 monomers are involved in 61 short contacts:

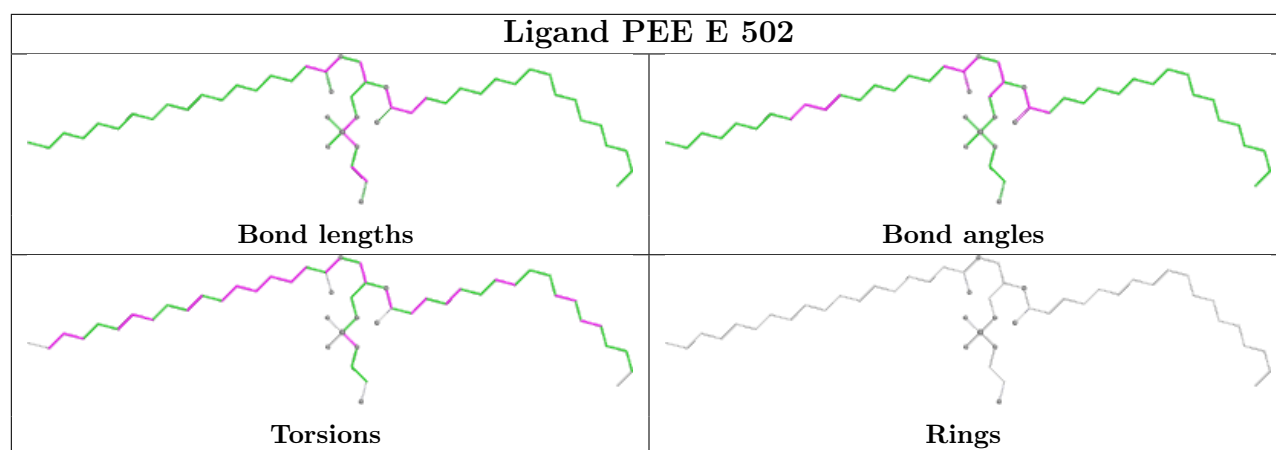
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	CDL	7	0
4	B	502	PEE	2	0
3	B	501	CDL	11	0
3	E	501	CDL	9	0
4	D	502	PEE	7	0
4	C	502	PEE	2	0
3	D	501	CDL	12	0
4	A	502	PEE	6	0
3	A	501	CDL	8	0
4	E	502	PEE	3	0

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.

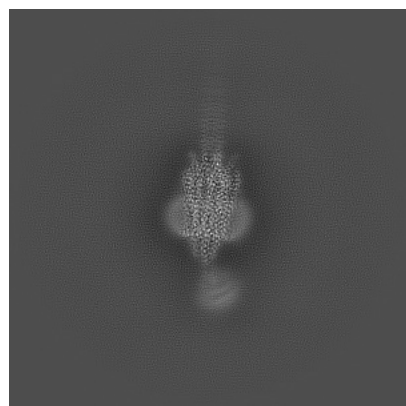
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18756. These allow visual inspection of the internal detail of the map and identification of artifacts.

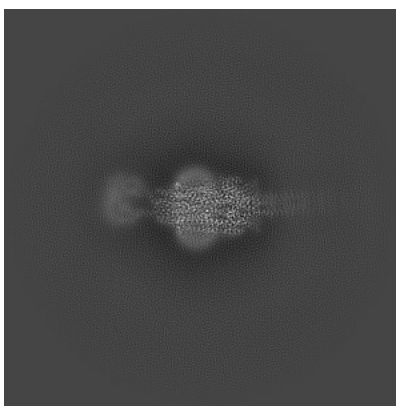
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

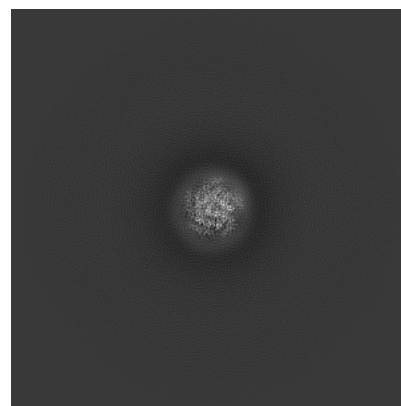
6.1.1 Primary map



X

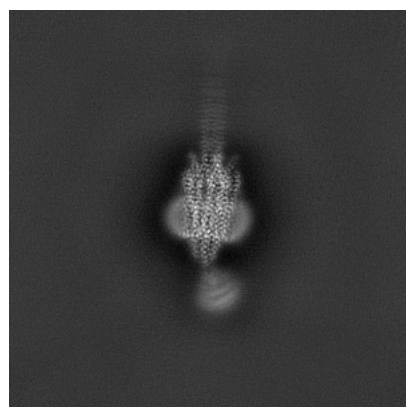


Y

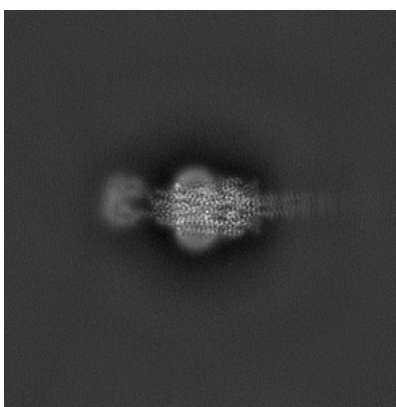


Z

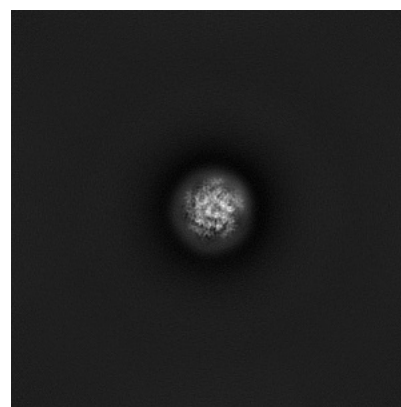
6.1.2 Raw map



X



Y

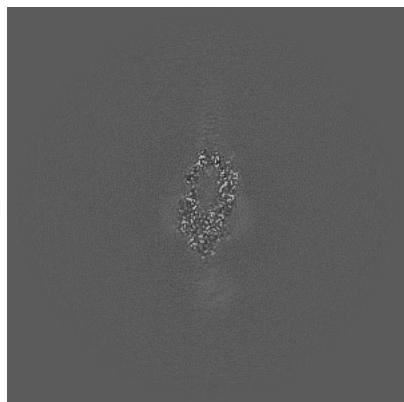


Z

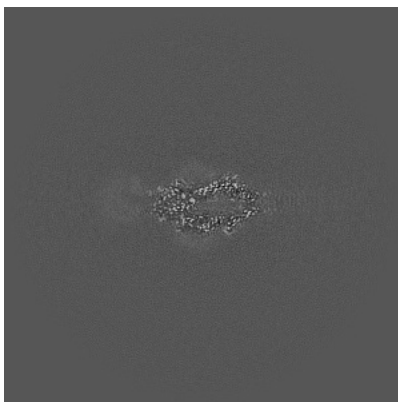
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

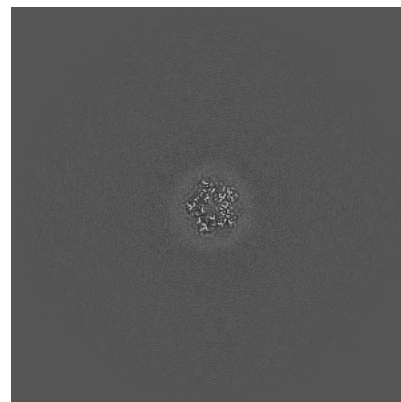
6.2.1 Primary map



X Index: 250



Y Index: 250

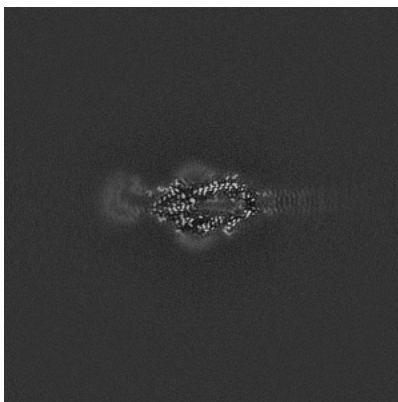


Z Index: 250

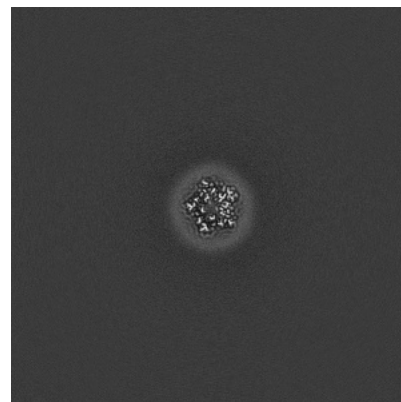
6.2.2 Raw map



X Index: 250



Y Index: 250

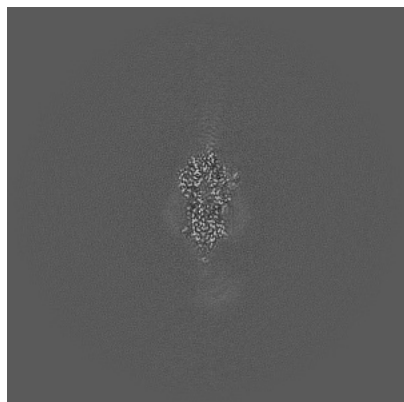


Z Index: 250

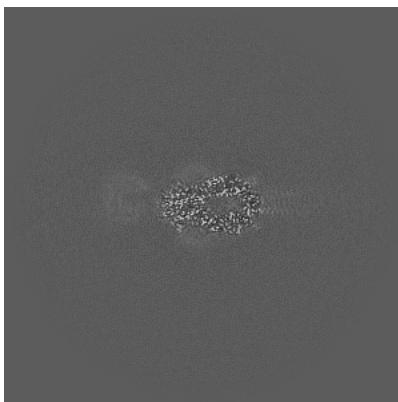
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

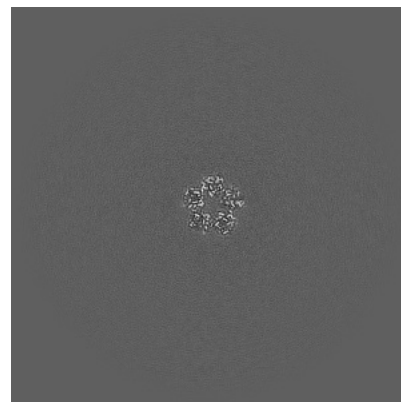
6.3.1 Primary map



X Index: 265

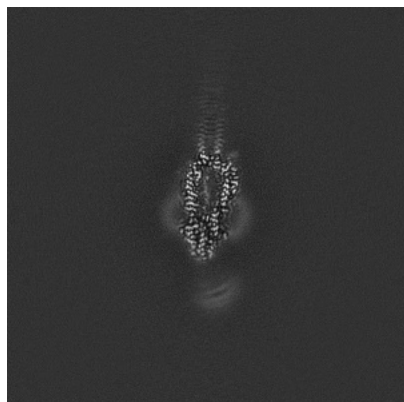


Y Index: 259

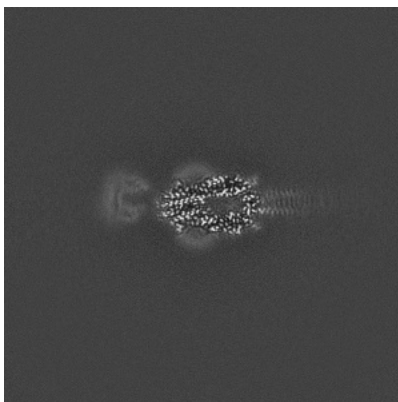


Z Index: 280

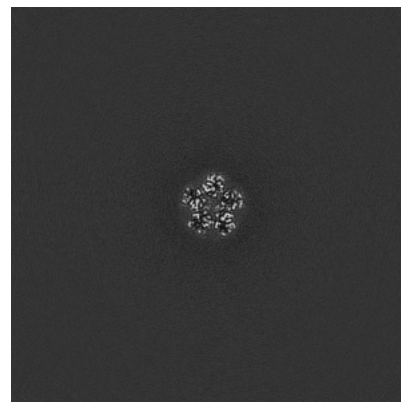
6.3.2 Raw map



X Index: 258



Y Index: 259

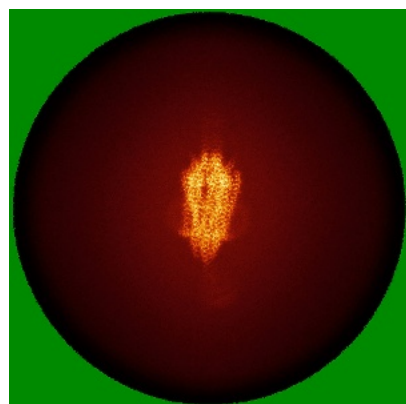


Z Index: 286

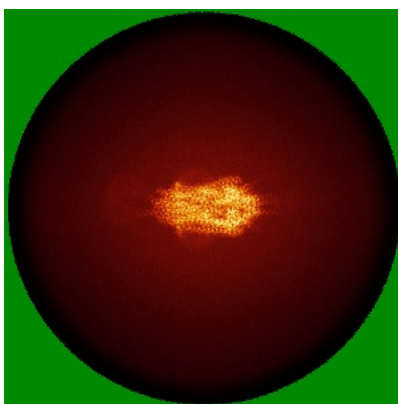
The images above show the largest variance slices of the map in three orthogonal directions.

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

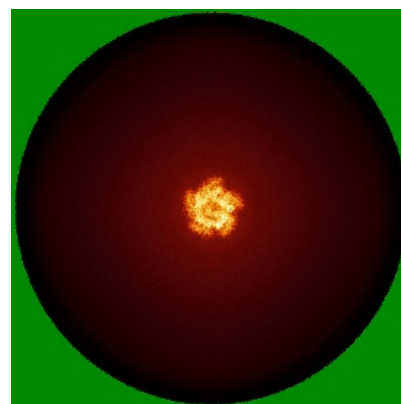
6.4.1 Primary map



X

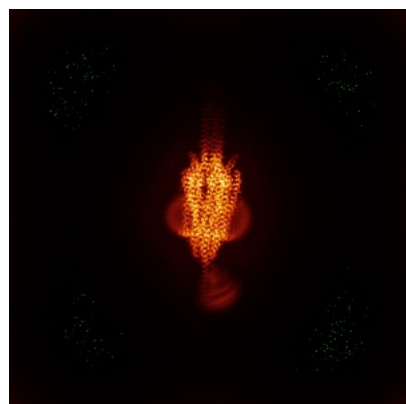


Y

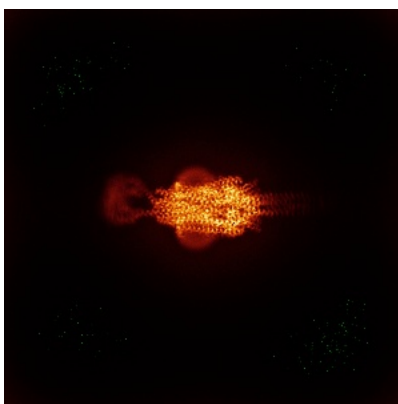


Z

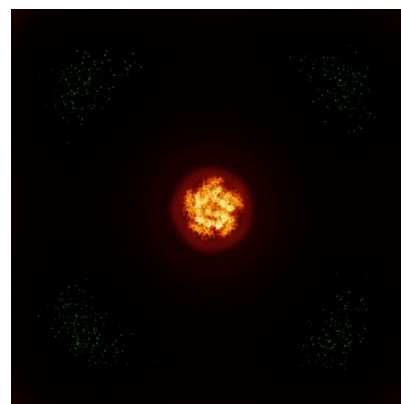
6.4.2 Raw map



X



Y

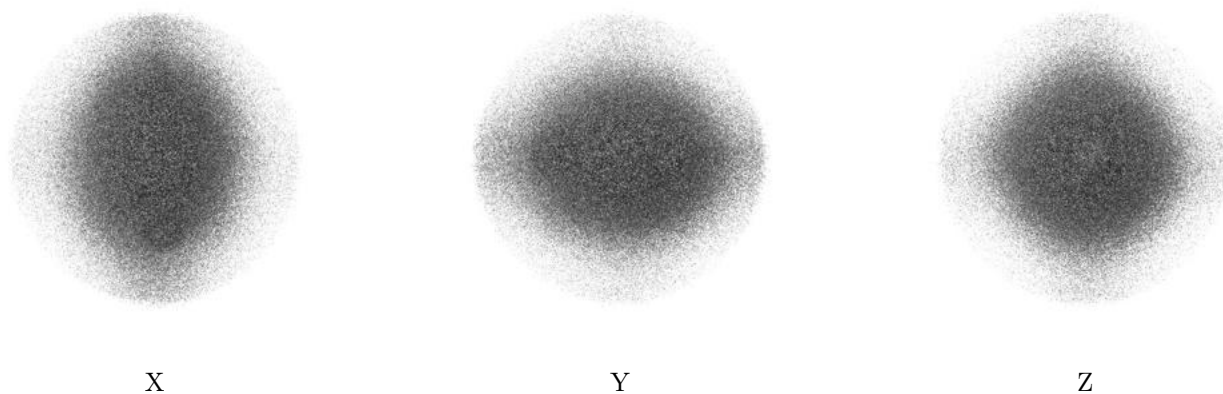


Z

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.

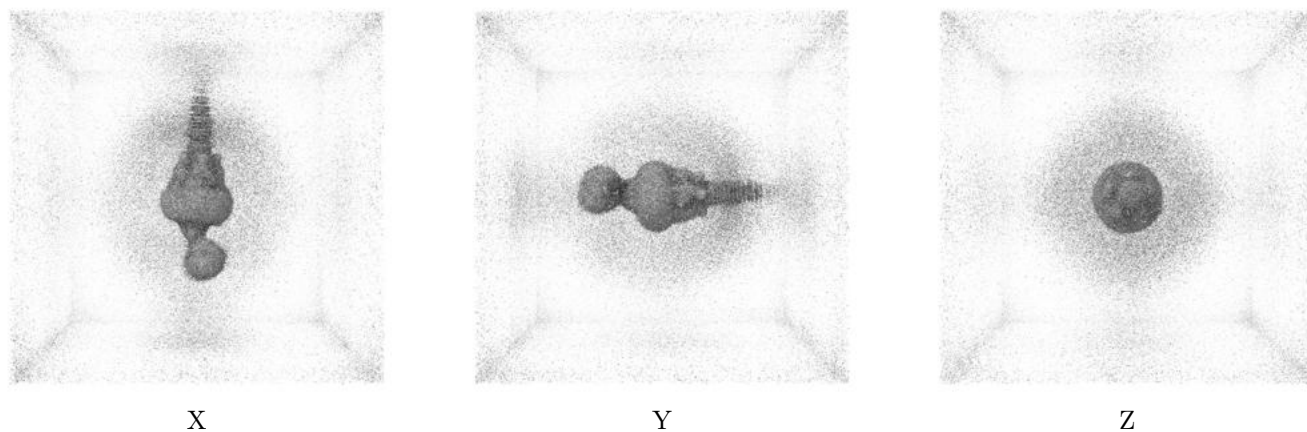
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

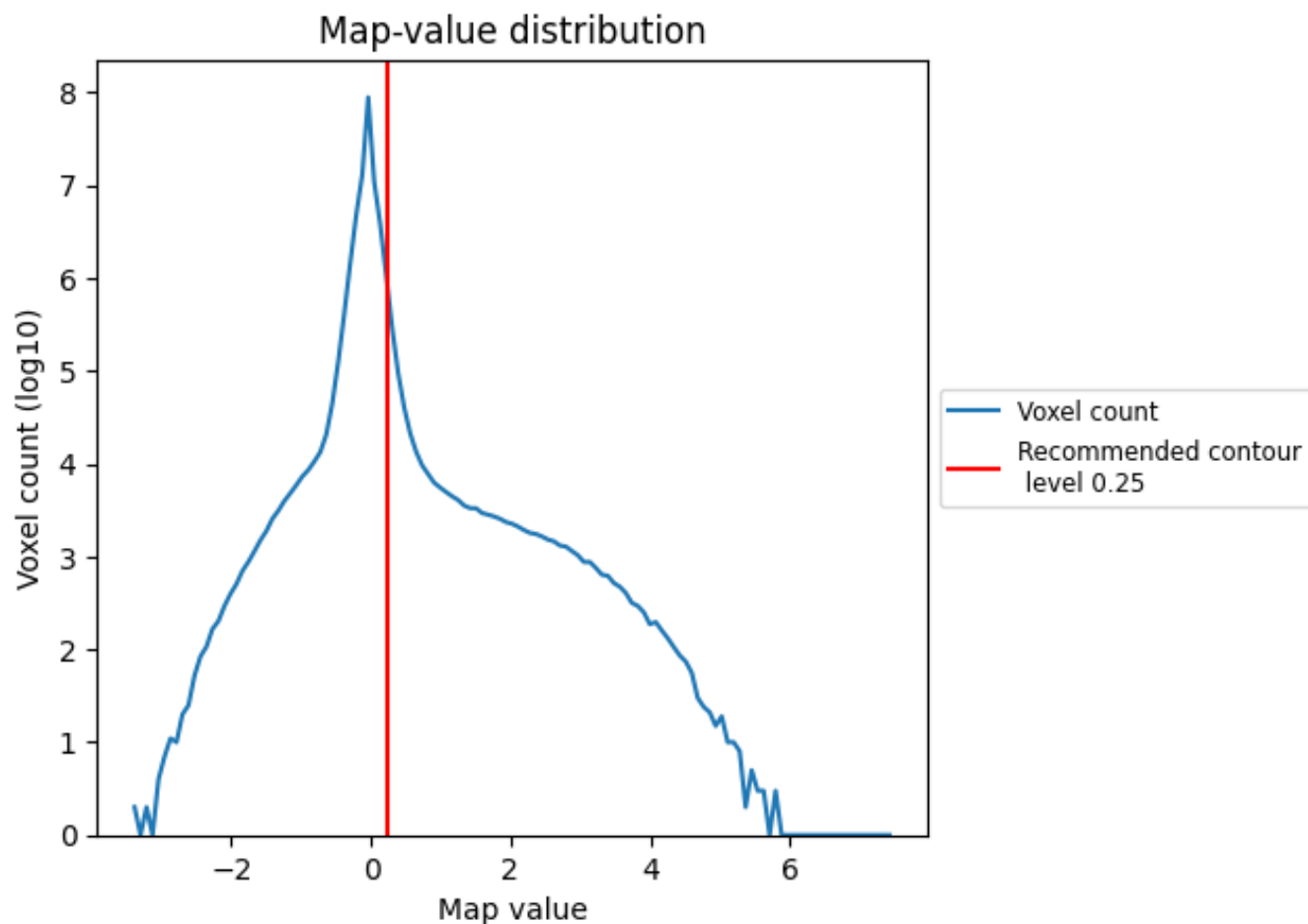
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

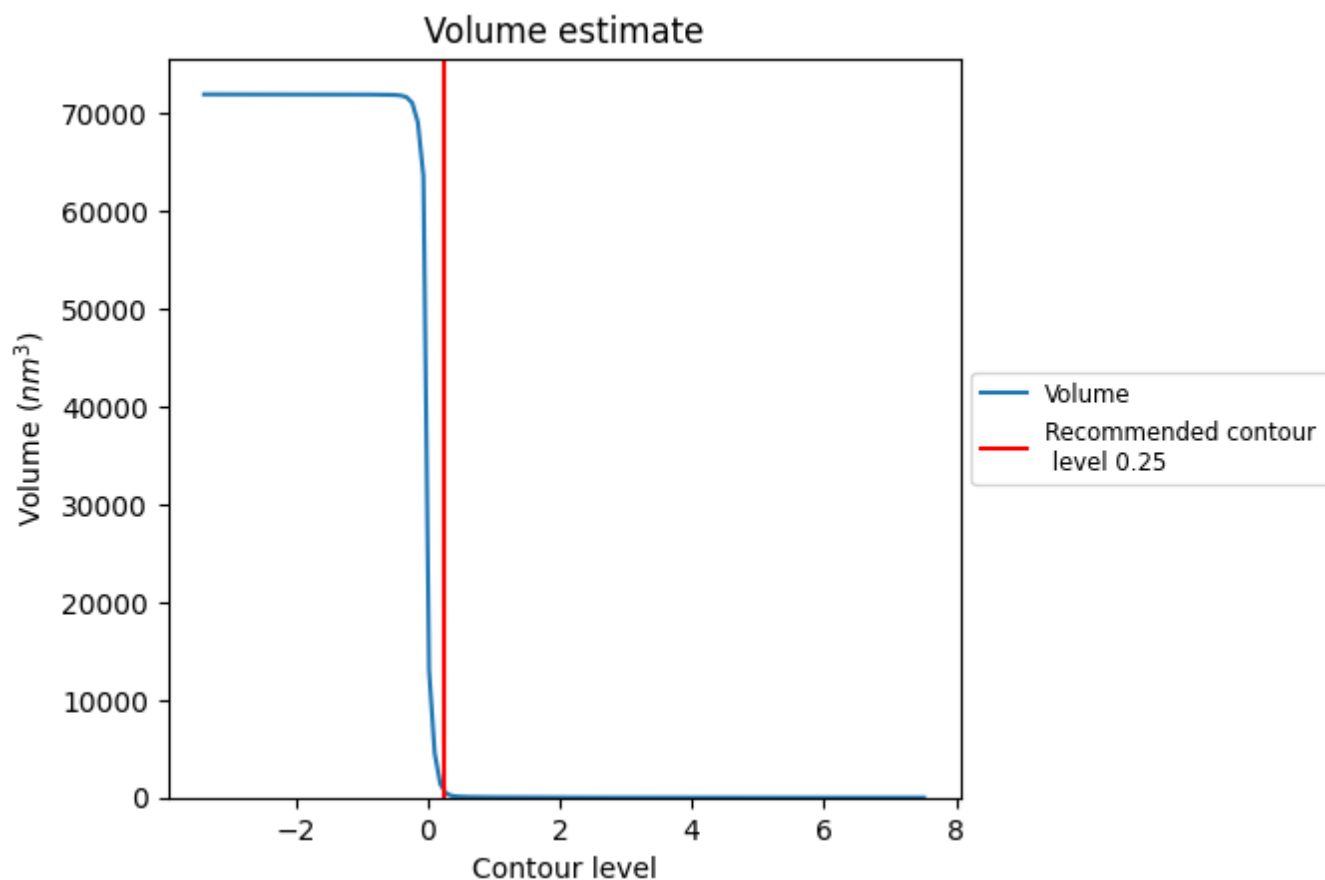
This section contains the results of statistical analysis of the map.

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.

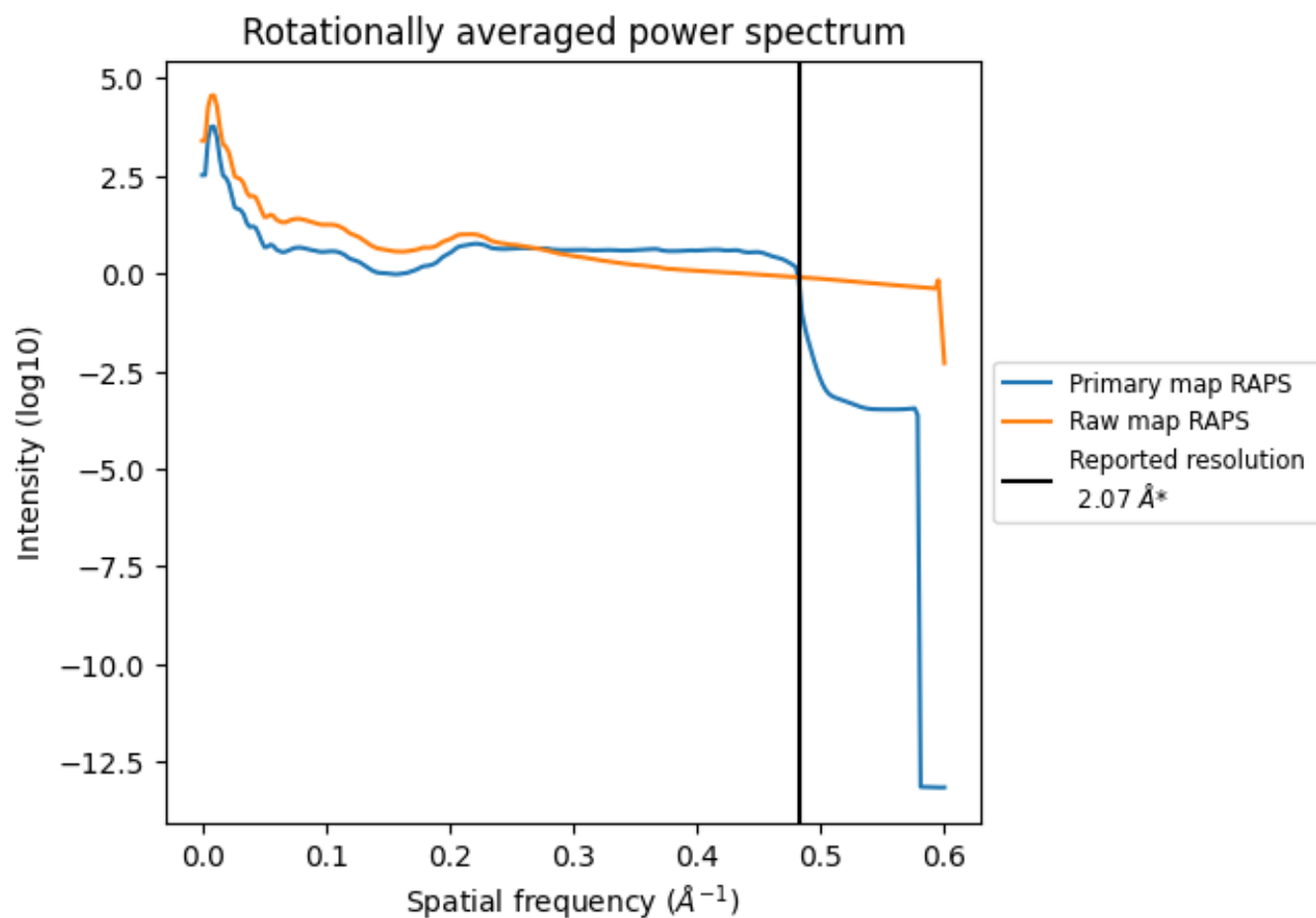
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 756 nm^3 ; this corresponds to an approximate mass of 683 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 ⓘ

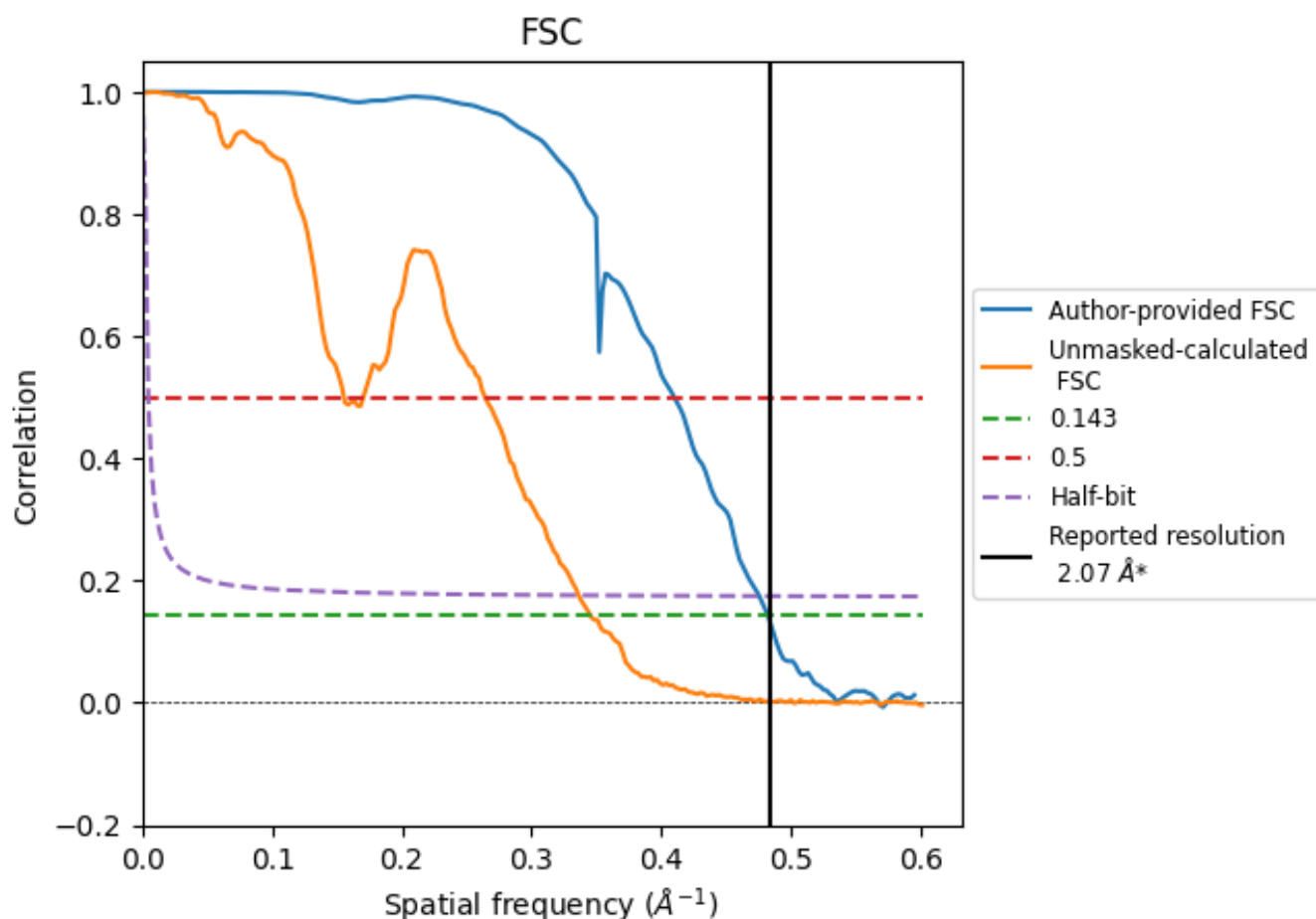


*Reported resolution corresponds to spatial frequency of 0.483 Å⁻¹

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 0.483 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

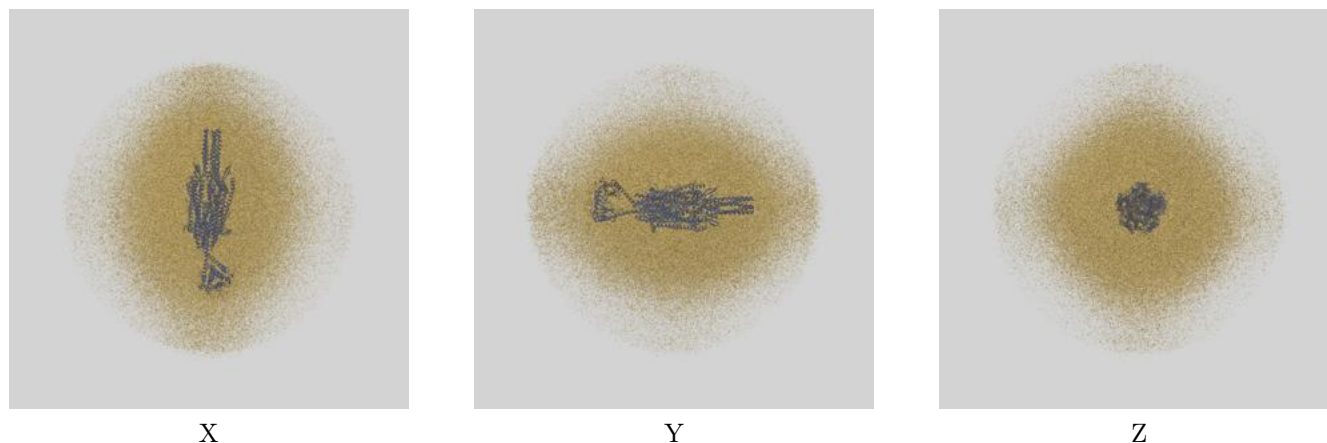
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.07	-	-
Author-provided FSC curve	2.07	2.44	2.10
Unmasked-calculated*	2.90	6.43	2.97

*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 2.90 differs from the reported value 2.07 by more than 10 %

9 Map-model fit [i](#)

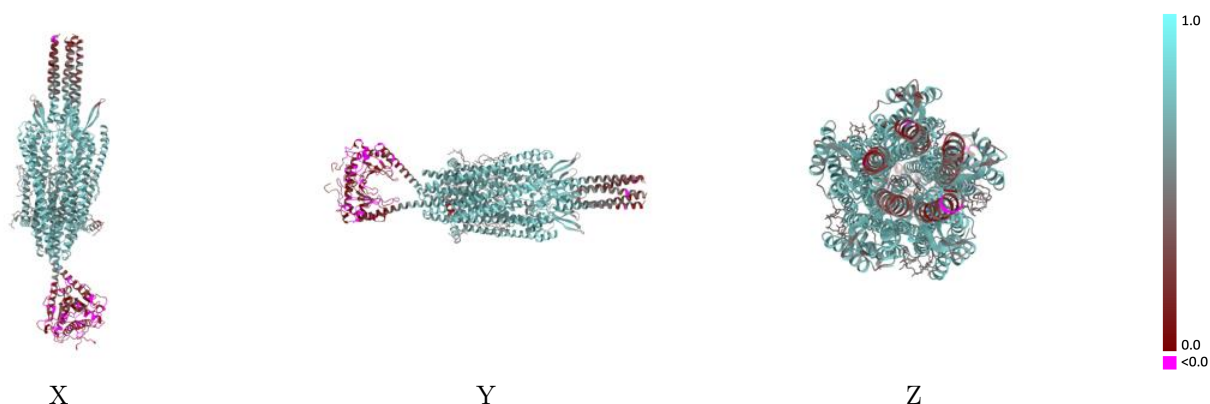
This section contains information regarding the fit between EMDB map EMD-18756 and PDB model 8QYK. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

9.1 Map-model overlay [i](#)



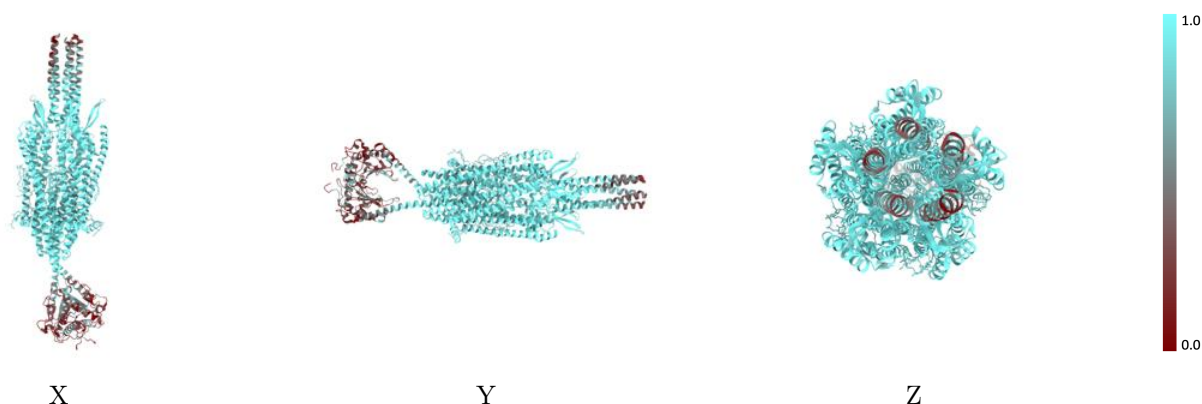
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



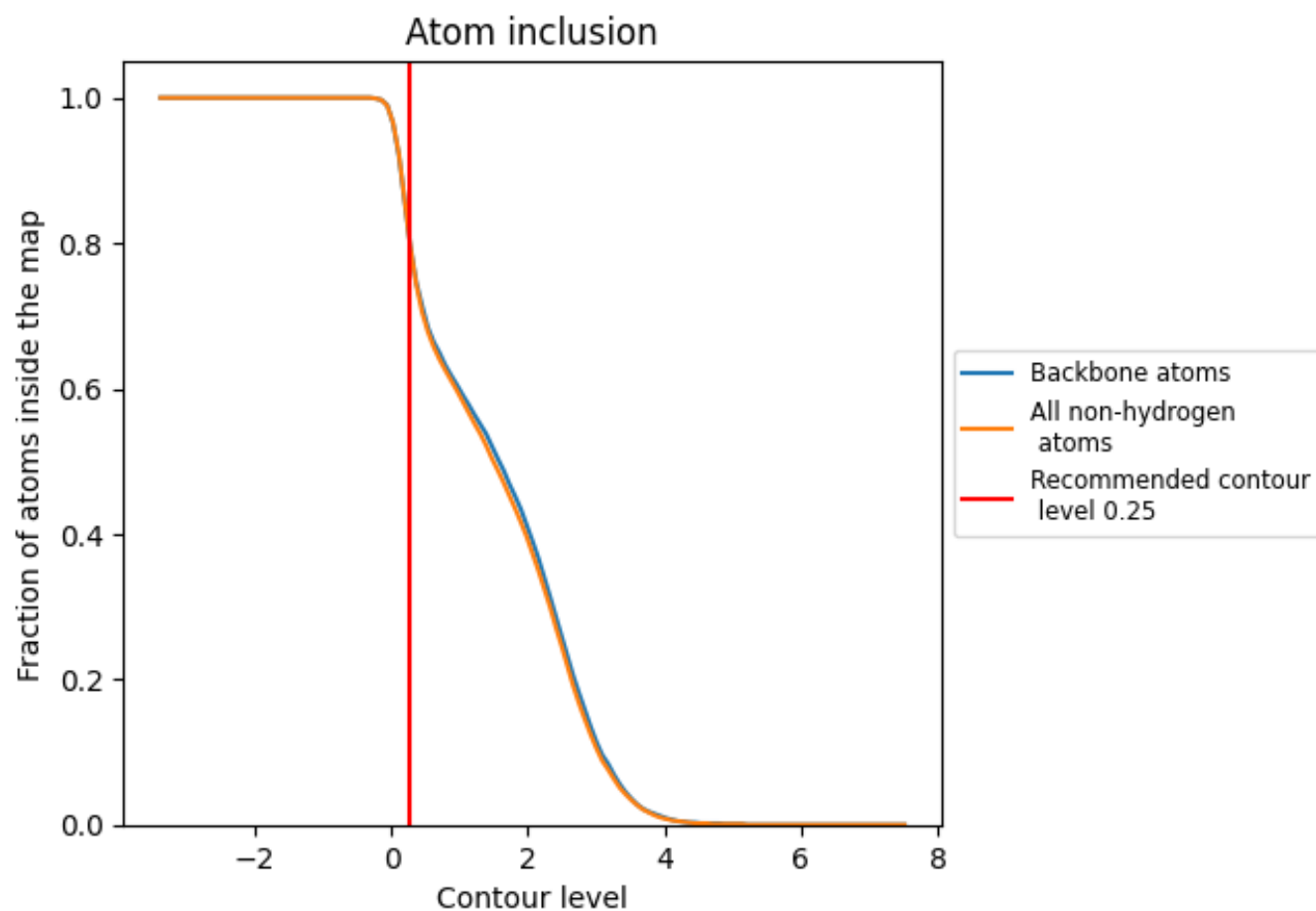
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 82% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8160	0.5440
A	0.9380	0.6530
B	0.9330	0.6530
C	0.9340	0.6690
D	0.9200	0.6410
E	0.9400	0.6660
F	0.4830	0.2260
G	0.4750	0.2100

1.0

0.0

<0.0