



Full wwPDB EM Validation Report ⓘ

Aug 19, 2026 – 03:35 pm BST

PDB ID : 9QHQ / pdb_00009qhq
EMDB ID : EMD-53177
Title : Cryo-EM structure of mouse TRPM3 alpha 2 in with agonists CIM-0216 and Pregnenolone sulfate (PregS)
Authors : Shkumatov, A.V.; Schenck, S.; Brunner, J.D.
Deposited on : 2025-03-16
Resolution : 3.07 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:

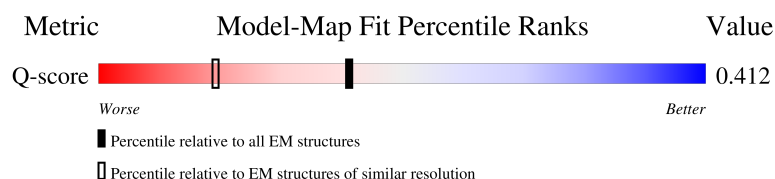
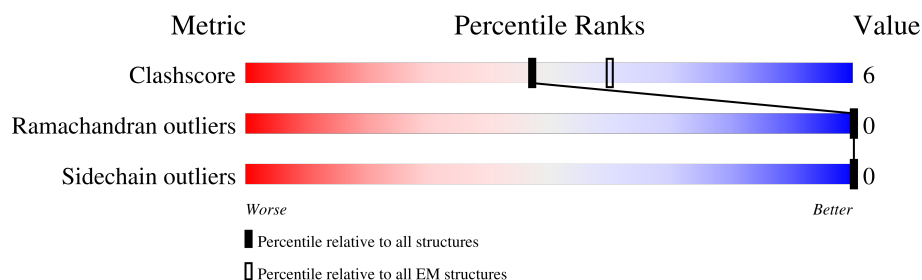
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.07 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	13977 (2.57 - 3.57)

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	1409	16% 58% 10% 32%
1	B	1409	15% 58% 9% 32%
1	C	1409	16% 59% 9% 32%
1	D	1409	15% 59% 9% 32%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 63184 atoms, of which 31876 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 MKIAA1616 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	956	Total	C	H	N	O	S	0	0
			15617	5024	7871	1308	1355	59		
1	B	956	Total	C	H	N	O	S	0	0
			15617	5024	7871	1308	1355	59		
1	C	956	Total	C	H	N	O	S	0	0
			15617	5024	7871	1308	1355	59		
1	D	956	Total	C	H	N	O	S	0	0
			15617	5024	7871	1308	1355	59		

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q69ZE8
A	1	SER	-	expression tag	UNP Q69ZE8
A	1345	ALA	-	expression tag	UNP Q69ZE8
A	1346	LEU	-	expression tag	UNP Q69ZE8
A	1347	GLU	-	expression tag	UNP Q69ZE8
A	1348	VAL	-	expression tag	UNP Q69ZE8
A	1349	LEU	-	expression tag	UNP Q69ZE8
A	1350	PHE	-	expression tag	UNP Q69ZE8
A	1351	GLN	-	expression tag	UNP Q69ZE8
A	1352	GLY	-	expression tag	UNP Q69ZE8
A	1353	PRO	-	expression tag	UNP Q69ZE8
A	1354	GLN	-	expression tag	UNP Q69ZE8
A	1355	GLY	-	expression tag	UNP Q69ZE8
A	1356	THR	-	expression tag	UNP Q69ZE8
A	1357	GLU	-	expression tag	UNP Q69ZE8
A	1358	GLN	-	expression tag	UNP Q69ZE8
A	1359	LYS	-	expression tag	UNP Q69ZE8
A	1360	LEU	-	expression tag	UNP Q69ZE8
A	1361	ILE	-	expression tag	UNP Q69ZE8
A	1362	SER	-	expression tag	UNP Q69ZE8
A	1363	GLU	-	expression tag	UNP Q69ZE8
A	1364	GLU	-	expression tag	UNP Q69ZE8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1365	ASP	-	expression tag	UNP Q69ZE8
A	1366	LEU	-	expression tag	UNP Q69ZE8
A	1367	ARG	-	expression tag	UNP Q69ZE8
A	1368	GLY	-	expression tag	UNP Q69ZE8
A	1369	ALA	-	expression tag	UNP Q69ZE8
A	1370	SER	-	expression tag	UNP Q69ZE8
A	1371	MET	-	expression tag	UNP Q69ZE8
A	1372	ASP	-	expression tag	UNP Q69ZE8
A	1373	GLU	-	expression tag	UNP Q69ZE8
A	1374	LYS	-	expression tag	UNP Q69ZE8
A	1375	THR	-	expression tag	UNP Q69ZE8
A	1376	THR	-	expression tag	UNP Q69ZE8
A	1377	GLY	-	expression tag	UNP Q69ZE8
A	1378	TRP	-	expression tag	UNP Q69ZE8
A	1379	ARG	-	expression tag	UNP Q69ZE8
A	1380	GLY	-	expression tag	UNP Q69ZE8
A	1381	GLY	-	expression tag	UNP Q69ZE8
A	1382	HIS	-	expression tag	UNP Q69ZE8
A	1383	VAL	-	expression tag	UNP Q69ZE8
A	1384	VAL	-	expression tag	UNP Q69ZE8
A	1385	GLU	-	expression tag	UNP Q69ZE8
A	1386	GLY	-	expression tag	UNP Q69ZE8
A	1387	LEU	-	expression tag	UNP Q69ZE8
A	1388	ALA	-	expression tag	UNP Q69ZE8
A	1389	GLY	-	expression tag	UNP Q69ZE8
A	1390	GLU	-	expression tag	UNP Q69ZE8
A	1391	LEU	-	expression tag	UNP Q69ZE8
A	1392	GLU	-	expression tag	UNP Q69ZE8
A	1393	GLN	-	expression tag	UNP Q69ZE8
A	1394	LEU	-	expression tag	UNP Q69ZE8
A	1395	ARG	-	expression tag	UNP Q69ZE8
A	1396	ALA	-	expression tag	UNP Q69ZE8
A	1397	ARG	-	expression tag	UNP Q69ZE8
A	1398	LEU	-	expression tag	UNP Q69ZE8
A	1399	GLU	-	expression tag	UNP Q69ZE8
A	1400	HIS	-	expression tag	UNP Q69ZE8
A	1401	HIS	-	expression tag	UNP Q69ZE8
A	1402	PRO	-	expression tag	UNP Q69ZE8
A	1403	GLN	-	expression tag	UNP Q69ZE8
A	1404	GLY	-	expression tag	UNP Q69ZE8
A	1405	GLN	-	expression tag	UNP Q69ZE8
A	1406	ARG	-	expression tag	UNP Q69ZE8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1407	GLU	-	expression tag	UNP Q69ZE8
A	1408	PRO	-	expression tag	UNP Q69ZE8
B	0	MET	-	initiating methionine	UNP Q69ZE8
B	1	SER	-	expression tag	UNP Q69ZE8
B	1345	ALA	-	expression tag	UNP Q69ZE8
B	1346	LEU	-	expression tag	UNP Q69ZE8
B	1347	GLU	-	expression tag	UNP Q69ZE8
B	1348	VAL	-	expression tag	UNP Q69ZE8
B	1349	LEU	-	expression tag	UNP Q69ZE8
B	1350	PHE	-	expression tag	UNP Q69ZE8
B	1351	GLN	-	expression tag	UNP Q69ZE8
B	1352	GLY	-	expression tag	UNP Q69ZE8
B	1353	PRO	-	expression tag	UNP Q69ZE8
B	1354	GLN	-	expression tag	UNP Q69ZE8
B	1355	GLY	-	expression tag	UNP Q69ZE8
B	1356	THR	-	expression tag	UNP Q69ZE8
B	1357	GLU	-	expression tag	UNP Q69ZE8
B	1358	GLN	-	expression tag	UNP Q69ZE8
B	1359	LYS	-	expression tag	UNP Q69ZE8
B	1360	LEU	-	expression tag	UNP Q69ZE8
B	1361	ILE	-	expression tag	UNP Q69ZE8
B	1362	SER	-	expression tag	UNP Q69ZE8
B	1363	GLU	-	expression tag	UNP Q69ZE8
B	1364	GLU	-	expression tag	UNP Q69ZE8
B	1365	ASP	-	expression tag	UNP Q69ZE8
B	1366	LEU	-	expression tag	UNP Q69ZE8
B	1367	ARG	-	expression tag	UNP Q69ZE8
B	1368	GLY	-	expression tag	UNP Q69ZE8
B	1369	ALA	-	expression tag	UNP Q69ZE8
B	1370	SER	-	expression tag	UNP Q69ZE8
B	1371	MET	-	expression tag	UNP Q69ZE8
B	1372	ASP	-	expression tag	UNP Q69ZE8
B	1373	GLU	-	expression tag	UNP Q69ZE8
B	1374	LYS	-	expression tag	UNP Q69ZE8
B	1375	THR	-	expression tag	UNP Q69ZE8
B	1376	THR	-	expression tag	UNP Q69ZE8
B	1377	GLY	-	expression tag	UNP Q69ZE8
B	1378	TRP	-	expression tag	UNP Q69ZE8
B	1379	ARG	-	expression tag	UNP Q69ZE8
B	1380	GLY	-	expression tag	UNP Q69ZE8
B	1381	GLY	-	expression tag	UNP Q69ZE8
B	1382	HIS	-	expression tag	UNP Q69ZE8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1383	VAL	-	expression tag	UNP Q69ZE8
B	1384	VAL	-	expression tag	UNP Q69ZE8
B	1385	GLU	-	expression tag	UNP Q69ZE8
B	1386	GLY	-	expression tag	UNP Q69ZE8
B	1387	LEU	-	expression tag	UNP Q69ZE8
B	1388	ALA	-	expression tag	UNP Q69ZE8
B	1389	GLY	-	expression tag	UNP Q69ZE8
B	1390	GLU	-	expression tag	UNP Q69ZE8
B	1391	LEU	-	expression tag	UNP Q69ZE8
B	1392	GLU	-	expression tag	UNP Q69ZE8
B	1393	GLN	-	expression tag	UNP Q69ZE8
B	1394	LEU	-	expression tag	UNP Q69ZE8
B	1395	ARG	-	expression tag	UNP Q69ZE8
B	1396	ALA	-	expression tag	UNP Q69ZE8
B	1397	ARG	-	expression tag	UNP Q69ZE8
B	1398	LEU	-	expression tag	UNP Q69ZE8
B	1399	GLU	-	expression tag	UNP Q69ZE8
B	1400	HIS	-	expression tag	UNP Q69ZE8
B	1401	HIS	-	expression tag	UNP Q69ZE8
B	1402	PRO	-	expression tag	UNP Q69ZE8
B	1403	GLN	-	expression tag	UNP Q69ZE8
B	1404	GLY	-	expression tag	UNP Q69ZE8
B	1405	GLN	-	expression tag	UNP Q69ZE8
B	1406	ARG	-	expression tag	UNP Q69ZE8
B	1407	GLU	-	expression tag	UNP Q69ZE8
B	1408	PRO	-	expression tag	UNP Q69ZE8
C	0	MET	-	initiating methionine	UNP Q69ZE8
C	1	SER	-	expression tag	UNP Q69ZE8
C	1345	ALA	-	expression tag	UNP Q69ZE8
C	1346	LEU	-	expression tag	UNP Q69ZE8
C	1347	GLU	-	expression tag	UNP Q69ZE8
C	1348	VAL	-	expression tag	UNP Q69ZE8
C	1349	LEU	-	expression tag	UNP Q69ZE8
C	1350	PHE	-	expression tag	UNP Q69ZE8
C	1351	GLN	-	expression tag	UNP Q69ZE8
C	1352	GLY	-	expression tag	UNP Q69ZE8
C	1353	PRO	-	expression tag	UNP Q69ZE8
C	1354	GLN	-	expression tag	UNP Q69ZE8
C	1355	GLY	-	expression tag	UNP Q69ZE8
C	1356	THR	-	expression tag	UNP Q69ZE8
C	1357	GLU	-	expression tag	UNP Q69ZE8
C	1358	GLN	-	expression tag	UNP Q69ZE8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1359	LYS	-	expression tag	UNP Q69ZE8
C	1360	LEU	-	expression tag	UNP Q69ZE8
C	1361	ILE	-	expression tag	UNP Q69ZE8
C	1362	SER	-	expression tag	UNP Q69ZE8
C	1363	GLU	-	expression tag	UNP Q69ZE8
C	1364	GLU	-	expression tag	UNP Q69ZE8
C	1365	ASP	-	expression tag	UNP Q69ZE8
C	1366	LEU	-	expression tag	UNP Q69ZE8
C	1367	ARG	-	expression tag	UNP Q69ZE8
C	1368	GLY	-	expression tag	UNP Q69ZE8
C	1369	ALA	-	expression tag	UNP Q69ZE8
C	1370	SER	-	expression tag	UNP Q69ZE8
C	1371	MET	-	expression tag	UNP Q69ZE8
C	1372	ASP	-	expression tag	UNP Q69ZE8
C	1373	GLU	-	expression tag	UNP Q69ZE8
C	1374	LYS	-	expression tag	UNP Q69ZE8
C	1375	THR	-	expression tag	UNP Q69ZE8
C	1376	THR	-	expression tag	UNP Q69ZE8
C	1377	GLY	-	expression tag	UNP Q69ZE8
C	1378	TRP	-	expression tag	UNP Q69ZE8
C	1379	ARG	-	expression tag	UNP Q69ZE8
C	1380	GLY	-	expression tag	UNP Q69ZE8
C	1381	GLY	-	expression tag	UNP Q69ZE8
C	1382	HIS	-	expression tag	UNP Q69ZE8
C	1383	VAL	-	expression tag	UNP Q69ZE8
C	1384	VAL	-	expression tag	UNP Q69ZE8
C	1385	GLU	-	expression tag	UNP Q69ZE8
C	1386	GLY	-	expression tag	UNP Q69ZE8
C	1387	LEU	-	expression tag	UNP Q69ZE8
C	1388	ALA	-	expression tag	UNP Q69ZE8
C	1389	GLY	-	expression tag	UNP Q69ZE8
C	1390	GLU	-	expression tag	UNP Q69ZE8
C	1391	LEU	-	expression tag	UNP Q69ZE8
C	1392	GLU	-	expression tag	UNP Q69ZE8
C	1393	GLN	-	expression tag	UNP Q69ZE8
C	1394	LEU	-	expression tag	UNP Q69ZE8
C	1395	ARG	-	expression tag	UNP Q69ZE8
C	1396	ALA	-	expression tag	UNP Q69ZE8
C	1397	ARG	-	expression tag	UNP Q69ZE8
C	1398	LEU	-	expression tag	UNP Q69ZE8
C	1399	GLU	-	expression tag	UNP Q69ZE8
C	1400	HIS	-	expression tag	UNP Q69ZE8

Continued on next page...

Continued from previous page...

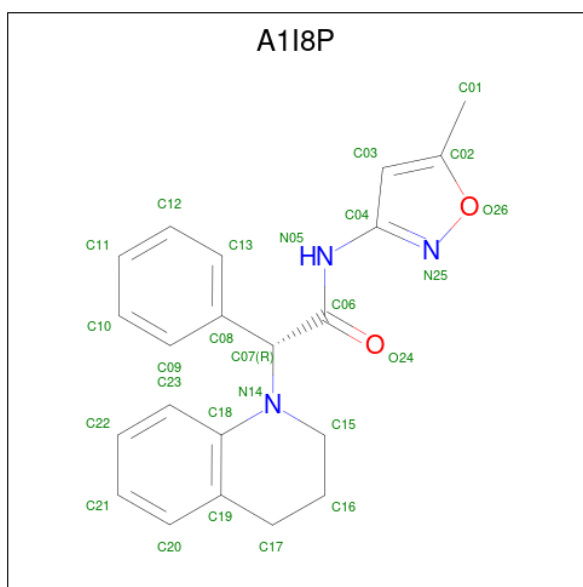
Chain	Residue	Modelled	Actual	Comment	Reference
C	1401	HIS	-	expression tag	UNP Q69ZE8
C	1402	PRO	-	expression tag	UNP Q69ZE8
C	1403	GLN	-	expression tag	UNP Q69ZE8
C	1404	GLY	-	expression tag	UNP Q69ZE8
C	1405	GLN	-	expression tag	UNP Q69ZE8
C	1406	ARG	-	expression tag	UNP Q69ZE8
C	1407	GLU	-	expression tag	UNP Q69ZE8
C	1408	PRO	-	expression tag	UNP Q69ZE8
D	0	MET	-	initiating methionine	UNP Q69ZE8
D	1	SER	-	expression tag	UNP Q69ZE8
D	1345	ALA	-	expression tag	UNP Q69ZE8
D	1346	LEU	-	expression tag	UNP Q69ZE8
D	1347	GLU	-	expression tag	UNP Q69ZE8
D	1348	VAL	-	expression tag	UNP Q69ZE8
D	1349	LEU	-	expression tag	UNP Q69ZE8
D	1350	PHE	-	expression tag	UNP Q69ZE8
D	1351	GLN	-	expression tag	UNP Q69ZE8
D	1352	GLY	-	expression tag	UNP Q69ZE8
D	1353	PRO	-	expression tag	UNP Q69ZE8
D	1354	GLN	-	expression tag	UNP Q69ZE8
D	1355	GLY	-	expression tag	UNP Q69ZE8
D	1356	THR	-	expression tag	UNP Q69ZE8
D	1357	GLU	-	expression tag	UNP Q69ZE8
D	1358	GLN	-	expression tag	UNP Q69ZE8
D	1359	LYS	-	expression tag	UNP Q69ZE8
D	1360	LEU	-	expression tag	UNP Q69ZE8
D	1361	ILE	-	expression tag	UNP Q69ZE8
D	1362	SER	-	expression tag	UNP Q69ZE8
D	1363	GLU	-	expression tag	UNP Q69ZE8
D	1364	GLU	-	expression tag	UNP Q69ZE8
D	1365	ASP	-	expression tag	UNP Q69ZE8
D	1366	LEU	-	expression tag	UNP Q69ZE8
D	1367	ARG	-	expression tag	UNP Q69ZE8
D	1368	GLY	-	expression tag	UNP Q69ZE8
D	1369	ALA	-	expression tag	UNP Q69ZE8
D	1370	SER	-	expression tag	UNP Q69ZE8
D	1371	MET	-	expression tag	UNP Q69ZE8
D	1372	ASP	-	expression tag	UNP Q69ZE8
D	1373	GLU	-	expression tag	UNP Q69ZE8
D	1374	LYS	-	expression tag	UNP Q69ZE8
D	1375	THR	-	expression tag	UNP Q69ZE8
D	1376	THR	-	expression tag	UNP Q69ZE8

Continued on next page...

Continued from previous page...

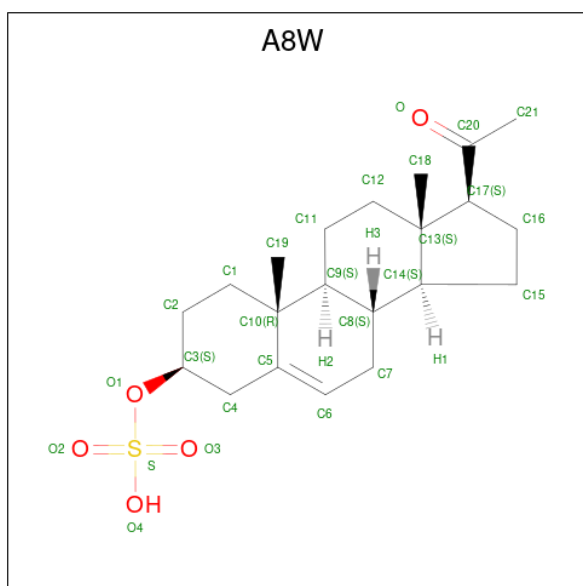
Chain	Residue	Modelled	Actual	Comment	Reference
D	1377	GLY	-	expression tag	UNP Q69ZE8
D	1378	TRP	-	expression tag	UNP Q69ZE8
D	1379	ARG	-	expression tag	UNP Q69ZE8
D	1380	GLY	-	expression tag	UNP Q69ZE8
D	1381	GLY	-	expression tag	UNP Q69ZE8
D	1382	HIS	-	expression tag	UNP Q69ZE8
D	1383	VAL	-	expression tag	UNP Q69ZE8
D	1384	VAL	-	expression tag	UNP Q69ZE8
D	1385	GLU	-	expression tag	UNP Q69ZE8
D	1386	GLY	-	expression tag	UNP Q69ZE8
D	1387	LEU	-	expression tag	UNP Q69ZE8
D	1388	ALA	-	expression tag	UNP Q69ZE8
D	1389	GLY	-	expression tag	UNP Q69ZE8
D	1390	GLU	-	expression tag	UNP Q69ZE8
D	1391	LEU	-	expression tag	UNP Q69ZE8
D	1392	GLU	-	expression tag	UNP Q69ZE8
D	1393	GLN	-	expression tag	UNP Q69ZE8
D	1394	LEU	-	expression tag	UNP Q69ZE8
D	1395	ARG	-	expression tag	UNP Q69ZE8
D	1396	ALA	-	expression tag	UNP Q69ZE8
D	1397	ARG	-	expression tag	UNP Q69ZE8
D	1398	LEU	-	expression tag	UNP Q69ZE8
D	1399	GLU	-	expression tag	UNP Q69ZE8
D	1400	HIS	-	expression tag	UNP Q69ZE8
D	1401	HIS	-	expression tag	UNP Q69ZE8
D	1402	PRO	-	expression tag	UNP Q69ZE8
D	1403	GLN	-	expression tag	UNP Q69ZE8
D	1404	GLY	-	expression tag	UNP Q69ZE8
D	1405	GLN	-	expression tag	UNP Q69ZE8
D	1406	ARG	-	expression tag	UNP Q69ZE8
D	1407	GLU	-	expression tag	UNP Q69ZE8
D	1408	PRO	-	expression tag	UNP Q69ZE8

- Molecule 2 is (2 {R})-2-(3,4-dihydro-2 {H}-quinolin-1-yl)- {N}-(5-methyl-1,2-oxazol-3-yl)-2-phenyl-ethanamide (CCD ID: A1I8P) (formula: C₂₁H₂₁N₃O₂) (labeled as "Ligand of Interest" by depositor).



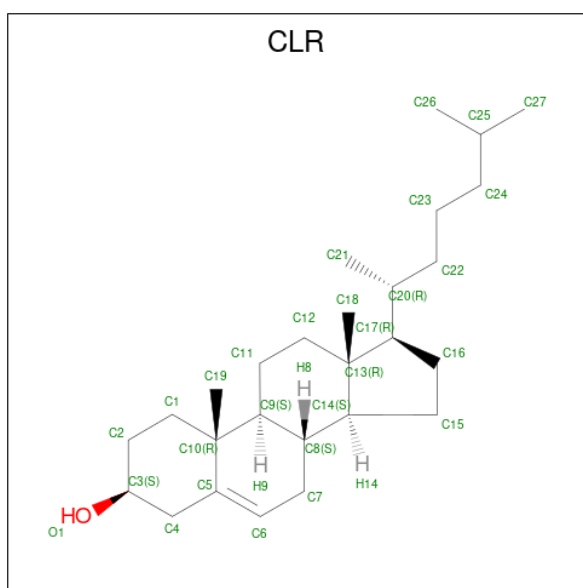
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	H	N	O	0
			47	21	21	3	2	
2	B	1	Total	C	H	N	O	0
			47	21	21	3	2	
2	C	1	Total	C	H	N	O	0
			47	21	21	3	2	
2	D	1	Total	C	H	N	O	0
			47	21	21	3	2	

- Molecule 3 is Pregnenolone sulfate (CCD ID: A8W) (formula: $C_{21}H_{32}O_5S$) (labeled as "Ligand of Interest" by depositor).

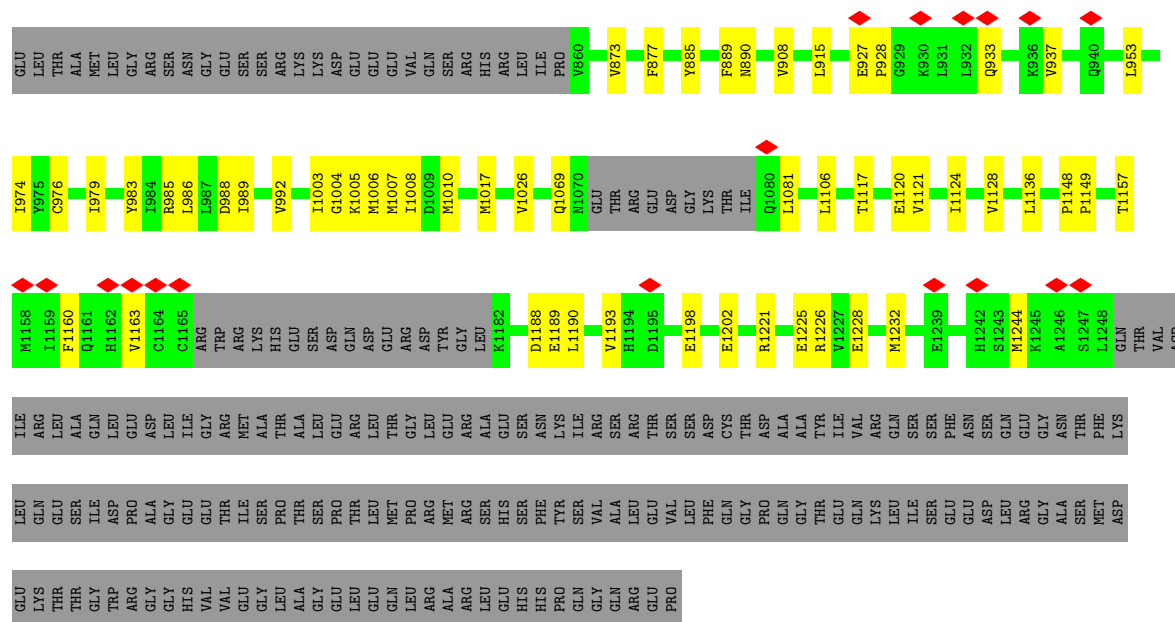


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	O	S	0
			58	21	31	5	1	
3	B	1	Total	C	H	O	S	0
			58	21	31	5	1	
3	C	1	Total	C	H	O	S	0
			58	21	31	5	1	
3	D	1	Total	C	H	O	S	0
			58	21	31	5	1	

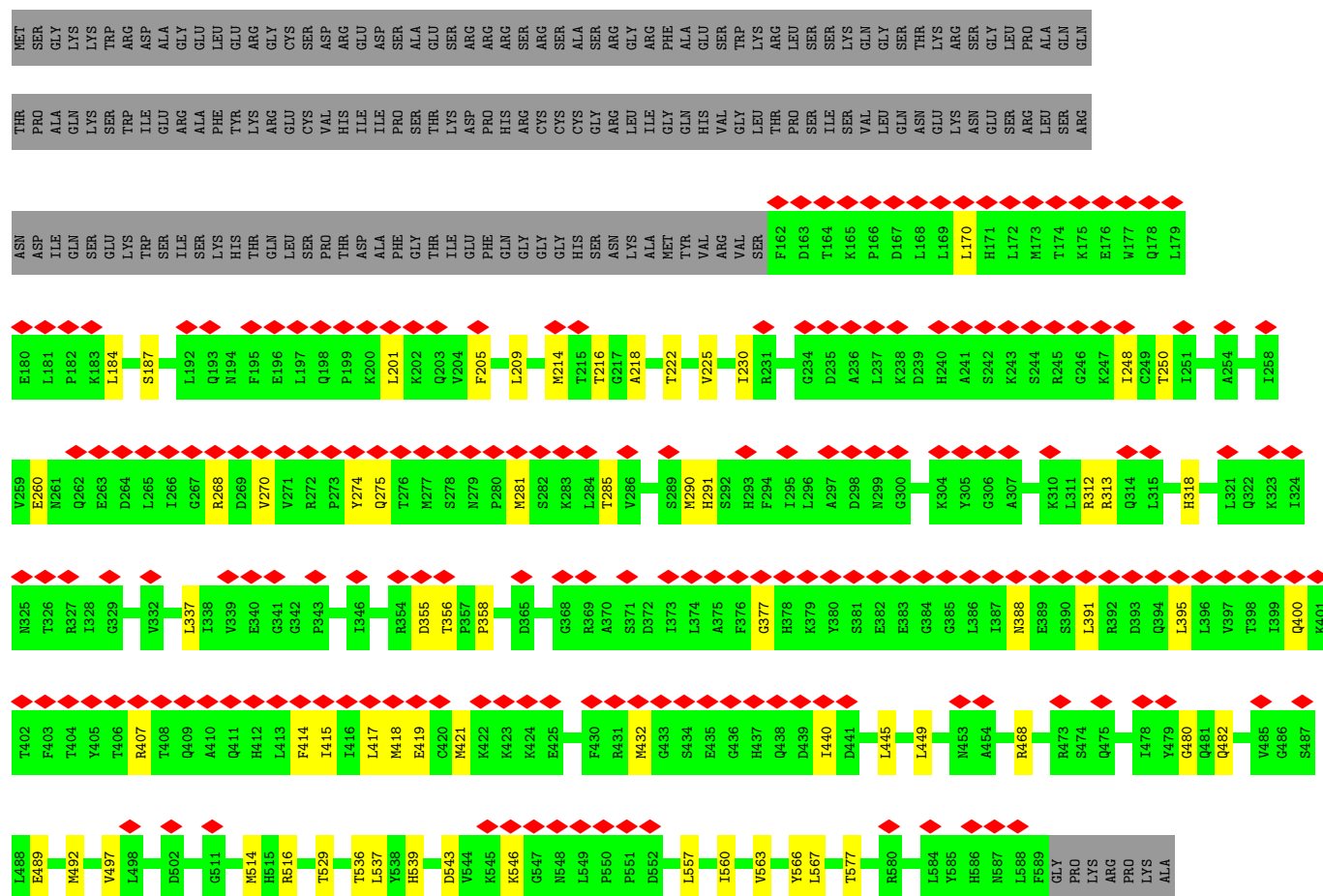
- Molecule 4 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).

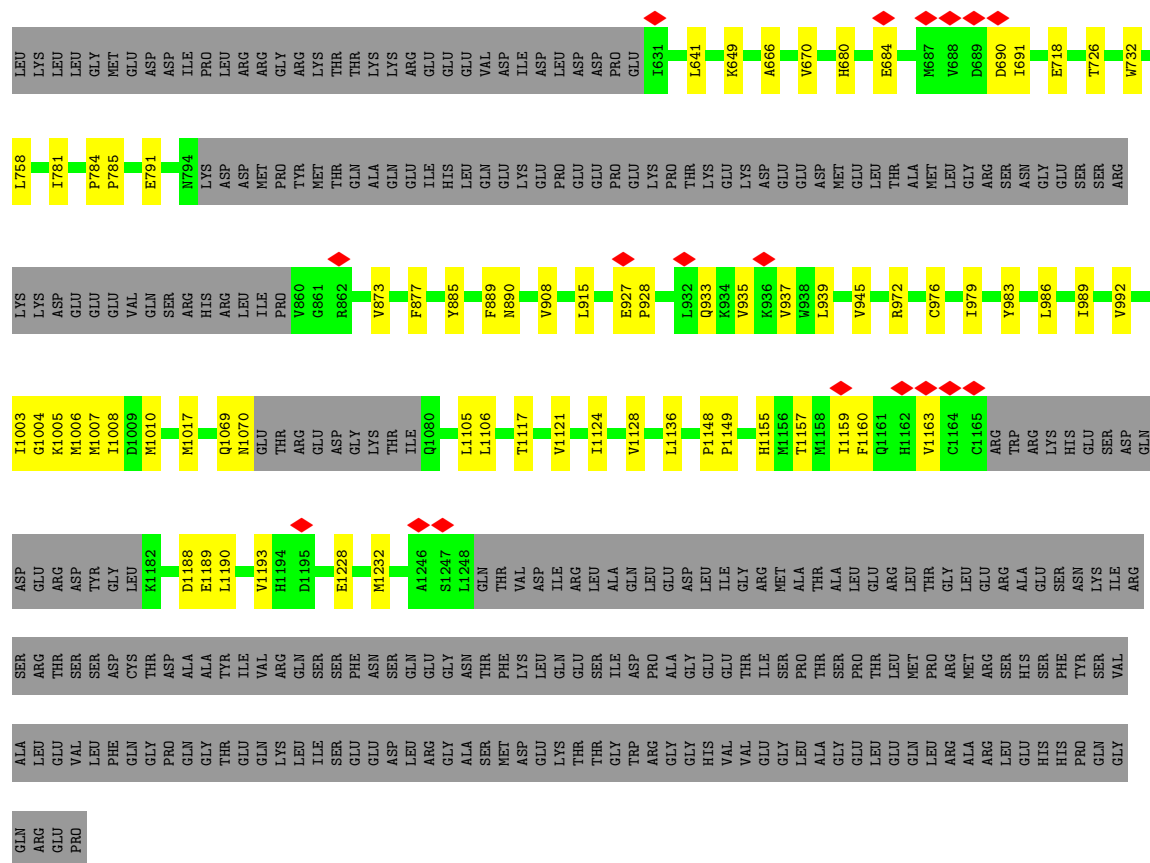


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	H	O		0
			74	27	46	1		
4	A	1	Total	C	H	O		0
			74	27	46	1		
4	C	1	Total	C	H	O		0
			74	27	46	1		
4	D	1	Total	C	H	O		0
			74	27	46	1		

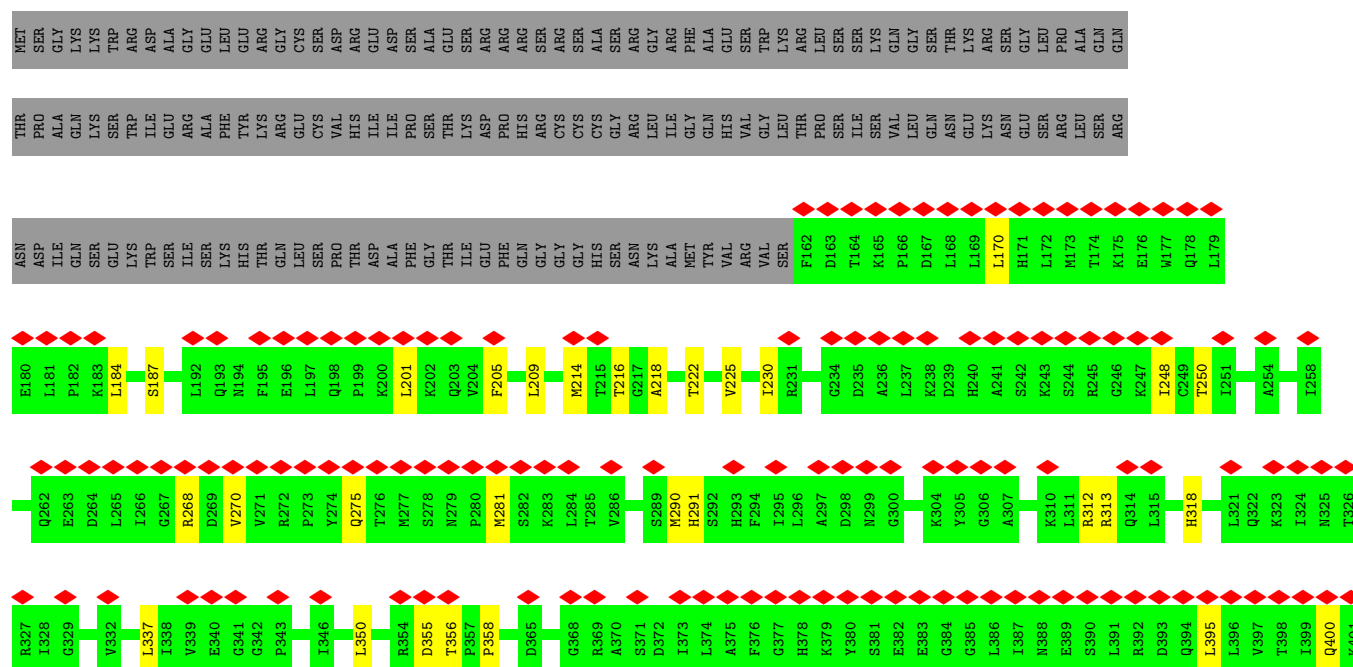


• Molecule 1: MKIAA1616 protein





• Molecule 1: MKIAA1616 protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58787	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	62	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.368	Depositor
Minimum map value	-0.166	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0551	Depositor
Map size ($\text{\AA}$)	358.8, 358.8, 358.8	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.69, 0.69, 0.69	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: CLR, A1I8P, A8W

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	0.15	0/7923	0.33	0/10714
1	B	0.15	0/7923	0.33	0/10714
1	C	0.15	0/7923	0.32	0/10714
1	D	0.15	0/7923	0.32	0/10714
All	All	0.15	0/31692	0.32	0/42856

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7746	7871	7881	98	0
1	B	7746	7871	7881	99	0
1	C	7746	7871	7881	98	0
1	D	7746	7871	7881	100	0
2	A	26	21	0	3	0
2	B	26	21	0	3	0
2	C	26	21	0	3	0
2	D	26	21	0	3	0
3	A	27	31	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	31	0	0	0
3	C	27	31	0	0	0
3	D	27	31	0	0	0
4	A	56	92	92	0	0
4	C	28	46	46	0	0
4	D	28	46	46	0	0
All	All	31308	31876	31708	378	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (378) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:985:ARG:NH1	1:A:988:ASP:OD2	2.07	0.88
1:D:976:CYS:O	1:D:979:ILE:HG22	1.79	0.83
1:C:976:CYS:O	1:C:979:ILE:HG22	1.78	0.83
1:A:976:CYS:O	1:A:979:ILE:HG22	1.78	0.81
1:B:976:CYS:O	1:B:979:ILE:HG22	1.79	0.81
1:D:890:ASN:OD1	1:D:979:ILE:HD11	1.87	0.74
1:C:568:MET:HE2	1:C:674:LEU:HD21	1.70	0.73
1:B:890:ASN:OD1	1:B:979:ILE:HD11	1.87	0.73
1:A:890:ASN:OD1	1:A:979:ILE:HD11	1.90	0.72
1:A:726:THR:CG2	1:A:758:LEU:HD11	2.21	0.71
1:D:718:GLU:N	1:D:718:GLU:OE2	2.25	0.68
1:C:1235:GLU:OE2	1:D:1233:ARG:NH1	2.26	0.68
1:A:1188:ASP:OD1	1:A:1189:GLU:N	2.28	0.67
1:B:889:PHE:HD1	1:B:908:VAL:HG11	1.61	0.65
1:C:781:ILE:HD12	1:C:877:PHE:CD1	2.31	0.65
1:A:1003:ILE:O	1:A:1007:MET:HG2	1.97	0.64
1:A:173:MET:HE1	1:A:251:ILE:HD12	1.80	0.63
1:A:726:THR:HG23	1:A:758:LEU:HD11	1.81	0.63
1:B:1003:ILE:O	1:B:1007:MET:HG2	1.99	0.63
1:D:885:TYR:HE1	1:D:908:VAL:HG13	1.63	0.63
1:B:718:GLU:OE2	1:B:718:GLU:N	2.30	0.63
1:C:568:MET:HE1	1:C:670:VAL:HG13	1.81	0.62
1:C:1157:THR:HA	1:C:1160:PHE:CE1	2.34	0.62
1:D:1003:ILE:O	1:D:1007:MET:HG2	1.99	0.62
1:A:222:THR:HG22	1:A:230:ILE:HD12	1.81	0.62
1:A:365:ASP:OD2	1:A:366:GLY:N	2.32	0.62
1:B:885:TYR:HE1	1:B:908:VAL:HG13	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1157:THR:HA	1:B:1160:PHE:CE1	2.34	0.62
1:C:214:MET:HA	1:C:214:MET:HE2	1.81	0.62
1:D:889:PHE:HD1	1:D:908:VAL:HG11	1.63	0.62
1:D:222:THR:HG22	1:D:230:ILE:HD12	1.82	0.61
1:B:680:HIS:NE2	1:B:684:GLU:OE2	2.33	0.61
1:A:1006:MET:N	1:A:1006:MET:HE2	2.15	0.61
1:B:214:MET:HE2	1:B:214:MET:HA	1.83	0.61
1:B:781:ILE:HD12	1:B:877:PHE:CD1	2.34	0.61
1:D:579:LYS:HE3	1:D:579:LYS:HA	1.81	0.61
1:B:222:THR:HG22	1:B:230:ILE:HD12	1.83	0.61
1:C:222:THR:HG22	1:C:230:ILE:HD12	1.83	0.61
1:C:579:LYS:HE3	1:C:579:LYS:HA	1.81	0.61
1:D:680:HIS:NE2	1:D:684:GLU:OE2	2.34	0.61
1:A:1157:THR:HA	1:A:1160:PHE:CE1	2.36	0.61
1:D:690:ASP:OD1	1:D:691:ILE:N	2.34	0.61
1:A:680:HIS:NE2	1:A:684:GLU:OE2	2.33	0.60
1:A:268:ARG:O	1:A:270:VAL:HG13	2.02	0.60
1:C:666:ALA:O	1:C:670:VAL:HG23	2.02	0.60
1:D:268:ARG:O	1:D:270:VAL:HG13	2.02	0.59
1:B:268:ARG:O	1:B:270:VAL:HG13	2.03	0.59
1:C:680:HIS:NE2	1:C:684:GLU:OE2	2.35	0.59
1:C:268:ARG:O	1:C:270:VAL:HG13	2.02	0.59
1:A:690:ASP:OD1	1:A:691:ILE:N	2.36	0.59
1:A:345:VAL:O	1:A:349:VAL:HG23	2.03	0.58
1:B:690:ASP:OD1	1:B:691:ILE:N	2.36	0.58
1:D:781:ILE:HD12	1:D:877:PHE:CD1	2.39	0.58
1:D:1005:LYS:HD3	1:D:1121:VAL:HG13	1.86	0.58
1:C:690:ASP:OD1	1:C:691:ILE:N	2.37	0.57
1:B:1005:LYS:HD3	1:B:1121:VAL:HG13	1.87	0.57
1:A:1005:LYS:HD3	1:A:1121:VAL:HG13	1.87	0.57
1:C:890:ASN:OD1	1:C:979:ILE:HD11	2.04	0.57
1:B:889:PHE:CD1	1:B:908:VAL:HG11	2.39	0.56
1:D:281:MET:SD	1:D:281:MET:N	2.78	0.56
1:B:281:MET:SD	1:B:281:MET:N	2.78	0.56
1:C:281:MET:SD	1:C:281:MET:N	2.78	0.56
1:A:560:ILE:HD11	1:A:647:LEU:HD13	1.87	0.55
1:C:1117:THR:O	1:C:1121:VAL:HG23	2.06	0.55
1:D:214:MET:HE2	1:D:214:MET:HA	1.88	0.55
1:D:889:PHE:CD1	1:D:908:VAL:HG11	2.40	0.55
1:A:281:MET:SD	1:A:281:MET:N	2.78	0.55
1:D:1006:MET:N	1:D:1006:MET:HE2	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1160:PHE:HA	1:A:1163:VAL:HG12	1.88	0.55
1:A:445:LEU:O	1:A:449:LEU:HD23	2.07	0.55
1:C:890:ASN:ND2	1:C:983:TYR:OH	2.37	0.55
1:B:1006:MET:N	1:B:1006:MET:HE2	2.22	0.55
1:C:214:MET:HE3	1:C:248:ILE:HG12	1.89	0.54
1:D:1159:ILE:O	1:D:1162:HIS:ND1	2.41	0.54
1:A:516:ARG:NH1	1:B:275:GLN:OE1	2.41	0.53
1:A:1120:GLU:O	1:A:1124:ILE:HD12	2.08	0.53
1:B:1004:GLY:O	1:B:1008:ILE:HD12	2.08	0.53
1:B:986:LEU:HD23	1:B:989:ILE:HD12	1.89	0.53
1:B:1160:PHE:HA	1:B:1163:VAL:HG12	1.91	0.53
1:C:1160:PHE:HA	1:C:1163:VAL:HG12	1.89	0.53
1:B:214:MET:HE3	1:B:248:ILE:HG12	1.92	0.52
1:C:986:LEU:HD23	1:C:989:ILE:HD12	1.90	0.52
1:A:889:PHE:CD1	1:A:908:VAL:HG11	2.45	0.52
1:A:781:ILE:HD12	1:A:877:PHE:CD1	2.44	0.52
1:A:1004:GLY:O	1:A:1008:ILE:HD12	2.09	0.52
1:C:1120:GLU:O	1:C:1124:ILE:HD12	2.10	0.52
1:D:497:VAL:HG13	1:D:529:THR:HG21	1.92	0.52
1:B:890:ASN:ND2	1:B:983:TYR:OH	2.36	0.52
1:A:214:MET:HA	1:A:214:MET:HE2	1.92	0.52
1:D:885:TYR:CE1	1:D:908:VAL:HG13	2.45	0.52
1:A:497:VAL:HG13	1:A:529:THR:HG21	1.92	0.52
1:C:497:VAL:HG13	1:C:529:THR:HG21	1.92	0.51
1:A:563:VAL:O	1:A:567:LEU:HD23	2.10	0.51
1:B:497:VAL:HG13	1:B:529:THR:HG21	1.92	0.51
1:A:187:SER:OG	1:A:312:ARG:NH2	2.41	0.51
1:A:889:PHE:HD1	1:A:908:VAL:HG11	1.74	0.51
1:B:1005:LYS:CD	1:B:1121:VAL:HG13	2.41	0.51
1:D:986:LEU:HD23	1:D:989:ILE:HD12	1.91	0.51
1:A:275:GLN:OE1	1:C:516:ARG:NH1	2.44	0.51
1:A:415:ILE:O	1:A:419:GLU:OE1	2.29	0.51
1:D:1005:LYS:CD	1:D:1121:VAL:HG13	2.41	0.51
1:B:415:ILE:O	1:B:419:GLU:OE1	2.29	0.51
1:A:1005:LYS:CD	1:A:1121:VAL:HG13	2.40	0.51
1:A:1017:MET:SD	1:A:1106:LEU:HD12	2.51	0.51
1:B:395:LEU:HD21	1:B:417:LEU:HD23	1.93	0.51
1:B:418:MET:HA	1:B:418:MET:HE2	1.92	0.50
1:B:356:THR:O	1:B:358:PRO:HD3	2.12	0.50
1:B:377:GLY:C	1:B:421:MET:HE3	2.37	0.50
1:B:885:TYR:CE1	1:B:908:VAL:HG13	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:ILE:O	1:D:419:GLU:OE1	2.29	0.50
1:A:536:THR:HG22	1:A:536:THR:O	2.12	0.50
1:B:514:MET:HE2	1:B:641:LEU:HD11	1.94	0.50
1:C:563:VAL:O	1:C:567:LEU:HD23	2.11	0.50
1:D:536:THR:HG22	1:D:536:THR:O	2.12	0.50
1:A:480:GLY:O	1:A:482:GLN:NE2	2.45	0.50
1:C:415:ILE:O	1:C:419:GLU:OE1	2.29	0.50
1:C:773:SER:O	1:C:777:VAL:HG23	2.11	0.50
1:D:356:THR:O	1:D:358:PRO:HD3	2.12	0.50
1:D:690:ASP:OD1	1:D:691:ILE:HG23	2.12	0.49
1:B:781:ILE:HD11	1:B:873:VAL:HG13	1.93	0.49
1:D:989:ILE:HG13	2:D:1503:A1I8P:C21	2.43	0.49
1:D:1188:ASP:OD2	1:D:1189:GLU:N	2.45	0.49
1:C:356:THR:O	1:C:358:PRO:HD3	2.12	0.49
1:B:536:THR:HG22	1:B:536:THR:O	2.11	0.49
1:C:992:VAL:HG22	1:C:1136:LEU:HD21	1.93	0.49
1:B:516:ARG:NH1	1:D:275:GLN:OE1	2.45	0.49
1:B:1188:ASP:OD2	1:B:1189:GLU:N	2.45	0.49
1:A:356:THR:O	1:A:358:PRO:HD3	2.12	0.49
1:B:1148:PRO:N	1:B:1149:PRO:HD2	2.28	0.49
1:B:563:VAL:O	1:B:567:LEU:HD23	2.13	0.49
1:B:989:ILE:HG13	2:B:1502:A1I8P:C21	2.43	0.49
1:C:781:ILE:HD12	1:C:877:PHE:HD1	1.74	0.49
1:A:514:MET:HE2	1:A:641:LEU:HD11	1.94	0.48
1:A:885:TYR:HE1	1:A:908:VAL:HG13	1.78	0.48
1:C:1232:MET:N	1:C:1232:MET:HE2	2.28	0.48
1:D:563:VAL:O	1:D:567:LEU:HD23	2.13	0.48
1:D:184:LEU:CD2	1:D:216:THR:HG21	2.43	0.48
1:D:1148:PRO:N	1:D:1149:PRO:HD2	2.29	0.48
1:A:1232:MET:N	1:A:1232:MET:HE2	2.28	0.48
1:D:992:VAL:HG22	1:D:1136:LEU:HD21	1.94	0.48
1:D:1159:ILE:HA	1:D:1162:HIS:HD1	1.79	0.48
1:C:1188:ASP:OD1	1:C:1189:GLU:N	2.45	0.48
1:B:972:ARG:NH1	1:D:1030:ALA:O	2.47	0.48
1:C:1148:PRO:N	1:C:1149:PRO:HD2	2.28	0.48
1:A:543:ASP:O	1:A:546:LYS:HE3	2.14	0.48
1:B:537:LEU:HD11	1:B:560:ILE:CD1	2.44	0.48
1:B:992:VAL:HG22	1:B:1136:LEU:HD21	1.94	0.48
1:C:537:LEU:HD11	1:C:560:ILE:CD1	2.44	0.48
1:B:1017:MET:CE	1:B:1106:LEU:HD12	2.43	0.47
1:C:989:ILE:HG13	2:C:1502:A1I8P:C21	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1017:MET:CE	1:D:1106:LEU:HD12	2.44	0.47
1:A:400:GLN:OE1	1:A:407:ARG:NH1	2.48	0.47
1:B:543:ASP:O	1:B:546:LYS:HE3	2.14	0.47
1:D:395:LEU:HD21	1:D:417:LEU:HD23	1.96	0.47
1:D:537:LEU:HD11	1:D:560:ILE:CD1	2.44	0.47
1:A:992:VAL:HG22	1:A:1136:LEU:HD21	1.96	0.47
1:D:890:ASN:ND2	1:D:983:TYR:OH	2.37	0.47
1:A:666:ALA:O	1:A:670:VAL:HG23	2.14	0.47
1:B:1232:MET:HE2	1:B:1232:MET:N	2.28	0.47
1:D:1232:MET:N	1:D:1232:MET:HE2	2.28	0.47
1:A:1148:PRO:N	1:A:1149:PRO:HD2	2.30	0.47
1:B:170:LEU:HD22	1:B:318:HIS:CD2	2.50	0.47
1:C:418:MET:HE2	1:C:418:MET:HA	1.97	0.47
1:D:418:MET:HE2	1:D:418:MET:HA	1.97	0.47
1:D:543:ASP:O	1:D:546:LYS:HE3	2.14	0.47
1:C:275:GLN:OE1	1:D:516:ARG:NH1	2.48	0.47
1:C:395:LEU:HD21	1:C:417:LEU:HD23	1.96	0.47
1:C:568:MET:HE1	1:C:670:VAL:CG1	2.45	0.47
1:C:649:LYS:HG3	1:C:649:LYS:O	2.16	0.47
1:D:965:GLN:OE1	1:D:969:SER:OG	2.33	0.46
1:B:649:LYS:O	1:B:649:LYS:HG3	2.15	0.46
1:C:543:ASP:O	1:C:546:LYS:HE3	2.15	0.46
1:C:726:THR:HG22	1:C:758:LEU:HD21	1.98	0.46
1:C:1002:MET:HG3	1:C:1121:VAL:HG12	1.96	0.46
1:D:170:LEU:HD22	1:D:318:HIS:CD2	2.51	0.46
1:C:480:GLY:O	1:C:482:GLN:NE2	2.49	0.46
1:A:250:THR:HG22	1:A:291:HIS:CD2	2.51	0.46
1:A:781:ILE:HD11	1:A:873:VAL:HG13	1.98	0.46
1:B:480:GLY:O	1:B:482:GLN:NE2	2.49	0.46
1:D:726:THR:HG22	1:D:758:LEU:HD21	1.98	0.46
1:D:468:ARG:HA	1:D:468:ARG:NE	2.31	0.46
1:D:726:THR:CG2	1:D:758:LEU:HD21	2.46	0.46
1:B:726:THR:HG22	1:B:758:LEU:HD21	1.98	0.46
1:D:187:SER:OG	1:D:312:ARG:NH2	2.42	0.46
1:A:989:ILE:HG13	2:A:1501:A1I8P:C21	2.46	0.46
1:C:170:LEU:HD22	1:C:318:HIS:CD2	2.51	0.46
1:C:935:VAL:HG13	1:C:939:LEU:HD23	1.98	0.46
1:D:935:VAL:HG13	1:D:939:LEU:HD23	1.98	0.46
1:A:1010:MET:HG3	1:B:1105:LEU:HD13	1.99	0.45
1:B:1017:MET:HE1	1:B:1106:LEU:HD12	1.98	0.45
1:D:649:LYS:O	1:D:649:LYS:HG3	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:666:ALA:O	1:D:670:VAL:HG23	2.15	0.45
1:B:468:ARG:NE	1:B:468:ARG:HA	2.31	0.45
1:B:666:ALA:O	1:B:670:VAL:HG23	2.16	0.45
1:C:1030:ALA:O	1:D:972:ARG:NH1	2.49	0.45
1:B:184:LEU:CD2	1:B:216:THR:HG21	2.45	0.45
1:A:170:LEU:HD22	1:A:318:HIS:CD2	2.51	0.45
1:B:184:LEU:HB3	1:B:218:ALA:HB2	1.98	0.45
1:C:468:ARG:HA	1:C:468:ARG:NE	2.31	0.45
1:D:480:GLY:O	1:D:482:GLN:NE2	2.48	0.45
1:D:670:VAL:HG21	1:D:732:TRP:CE3	2.52	0.45
1:A:395:LEU:HD21	1:A:417:LEU:HD23	1.99	0.45
1:D:337:LEU:HD11	1:D:440:ILE:HD11	1.99	0.45
1:C:915:LEU:HD13	2:C:1502:A1I8P:C03	2.47	0.45
1:D:184:LEU:HB3	1:D:218:ALA:HB2	1.97	0.45
1:C:184:LEU:CD2	1:C:216:THR:HG21	2.46	0.45
1:C:791:GLU:OE1	1:C:791:GLU:N	2.50	0.45
1:D:791:GLU:N	1:D:791:GLU:OE1	2.50	0.45
1:D:1017:MET:HE1	1:D:1106:LEU:HD12	1.98	0.45
1:A:791:GLU:N	1:A:791:GLU:OE1	2.49	0.45
1:A:768:ARG:O	1:A:770:ARG:NH1	2.50	0.45
1:B:935:VAL:HG13	1:B:939:LEU:HD23	1.99	0.45
1:C:726:THR:CG2	1:C:758:LEU:HD21	2.47	0.45
1:C:939:LEU:HD13	1:C:945:VAL:HG22	1.99	0.45
1:D:939:LEU:HD13	1:D:945:VAL:HG22	1.99	0.45
1:A:577:THR:O	1:A:577:THR:HG22	2.17	0.44
1:A:1124:ILE:O	1:A:1128:VAL:HG23	2.16	0.44
1:B:337:LEU:HD11	1:B:440:ILE:HD11	1.99	0.44
1:B:1124:ILE:O	1:B:1128:VAL:HG23	2.18	0.44
1:B:400:GLN:OE1	1:B:407:ARG:NH1	2.50	0.44
1:D:222:THR:CG2	1:D:230:ILE:HD12	2.47	0.44
1:D:400:GLN:OE1	1:D:407:ARG:NH1	2.50	0.44
1:A:468:ARG:HA	1:A:468:ARG:NE	2.31	0.44
1:A:1190:LEU:O	1:A:1193:VAL:HG12	2.17	0.44
1:B:577:THR:HG22	1:B:577:THR:O	2.18	0.44
1:C:337:LEU:HD11	1:C:440:ILE:HD11	1.99	0.44
1:B:939:LEU:HD13	1:B:945:VAL:HG22	1.99	0.44
1:C:400:GLN:OE1	1:C:407:ARG:NH1	2.50	0.44
1:C:867:PHE:O	1:C:873:VAL:HG21	2.18	0.44
1:A:184:LEU:CD2	1:A:216:THR:HG21	2.48	0.44
1:A:184:LEU:HB3	1:A:218:ALA:HB2	1.98	0.44
1:C:1100:LEU:CD1	1:D:1010:MET:HE1	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:LEU:HD13	2:A:1501:A1I8P:C03	2.48	0.44
1:B:726:THR:CG2	1:B:758:LEU:HD21	2.47	0.44
1:C:577:THR:HG22	1:C:577:THR:O	2.18	0.44
1:D:209:LEU:HD23	1:D:209:LEU:C	2.43	0.44
1:A:259:VAL:HG12	1:A:287:LEU:HD21	1.98	0.44
1:C:445:LEU:O	1:C:449:LEU:HD23	2.17	0.44
1:A:259:VAL:HG23	1:A:262:GLN:HB3	2.00	0.44
1:B:250:THR:HG22	1:B:291:HIS:CD2	2.53	0.44
1:A:313:ARG:NH2	1:A:355:ASP:OD2	2.50	0.43
1:B:791:GLU:N	1:B:791:GLU:OE1	2.50	0.43
1:C:933:GLN:O	1:C:937:VAL:HG12	2.18	0.43
1:A:537:LEU:HD11	1:A:560:ILE:CD1	2.48	0.43
1:B:201:LEU:HD13	1:B:432:MET:CE	2.48	0.43
1:B:445:LEU:O	1:B:449:LEU:HD23	2.18	0.43
1:C:222:THR:CG2	1:C:230:ILE:HD12	2.48	0.43
1:D:1124:ILE:O	1:D:1128:VAL:HG23	2.18	0.43
1:D:201:LEU:HD13	1:D:432:MET:CE	2.48	0.43
1:D:445:LEU:O	1:D:449:LEU:HD23	2.18	0.43
1:D:577:THR:O	1:D:577:THR:HG22	2.17	0.43
1:B:670:VAL:HG21	1:B:732:TRP:CE3	2.54	0.43
1:D:250:THR:HG22	1:D:291:HIS:CD2	2.53	0.43
1:D:313:ARG:NH2	1:D:355:ASP:OD2	2.49	0.43
1:D:933:GLN:O	1:D:937:VAL:HG12	2.18	0.43
1:A:185:LEU:HD11	1:A:319:ILE:CG2	2.49	0.43
1:B:209:LEU:HD23	1:B:209:LEU:C	2.43	0.43
1:A:1117:THR:O	1:A:1121:VAL:HG23	2.19	0.43
1:B:1155:HIS:O	1:B:1159:ILE:HG12	2.18	0.43
1:C:184:LEU:HB3	1:C:218:ALA:HB2	1.99	0.43
1:C:209:LEU:C	1:C:209:LEU:HD23	2.43	0.43
1:A:566:TYR:HD1	1:A:567:LEU:HD22	1.83	0.43
1:A:1244:MET:SD	1:A:1244:MET:C	3.01	0.43
1:B:260:GLU:O	1:B:274:TYR:OH	2.24	0.43
1:B:784:PRO:N	1:B:785:PRO:HD2	2.33	0.43
1:B:1010:MET:HE1	1:D:1100:LEU:CD1	2.49	0.43
1:B:989:ILE:HG13	2:B:1502:A1I8P:C20	2.49	0.43
1:D:784:PRO:N	1:D:785:PRO:HD2	2.33	0.43
1:D:989:ILE:HG13	2:D:1503:A1I8P:C20	2.49	0.43
1:D:1190:LEU:O	1:D:1193:VAL:HG12	2.19	0.43
1:A:784:PRO:N	1:A:785:PRO:HD2	2.34	0.43
1:B:781:ILE:HD12	1:B:877:PHE:HD1	1.81	0.43
1:B:933:GLN:O	1:B:937:VAL:HG12	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:989:ILE:HG13	2:C:1502:A1I8P:C20	2.49	0.43
1:B:313:ARG:NH2	1:B:355:ASP:OD2	2.50	0.43
1:C:250:THR:HG22	1:C:291:HIS:CD2	2.54	0.43
1:C:313:ARG:NH2	1:C:355:ASP:OD2	2.49	0.43
1:C:784:PRO:N	1:C:785:PRO:HD2	2.34	0.43
1:C:1100:LEU:HD11	1:D:1010:MET:HE1	2.01	0.43
1:C:1124:ILE:O	1:C:1128:VAL:HG23	2.19	0.43
1:C:1190:LEU:O	1:C:1193:VAL:HG12	2.19	0.43
1:B:418:MET:HE2	1:B:418:MET:CA	2.49	0.42
1:B:489:GLU:O	1:B:492:MET:HG2	2.18	0.42
1:B:915:LEU:HD13	2:B:1502:A1I8P:C03	2.49	0.42
1:C:201:LEU:HD13	1:C:432:MET:CE	2.49	0.42
1:A:489:GLU:O	1:A:492:MET:HG2	2.18	0.42
1:B:557:LEU:O	1:B:560:ILE:HG22	2.20	0.42
1:B:986:LEU:CD2	1:B:989:ILE:HD12	2.49	0.42
1:C:927:GLU:N	1:C:928:PRO:CD	2.83	0.42
1:C:986:LEU:CD2	1:C:989:ILE:HD12	2.49	0.42
1:D:1117:THR:O	1:D:1121:VAL:HG23	2.20	0.42
1:A:1226:ARG:CZ	1:B:1228:GLU:OE2	2.67	0.42
1:B:222:THR:CG2	1:B:230:ILE:HD12	2.47	0.42
1:B:260:GLU:N	1:B:285:THR:O	2.51	0.42
1:C:895:VAL:O	1:C:896:LYS:HB3	2.20	0.42
1:D:290:MET:N	1:D:290:MET:SD	2.93	0.42
1:D:557:LEU:O	1:D:560:ILE:HG22	2.20	0.42
1:A:377:GLY:C	1:A:421:MET:HE3	2.44	0.42
1:C:557:LEU:O	1:C:560:ILE:HG22	2.20	0.42
1:A:350:LEU:HB2	1:A:420:CYS:SG	2.59	0.42
1:D:986:LEU:CD2	1:D:989:ILE:HD12	2.50	0.42
1:B:290:MET:N	1:B:290:MET:SD	2.93	0.42
1:C:568:MET:HG3	1:C:572:TYR:CD2	2.55	0.42
1:C:187:SER:OG	1:C:312:ARG:NH2	2.42	0.42
1:A:557:LEU:O	1:A:560:ILE:HG22	2.20	0.42
1:A:1148:PRO:HG2	1:A:1149:PRO:HD3	2.01	0.42
1:B:1190:LEU:O	1:B:1193:VAL:HG12	2.19	0.42
1:C:784:PRO:O	1:C:787:ILE:HD12	2.19	0.42
1:A:290:MET:N	1:A:290:MET:SD	2.93	0.42
1:A:985:ARG:O	1:A:985:ARG:HG3	2.19	0.42
1:B:927:GLU:N	1:B:928:PRO:CD	2.83	0.42
1:C:225:VAL:O	1:C:230:ILE:HG21	2.20	0.42
1:C:517:PHE:O	1:C:522:ARG:NH1	2.50	0.42
1:C:680:HIS:O	1:C:684:GLU:OE1	2.38	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1117:THR:O	1:B:1121:VAL:HG23	2.20	0.41
1:C:566:TYR:HD1	1:C:567:LEU:HD22	1.85	0.41
1:D:205:PHE:CZ	1:D:337:LEU:HD21	2.55	0.41
1:D:260:GLU:N	1:D:285:THR:O	2.51	0.41
1:D:915:LEU:HD13	2:D:1503:A1I8P:C03	2.50	0.41
1:A:670:VAL:HG21	1:A:732:TRP:CE3	2.56	0.41
1:A:986:LEU:HD23	1:A:989:ILE:HD12	2.01	0.41
1:B:395:LEU:HD23	1:B:414:PHE:CD1	2.55	0.41
1:B:1010:MET:HE1	1:D:1100:LEU:HD11	2.01	0.41
1:D:680:HIS:O	1:D:684:GLU:OE1	2.38	0.41
1:D:927:GLU:N	1:D:928:PRO:CD	2.83	0.41
1:A:933:GLN:O	1:A:937:VAL:HG12	2.19	0.41
1:A:1069:GLN:O	1:A:1081:LEU:HD12	2.20	0.41
1:A:388:ASN:OD1	1:A:391:LEU:HD13	2.21	0.41
1:A:649:LYS:O	1:A:649:LYS:HG3	2.19	0.41
1:A:707:VAL:HG23	1:A:746:HIS:NE2	2.35	0.41
1:A:1221:ARG:NH1	1:A:1225:GLU:OE1	2.53	0.41
1:A:1228:GLU:OE2	1:C:1226:ARG:CZ	2.68	0.41
1:C:290:MET:N	1:C:290:MET:SD	2.93	0.41
1:D:1148:PRO:HG2	1:D:1149:PRO:HD3	2.03	0.41
1:A:680:HIS:O	1:A:684:GLU:OE1	2.39	0.41
1:A:927:GLU:N	1:A:928:PRO:CD	2.84	0.41
1:C:690:ASP:OD1	1:C:691:ILE:HG23	2.21	0.41
1:C:707:VAL:HG23	1:C:746:HIS:NE2	2.36	0.41
1:C:889:PHE:HD2	1:C:979:ILE:HG13	1.86	0.41
1:B:225:VAL:O	1:B:230:ILE:HG21	2.20	0.41
1:D:536:THR:HG22	1:D:539:HIS:HB3	2.02	0.41
1:B:536:THR:HG22	1:B:539:HIS:HB3	2.02	0.41
1:C:424:LYS:HA	1:C:427:ILE:HD12	2.02	0.41
1:A:514:MET:CE	1:A:641:LEU:HD11	2.51	0.41
1:A:890:ASN:ND2	1:A:983:TYR:OH	2.40	0.41
1:B:388:ASN:OD1	1:B:391:LEU:HD13	2.21	0.41
1:B:566:TYR:HD1	1:B:567:LEU:HD22	1.85	0.41
1:C:678:MET:HE2	1:C:695:LEU:HD22	2.03	0.41
1:C:940:GLN:OE1	1:C:940:GLN:C	2.64	0.41
1:D:388:ASN:OD1	1:D:391:LEU:HD13	2.21	0.41
1:A:248:ILE:HD12	1:A:248:ILE:N	2.36	0.41
1:A:953:LEU:HG	1:A:974:ILE:HG23	2.02	0.41
1:A:989:ILE:HG13	2:A:1501:A1I8P:C20	2.51	0.41
1:A:1198:GLU:O	1:A:1202:GLU:HG3	2.21	0.41
1:B:205:PHE:CZ	1:B:337:LEU:HD21	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:680:HIS:O	1:B:684:GLU:OE1	2.39	0.41
1:C:781:ILE:HD11	1:C:873:VAL:HG13	2.03	0.41
1:C:1046:ILE:HD11	1:D:894:LEU:HD11	2.03	0.41
1:D:225:VAL:O	1:D:230:ILE:HG21	2.21	0.41
1:D:1069:GLN:HG3	1:D:1070:ASN:N	2.36	0.41
1:C:205:PHE:CZ	1:C:337:LEU:HD21	2.56	0.40
1:C:1069:GLN:HG3	1:C:1070:ASN:N	2.36	0.40
1:A:424:LYS:HA	1:A:427:ILE:HD12	2.03	0.40
1:B:514:MET:CE	1:B:641:LEU:HD11	2.51	0.40
1:D:424:LYS:HA	1:D:427:ILE:HD12	2.02	0.40
1:D:214:MET:HE3	1:D:248:ILE:HG13	2.03	0.40
1:D:566:TYR:HD1	1:D:567:LEU:HD22	1.85	0.40
1:A:1026:VAL:HG11	1:C:979:ILE:HD13	2.02	0.40
1:B:187:SER:OG	1:B:312:ARG:NH2	2.43	0.40
1:C:350:LEU:HB2	1:C:420:CYS:SG	2.62	0.40
1:C:1012:TYR:CD2	1:D:995:TYR:CE1	3.09	0.40
1:D:1198:GLU:O	1:D:1202:GLU:HG3	2.22	0.40
1:A:470:ASP:OD1	1:A:470:ASP:N	2.53	0.40
1:B:1069:GLN:HG3	1:B:1070:ASN:N	2.37	0.40
1:C:470:ASP:OD1	1:C:470:ASP:N	2.55	0.40
1:C:915:LEU:HD23	1:C:915:LEU:C	2.47	0.40
1:D:240:HIS:CE1	1:D:248:ILE:HD11	2.57	0.40
1:D:470:ASP:OD1	1:D:470:ASP:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	946/1409 (67%)	924 (98%)	22 (2%)	0	100	100
1	B	946/1409 (67%)	925 (98%)	21 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	946/1409 (67%)	925 (98%)	21 (2%)	0	100	100
1	D	946/1409 (67%)	927 (98%)	19 (2%)	0	100	100
All	All	3784/5636 (67%)	3701 (98%)	83 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	850/1247 (68%)	850 (100%)	0	100	100
1	B	850/1247 (68%)	850 (100%)	0	100	100
1	C	850/1247 (68%)	850 (100%)	0	100	100
1	D	850/1247 (68%)	850 (100%)	0	100	100
All	All	3400/4988 (68%)	3400 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	GLN
1	A	412	HIS
1	A	459	GLN
1	A	467	ASN
1	A	481	GLN
1	A	515	HIS
1	A	586	HIS
1	A	739	GLN
1	A	965	GLN
1	A	978	ASN
1	A	1115	ASN
1	B	412	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	586	HIS
1	B	739	GLN
1	B	965	GLN
1	C	412	HIS
1	C	586	HIS
1	C	739	GLN
1	C	1035	ASN
1	C	1115	ASN
1	D	412	HIS
1	D	586	HIS
1	D	739	GLN
1	D	1115	ASN
1	D	1132	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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	A8W	D	1502	-	30,30,30	3.79	18 (60%)	45,49,49	1.76	11 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1I8P	D	1503	-	29,29,29	2.72	9 (31%)	37,40,40	4.31	18 (48%)
3	A8W	A	1502	-	30,30,30	3.80	18 (60%)	45,49,49	1.79	12 (26%)
3	A8W	B	1501	-	30,30,30	3.81	18 (60%)	45,49,49	1.76	10 (22%)
2	A1I8P	A	1501	-	29,29,29	2.77	9 (31%)	37,40,40	4.32	18 (48%)
4	CLR	A	1503	-	31,31,31	0.39	0	48,48,48	0.53	0
4	CLR	A	1504	-	31,31,31	0.39	0	48,48,48	0.53	0
2	A1I8P	B	1502	-	29,29,29	2.72	9 (31%)	37,40,40	4.29	18 (48%)
4	CLR	C	1501	-	31,31,31	0.39	0	48,48,48	0.53	0
3	A8W	C	1503	-	30,30,30	3.80	18 (60%)	45,49,49	1.76	11 (24%)
4	CLR	D	1501	-	31,31,31	0.39	0	48,48,48	0.53	0
2	A1I8P	C	1502	-	29,29,29	2.73	9 (31%)	37,40,40	4.34	18 (48%)

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	A8W	D	1502	-	-	2/9/67/67	0/4/4/4
2	A1I8P	D	1503	-	-	4/16/26/26	0/4/4/4
3	A8W	A	1502	-	-	0/9/67/67	0/4/4/4
3	A8W	B	1501	-	-	2/9/67/67	0/4/4/4
2	A1I8P	A	1501	-	-	4/16/26/26	0/4/4/4
4	CLR	A	1503	-	-	0/10/68/68	0/4/4/4
4	CLR	A	1504	-	-	0/10/68/68	0/4/4/4
2	A1I8P	B	1502	-	-	4/16/26/26	0/4/4/4
4	CLR	C	1501	-	-	0/10/68/68	0/4/4/4
3	A8W	C	1503	-	-	2/9/67/67	0/4/4/4
4	CLR	D	1501	-	-	0/10/68/68	0/4/4/4
2	A1I8P	C	1502	-	-	4/16/26/26	0/4/4/4

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1502	A8W	C12-C13	-7.82	1.40	1.54
3	B	1501	A8W	C12-C13	-7.79	1.40	1.54
3	C	1503	A8W	C12-C13	-7.75	1.40	1.54
3	D	1502	A8W	C12-C13	-7.74	1.40	1.54
3	B	1501	A8W	C11-C9	7.11	1.65	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1501	A1I8P	C08-C07	7.09	1.60	1.52
2	C	1502	A1I8P	C08-C07	7.09	1.60	1.52
3	A	1502	A8W	C11-C9	7.08	1.65	1.53
3	C	1503	A8W	C11-C9	7.06	1.65	1.53
2	B	1502	A1I8P	C08-C07	7.05	1.60	1.52
3	D	1502	A8W	C11-C9	7.04	1.65	1.53
2	D	1503	A1I8P	C08-C07	7.04	1.60	1.52
3	B	1501	A8W	C8-C14	-6.85	1.40	1.53
3	C	1503	A8W	C8-C14	-6.85	1.40	1.53
3	A	1502	A8W	C8-C14	-6.83	1.40	1.53
3	D	1502	A8W	C8-C14	-6.79	1.40	1.53
2	A	1501	A1I8P	C04-N25	6.42	1.36	1.30
2	C	1502	A1I8P	C04-N25	6.40	1.36	1.30
2	B	1502	A1I8P	C04-N25	6.37	1.36	1.30
2	D	1503	A1I8P	C04-N25	6.33	1.36	1.30
3	A	1502	A8W	C8-C9	5.78	1.64	1.53
3	D	1502	A8W	C8-C9	5.75	1.64	1.53
3	C	1503	A8W	C8-C9	5.72	1.64	1.53
3	B	1501	A8W	C8-C9	5.68	1.64	1.53
3	B	1501	A8W	C17-C20	-5.52	1.44	1.51
3	A	1502	A8W	C17-C20	-5.51	1.44	1.51
3	C	1503	A8W	C17-C20	-5.48	1.44	1.51
3	D	1502	A8W	C17-C20	-5.46	1.44	1.51
3	A	1502	A8W	O1-C3	-5.42	1.37	1.48
3	C	1503	A8W	O1-C3	-5.41	1.37	1.48
3	B	1501	A8W	O1-C3	-5.38	1.37	1.48
3	D	1502	A8W	O1-C3	-5.36	1.37	1.48
3	B	1501	A8W	C10-C9	-5.27	1.47	1.56
3	A	1502	A8W	C16-C15	5.24	1.68	1.54
3	B	1501	A8W	C16-C15	5.24	1.68	1.54
3	C	1503	A8W	C16-C15	5.24	1.68	1.54
3	A	1502	A8W	C10-C9	-5.23	1.47	1.56
3	D	1502	A8W	C10-C9	-5.22	1.47	1.56
3	C	1503	A8W	C10-C9	-5.22	1.47	1.56
3	D	1502	A8W	C16-C15	5.19	1.68	1.54
2	C	1502	A1I8P	C06-N05	5.19	1.45	1.36
2	A	1501	A1I8P	C06-N05	5.13	1.45	1.36
2	B	1502	A1I8P	C06-N05	5.12	1.45	1.36
2	D	1503	A1I8P	C06-N05	5.08	1.45	1.36
2	A	1501	A1I8P	C03-C04	4.61	1.47	1.40
2	D	1503	A1I8P	C03-C04	4.60	1.47	1.40
2	A	1501	A1I8P	C07-N14	4.60	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1502	A1I8P	C03-C04	4.59	1.47	1.40
2	C	1502	A1I8P	C03-C04	4.57	1.47	1.40
2	C	1502	A1I8P	C07-N14	4.43	1.51	1.46
3	B	1501	A8W	C15-C14	4.38	1.63	1.54
3	D	1502	A8W	C15-C14	4.36	1.63	1.54
2	B	1502	A1I8P	C07-N14	4.35	1.51	1.46
3	C	1503	A8W	C15-C14	4.35	1.63	1.54
2	D	1503	A1I8P	C07-N14	4.33	1.51	1.46
3	D	1502	A8W	C12-C11	4.31	1.62	1.53
3	B	1501	A8W	C12-C11	4.31	1.62	1.53
3	A	1502	A8W	C15-C14	4.30	1.63	1.54
3	C	1503	A8W	C12-C11	4.27	1.62	1.53
3	A	1502	A8W	C12-C11	4.26	1.62	1.53
3	B	1501	A8W	C6-C5	-3.73	1.24	1.33
3	B	1501	A8W	C1-C10	3.72	1.61	1.54
3	C	1503	A8W	C6-C5	-3.72	1.24	1.33
3	C	1503	A8W	C10-C5	-3.71	1.45	1.52
3	D	1502	A8W	C6-C5	-3.70	1.24	1.33
3	D	1502	A8W	C10-C5	-3.69	1.45	1.52
3	A	1502	A8W	C10-C5	-3.69	1.45	1.52
3	D	1502	A8W	C1-C10	3.69	1.61	1.54
3	B	1501	A8W	C10-C5	-3.68	1.45	1.52
3	C	1503	A8W	C1-C10	3.67	1.61	1.54
3	A	1502	A8W	C1-C10	3.67	1.61	1.54
3	A	1502	A8W	C6-C5	-3.67	1.24	1.33
2	D	1503	A1I8P	O26-N25	-3.48	1.36	1.42
2	A	1501	A1I8P	O26-N25	-3.45	1.36	1.42
2	B	1502	A1I8P	O26-N25	-3.42	1.36	1.42
2	C	1502	A1I8P	O26-N25	-3.40	1.36	1.42
2	A	1501	A1I8P	C04-N05	3.35	1.44	1.39
2	D	1503	A1I8P	C04-N05	3.24	1.44	1.39
2	C	1502	A1I8P	C04-N05	3.22	1.44	1.39
2	B	1502	A1I8P	C04-N05	3.21	1.44	1.39
3	A	1502	A8W	C13-C14	-3.03	1.49	1.55
3	D	1502	A8W	C13-C14	-3.01	1.49	1.55
3	C	1503	A8W	C13-C14	-3.01	1.49	1.55
3	B	1501	A8W	C13-C14	-2.98	1.49	1.55
3	A	1502	A8W	O1-S	2.91	1.65	1.57
3	C	1503	A8W	O1-S	2.91	1.65	1.57
3	D	1502	A8W	O1-S	2.90	1.65	1.57
3	B	1501	A8W	O1-S	2.89	1.65	1.57
3	C	1503	A8W	C19-C10	2.73	1.59	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1501	A8W	C19-C10	2.70	1.59	1.54
2	A	1501	A1I8P	C18-N14	2.70	1.47	1.40
3	D	1502	A8W	C19-C10	2.69	1.59	1.54
3	A	1502	A8W	C19-C10	2.68	1.59	1.54
3	C	1503	A8W	C4-C5	2.47	1.57	1.51
3	D	1502	A8W	C4-C5	2.46	1.57	1.51
3	D	1502	A8W	C1-C2	2.46	1.58	1.53
3	A	1502	A8W	C1-C2	2.45	1.58	1.53
3	C	1503	A8W	C1-C2	2.44	1.58	1.53
3	B	1501	A8W	C1-C2	2.42	1.58	1.53
3	A	1502	A8W	C4-C5	2.41	1.56	1.51
3	B	1501	A8W	C4-C5	2.40	1.56	1.51
2	A	1501	A1I8P	C15-N14	2.35	1.50	1.46
2	B	1502	A1I8P	C18-N14	2.31	1.46	1.40
2	D	1503	A1I8P	C18-N14	2.30	1.46	1.40
2	C	1502	A1I8P	C18-N14	2.28	1.46	1.40
2	B	1502	A1I8P	C15-N14	2.22	1.50	1.46
2	D	1503	A1I8P	C15-N14	2.19	1.50	1.46
2	C	1502	A1I8P	C15-N14	2.14	1.50	1.46

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1501	A1I8P	C03-C04-N25	-15.20	103.52	112.29
2	D	1503	A1I8P	C03-C04-N25	-15.14	103.55	112.29
2	C	1502	A1I8P	C03-C04-N25	-15.13	103.55	112.29
2	B	1502	A1I8P	C03-C04-N25	-15.05	103.60	112.29
2	C	1502	A1I8P	O26-C02-C01	9.34	124.24	115.88
2	A	1501	A1I8P	O26-N25-C04	9.27	110.31	104.58
2	D	1503	A1I8P	O26-N25-C04	9.22	110.28	104.58
2	B	1502	A1I8P	O26-N25-C04	9.14	110.23	104.58
2	C	1502	A1I8P	O26-N25-C04	9.11	110.22	104.58
2	D	1503	A1I8P	O26-C02-C01	9.05	123.98	115.88
2	A	1501	A1I8P	O26-C02-C01	9.02	123.96	115.88
2	B	1502	A1I8P	O26-C02-C01	9.02	123.95	115.88
2	C	1502	A1I8P	C08-C07-N14	7.00	119.19	112.17
2	B	1502	A1I8P	C08-C07-N14	6.91	119.09	112.17
2	D	1503	A1I8P	C08-C07-N14	6.83	119.02	112.17
2	A	1501	A1I8P	C08-C07-N14	6.68	118.87	112.17
2	C	1502	A1I8P	C04-C03-C02	6.65	109.49	104.70
2	D	1503	A1I8P	C04-C03-C02	6.56	109.43	104.70
2	A	1501	A1I8P	C04-C03-C02	6.51	109.39	104.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1502	A1I8P	C04-C03-C02	6.49	109.37	104.70
2	A	1501	A1I8P	C20-C19-C18	5.92	126.10	118.22
2	D	1503	A1I8P	C20-C19-C18	5.86	126.02	118.22
2	C	1502	A1I8P	C20-C19-C18	5.86	126.01	118.22
2	B	1502	A1I8P	C20-C19-C18	5.82	125.97	118.22
2	A	1501	A1I8P	C23-C18-C19	-5.15	112.21	119.87
2	C	1502	A1I8P	C23-C18-C19	-5.01	112.43	119.87
2	D	1503	A1I8P	C23-C18-C19	-5.00	112.44	119.87
2	B	1502	A1I8P	C23-C18-C19	-4.99	112.46	119.87
2	C	1502	A1I8P	O24-C06-C07	-4.96	114.32	120.97
2	D	1503	A1I8P	O24-C06-C07	-4.88	114.43	120.97
2	B	1502	A1I8P	O24-C06-C07	-4.81	114.52	120.97
2	A	1501	A1I8P	O24-C06-C07	-4.81	114.53	120.97
2	C	1502	A1I8P	O26-C02-C03	-4.69	106.11	109.72
2	D	1503	A1I8P	O26-C02-C03	-4.67	106.13	109.72
2	B	1502	A1I8P	O26-C02-C03	-4.58	106.20	109.72
2	A	1501	A1I8P	O26-C02-C03	-4.56	106.21	109.72
3	A	1502	A8W	C15-C14-C8	-4.35	111.92	119.08
3	B	1501	A8W	C15-C14-C8	-4.33	111.94	119.08
3	C	1503	A8W	C15-C14-C8	-4.33	111.95	119.08
3	D	1502	A8W	C15-C14-C8	-4.30	112.00	119.08
3	A	1502	A8W	C12-C13-C17	-4.19	110.98	116.10
3	B	1501	A8W	C12-C13-C17	-4.05	111.15	116.10
3	C	1503	A8W	C12-C13-C17	-4.03	111.17	116.10
3	D	1502	A8W	C12-C13-C17	-3.96	111.26	116.10
3	A	1502	A8W	C7-C8-C9	-3.83	105.08	109.71
2	B	1502	A1I8P	O24-C06-N05	-3.76	116.65	122.57
2	C	1502	A1I8P	O24-C06-N05	-3.76	116.66	122.57
2	D	1503	A1I8P	O24-C06-N05	-3.75	116.66	122.57
2	A	1501	A1I8P	O24-C06-N05	-3.74	116.69	122.57
2	A	1501	A1I8P	C23-C18-N14	3.73	128.54	121.50
2	C	1502	A1I8P	C23-C18-N14	3.68	128.46	121.50
2	D	1503	A1I8P	C23-C18-N14	3.65	128.39	121.50
2	B	1502	A1I8P	C23-C18-N14	3.63	128.36	121.50
3	B	1501	A8W	C7-C8-C9	-3.43	105.56	109.71
3	C	1503	A8W	C7-C8-C9	-3.36	105.64	109.71
3	D	1502	A8W	C7-C8-C9	-3.31	105.70	109.71
3	A	1502	A8W	C8-C7-C6	-3.29	108.00	112.73
3	B	1501	A8W	C8-C7-C6	-3.13	108.24	112.73
2	C	1502	A1I8P	C02-O26-N25	3.12	110.61	108.66
2	D	1503	A1I8P	C02-O26-N25	3.10	110.61	108.66
2	B	1502	A1I8P	C02-O26-N25	3.08	110.59	108.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1502	A8W	C11-C9-C8	-3.06	107.35	111.75
3	C	1503	A8W	C8-C7-C6	-3.05	108.35	112.73
2	A	1501	A1I8P	C02-O26-N25	3.03	110.56	108.66
3	D	1502	A8W	C8-C7-C6	-2.95	108.49	112.73
3	C	1503	A8W	C11-C9-C8	-2.93	107.54	111.75
3	B	1501	A8W	C11-C9-C8	-2.87	107.62	111.75
2	C	1502	A1I8P	C13-C08-C07	2.82	124.90	120.71
2	B	1502	A1I8P	C13-C08-C07	2.82	124.89	120.71
2	D	1503	A1I8P	C13-C08-C07	2.80	124.86	120.71
3	C	1503	A8W	C4-C5-C6	-2.75	116.64	120.61
3	D	1502	A8W	C4-C5-C6	-2.75	116.65	120.61
3	B	1501	A8W	C4-C5-C6	-2.71	116.71	120.61
3	A	1502	A8W	C4-C5-C6	-2.70	116.72	120.61
2	A	1501	A1I8P	C13-C08-C07	2.67	124.67	120.71
3	A	1502	A8W	C11-C9-C8	-2.61	107.99	111.75
3	C	1503	A8W	C12-C13-C14	2.53	111.19	107.27
3	B	1501	A8W	C12-C13-C14	2.52	111.18	107.27
3	A	1502	A8W	C12-C13-C14	2.49	111.14	107.27
2	C	1502	A1I8P	C01-C02-C03	-2.47	129.64	134.09
3	D	1502	A8W	C12-C13-C14	2.47	111.10	107.27
2	B	1502	A1I8P	C09-C08-C13	-2.46	115.23	118.29
2	D	1503	A1I8P	C09-C08-C13	-2.45	115.24	118.29
2	A	1501	A1I8P	C09-C08-C13	-2.43	115.26	118.29
3	C	1503	A8W	C1-C10-C9	-2.42	105.35	108.73
3	D	1502	A8W	C1-C10-C9	-2.41	105.36	108.73
2	C	1502	A1I8P	C09-C08-C13	-2.41	115.28	118.29
3	B	1501	A8W	C1-C10-C9	-2.41	105.37	108.73
3	D	1502	A8W	C16-C17-C20	-2.37	110.61	114.23
2	A	1501	A1I8P	C01-C02-C03	-2.37	129.83	134.09
2	B	1502	A1I8P	C01-C02-C03	-2.35	129.85	134.09
3	A	1502	A8W	C1-C10-C9	-2.35	105.44	108.73
2	D	1503	A1I8P	C01-C02-C03	-2.33	129.89	134.09
2	A	1501	A1I8P	C22-C23-C18	2.32	123.14	118.26
2	C	1502	A1I8P	C22-C23-C18	2.27	123.02	118.26
2	B	1502	A1I8P	C22-C23-C18	2.26	123.01	118.26
2	D	1503	A1I8P	C22-C23-C18	2.26	123.01	118.26
3	C	1503	A8W	C16-C17-C20	-2.25	110.79	114.23
3	B	1501	A8W	C16-C17-C20	-2.19	110.89	114.23
3	A	1502	A8W	C13-C17-C20	-2.18	111.90	114.98
2	A	1501	A1I8P	C22-C21-C20	-2.17	116.89	120.19
3	D	1502	A8W	O4-S-O2	-2.14	101.04	108.49
2	C	1502	A1I8P	N05-C04-N25	2.14	129.66	123.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1502	A1I8P	C22-C21-C20	-2.13	116.95	120.19
3	B	1501	A8W	O4-S-O2	-2.12	101.12	108.49
3	C	1503	A8W	O4-S-O2	-2.12	101.12	108.49
3	A	1502	A8W	O4-S-O2	-2.11	101.16	108.49
2	C	1502	A1I8P	C22-C21-C20	-2.09	117.01	120.19
2	D	1503	A1I8P	N05-C04-N25	2.09	129.51	123.38
2	A	1501	A1I8P	N05-C04-N25	2.08	129.49	123.38
2	D	1503	A1I8P	C22-C21-C20	-2.06	117.05	120.19
3	A	1502	A8W	C2-C1-C10	-2.05	108.29	112.74
2	B	1502	A1I8P	N05-C04-N25	2.04	129.37	123.38
3	A	1502	A8W	C17-C13-C14	2.04	101.90	99.72
3	C	1503	A8W	C10-C5-C6	2.03	126.02	122.90
3	D	1502	A8W	C16-C15-C14	-2.02	101.12	105.13

There are no chirality outliers.

All (22) torsion outliers are listed below:

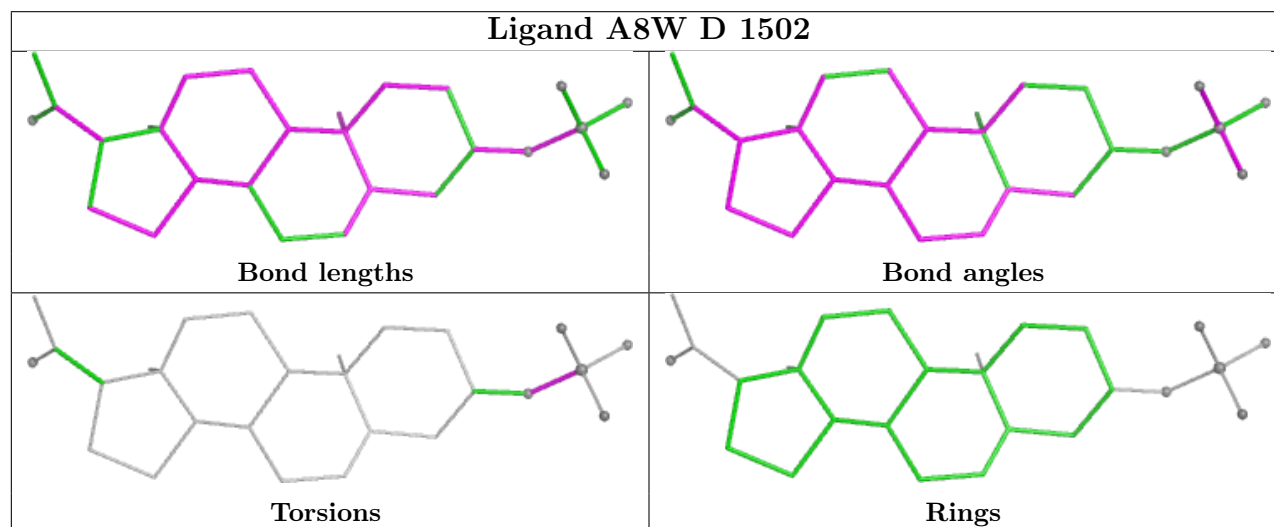
Mol	Chain	Res	Type	Atoms
2	A	1501	A1I8P	N05-C06-C07-N14
2	A	1501	A1I8P	C06-C07-N14-C15
2	B	1502	A1I8P	C06-C07-N14-C15
2	C	1502	A1I8P	C06-C07-N14-C15
2	D	1503	A1I8P	C06-C07-N14-C15
3	B	1501	A8W	C3-O1-S-O4
3	C	1503	A8W	C3-O1-S-O4
3	D	1502	A8W	C3-O1-S-O4
3	B	1501	A8W	C3-O1-S-O3
3	C	1503	A8W	C3-O1-S-O3
3	D	1502	A8W	C3-O1-S-O3
2	A	1501	A1I8P	O24-C06-C07-N14
2	B	1502	A1I8P	N05-C06-C07-N14
2	B	1502	A1I8P	O24-C06-C07-N14
2	C	1502	A1I8P	N05-C06-C07-N14
2	C	1502	A1I8P	O24-C06-C07-N14
2	D	1503	A1I8P	N05-C06-C07-N14
2	D	1503	A1I8P	O24-C06-C07-N14
2	A	1501	A1I8P	C08-C07-N14-C15
2	B	1502	A1I8P	C08-C07-N14-C15
2	C	1502	A1I8P	C08-C07-N14-C15
2	D	1503	A1I8P	C08-C07-N14-C15

There are no ring outliers.

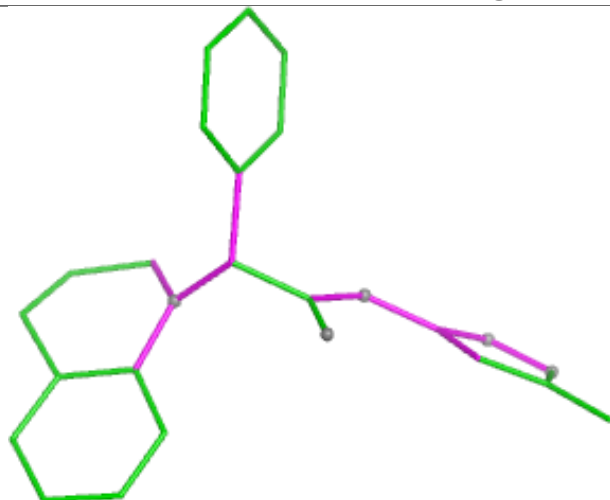
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1503	A1I8P	3	0
2	A	1501	A1I8P	3	0
2	B	1502	A1I8P	3	0
2	C	1502	A1I8P	3	0

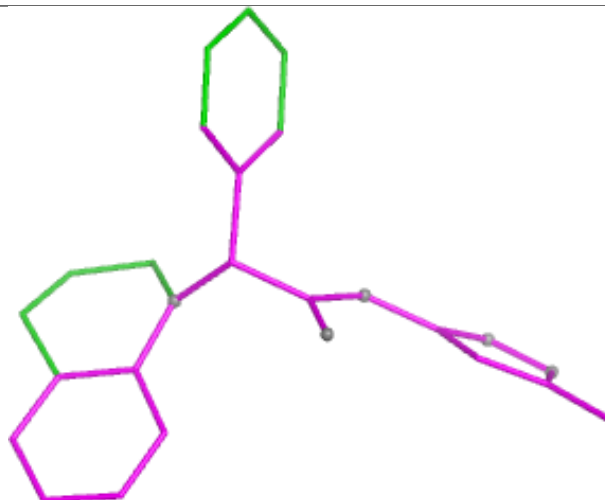
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



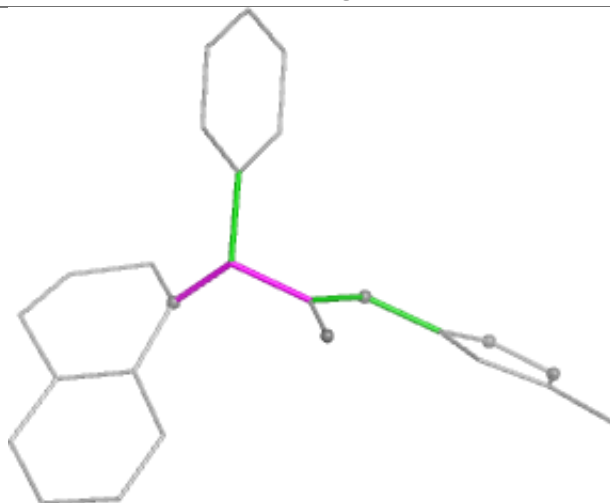
Ligand A1I8P D 1503



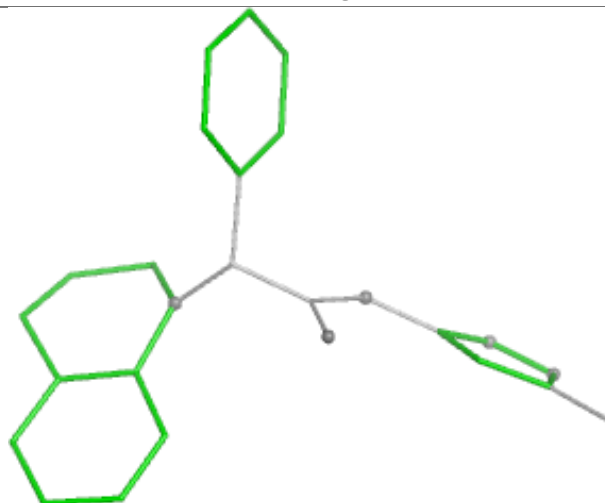
Bond lengths



Bond angles

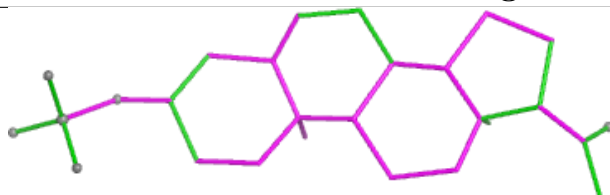


Torsions

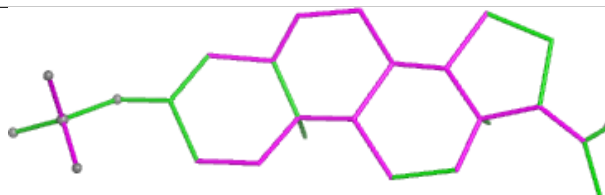


Rings

Ligand A8W A 1502



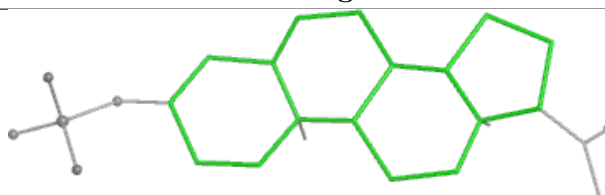
Bond lengths



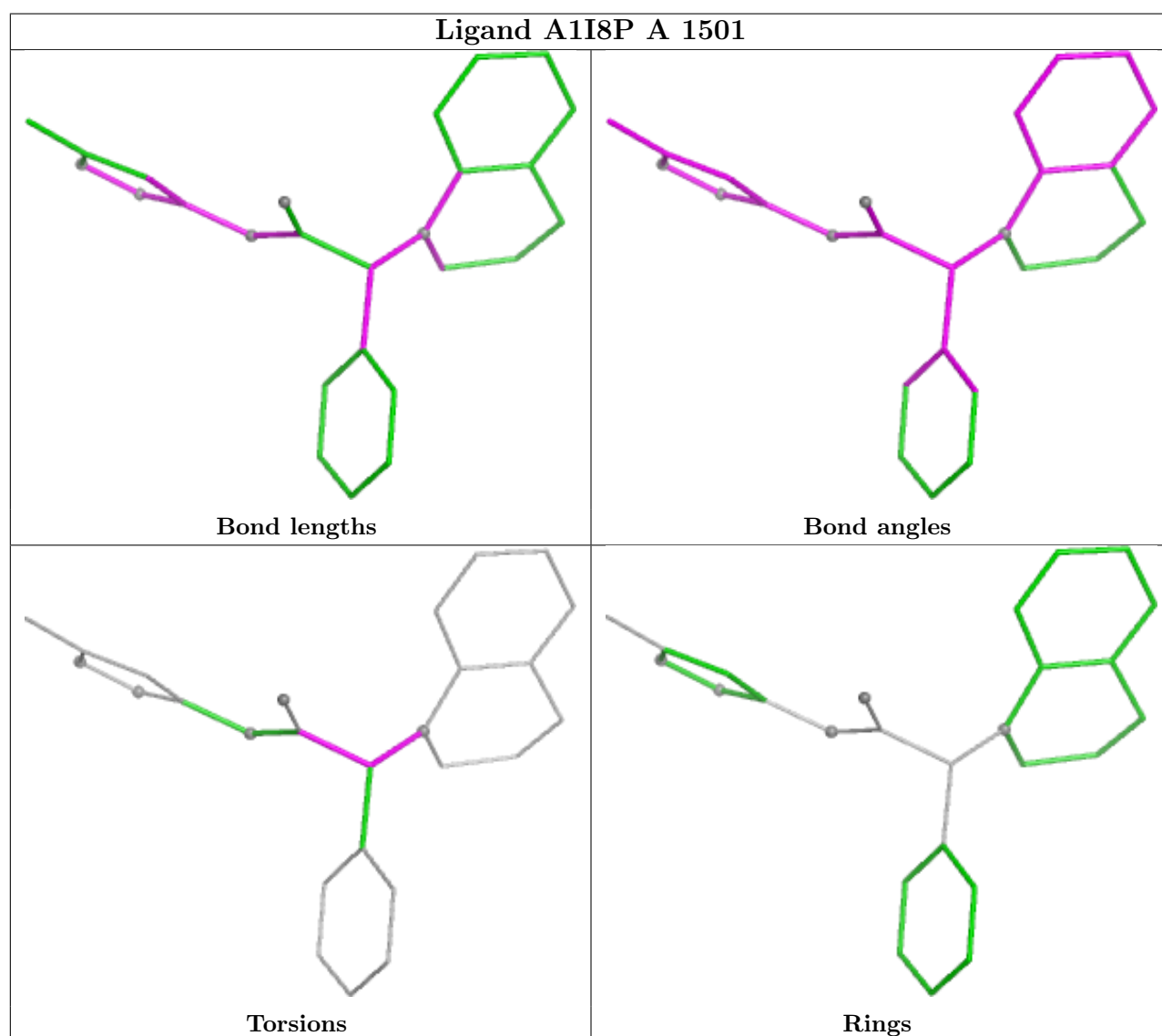
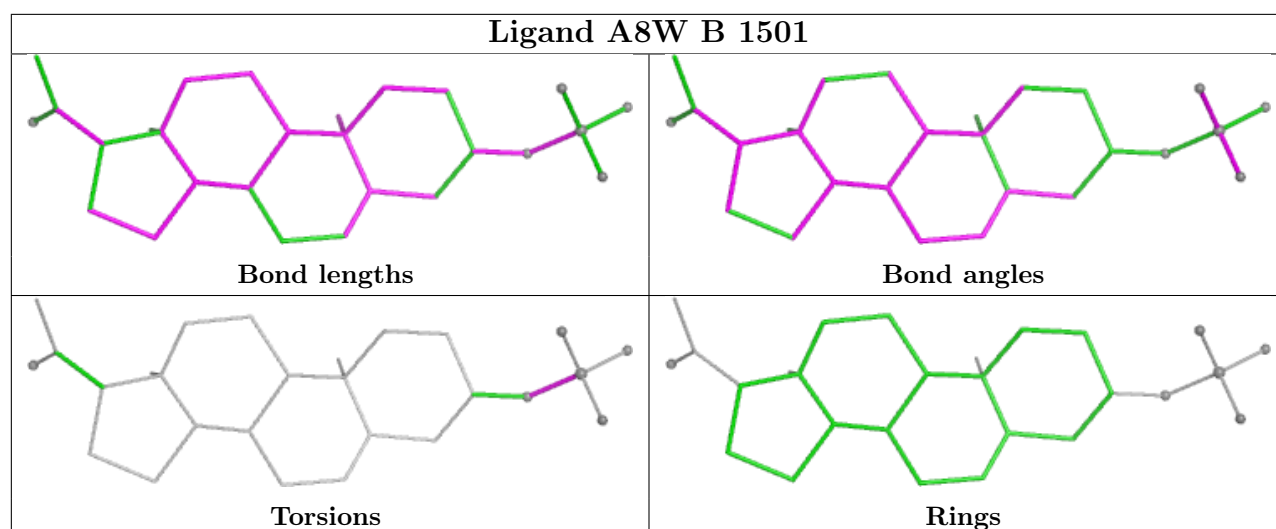
Bond angles



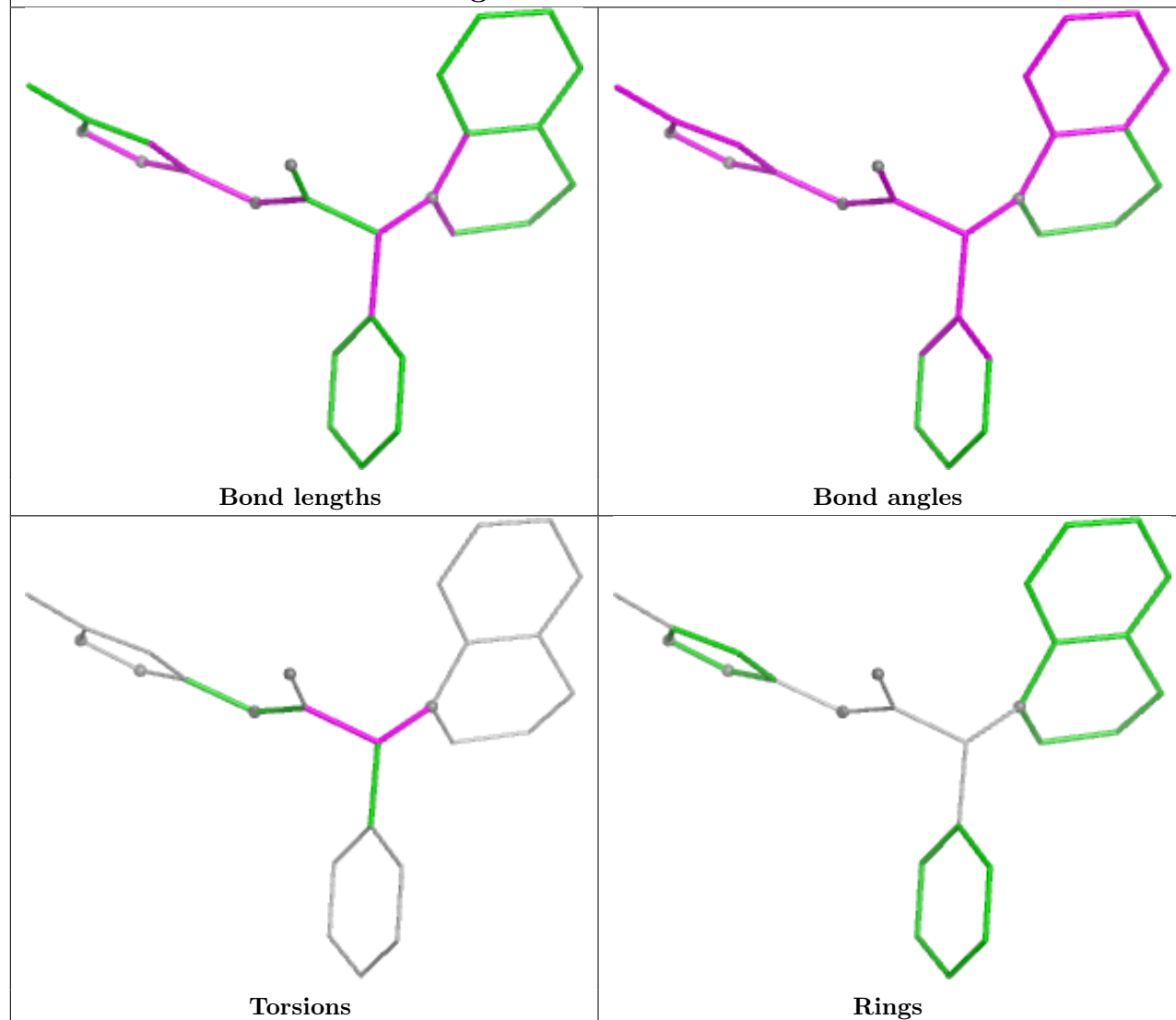
Torsions



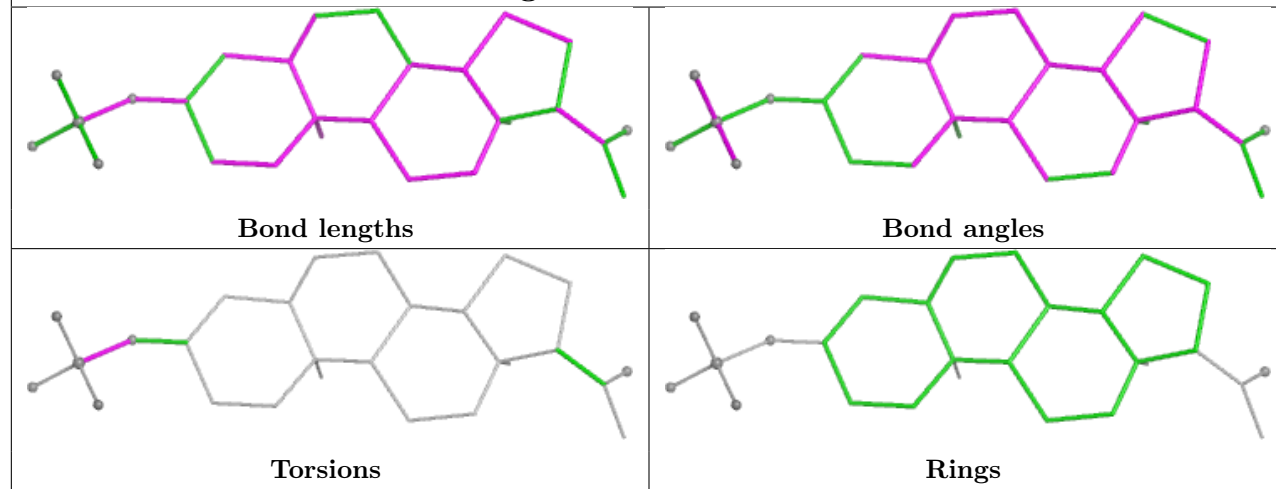
Rings

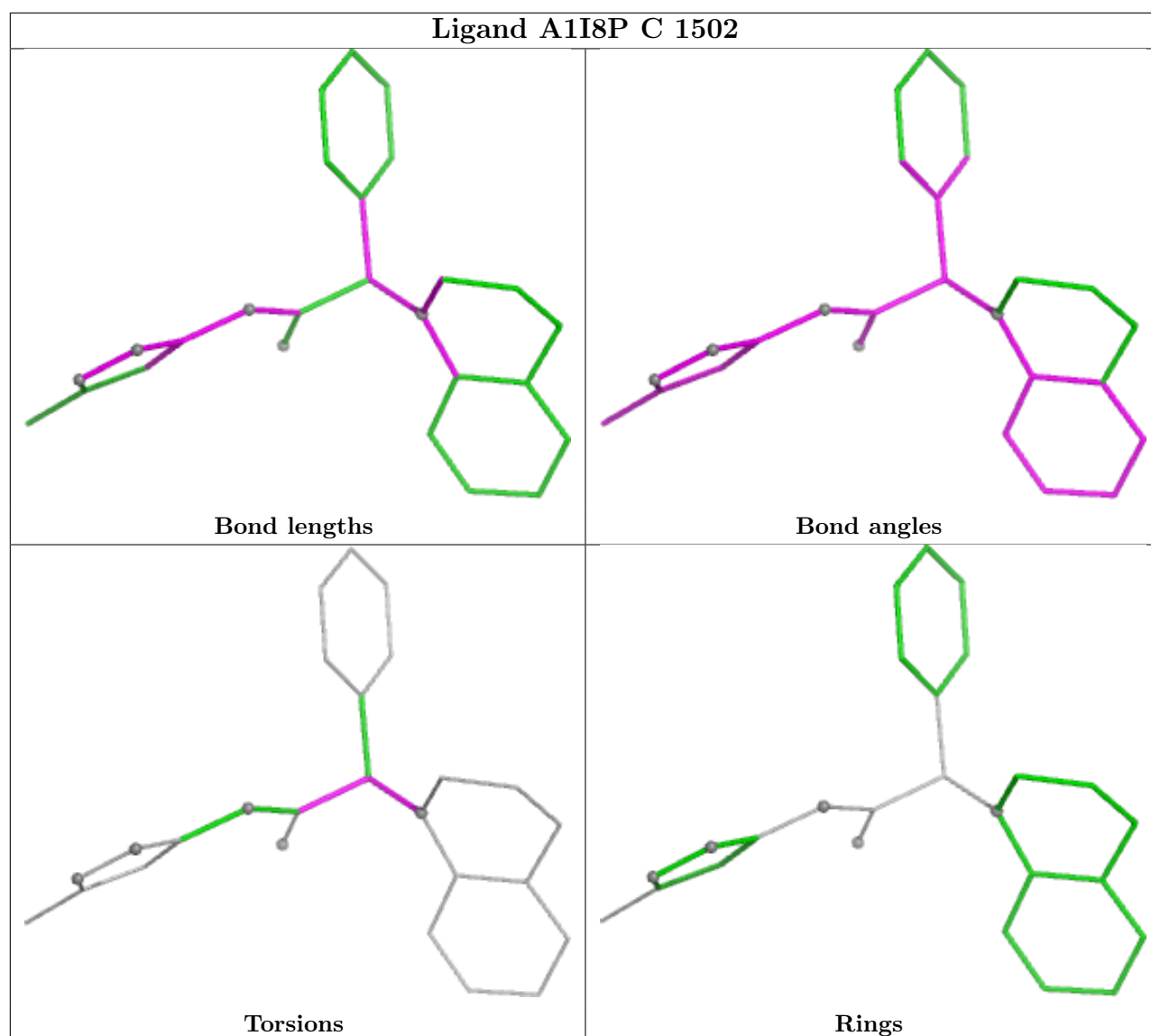


Ligand A1I8P B 1502



Ligand A8W C 1503





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.

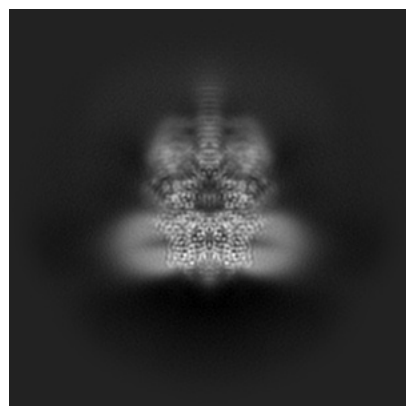
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53177. These allow visual inspection of the internal detail of the map and identification of artifacts.

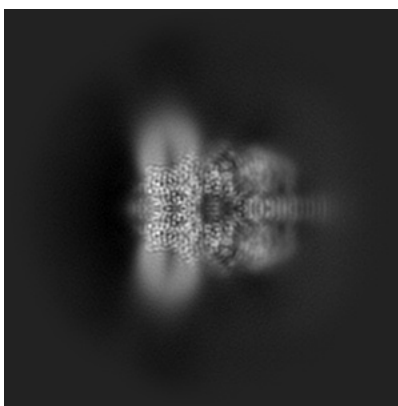
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

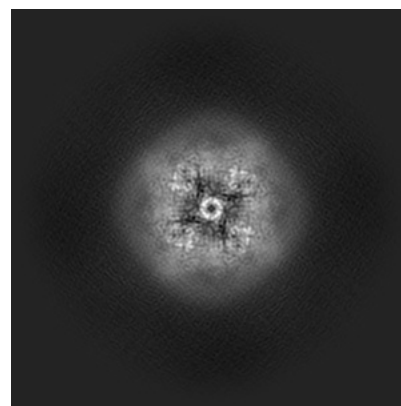
6.1.1 Primary map



X

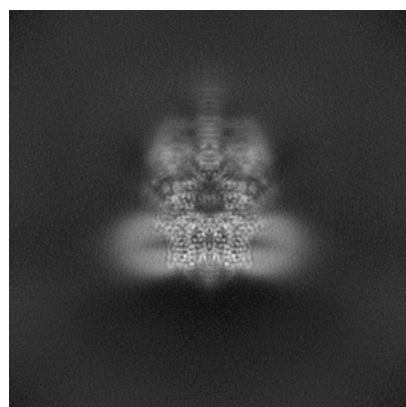


Y

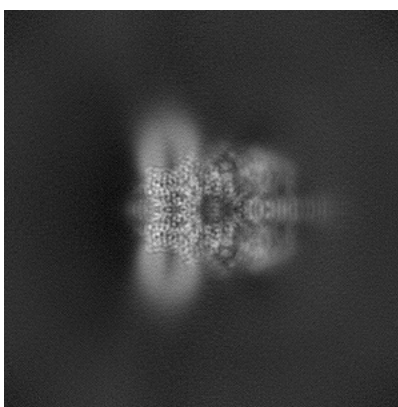


Z

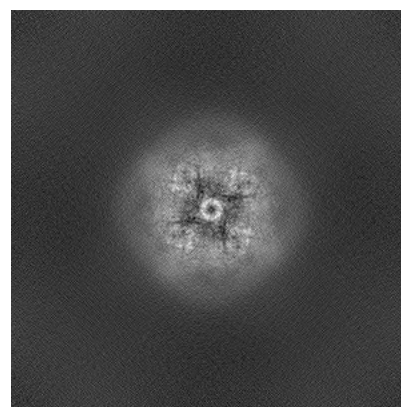
6.1.2 Raw map



X



Y

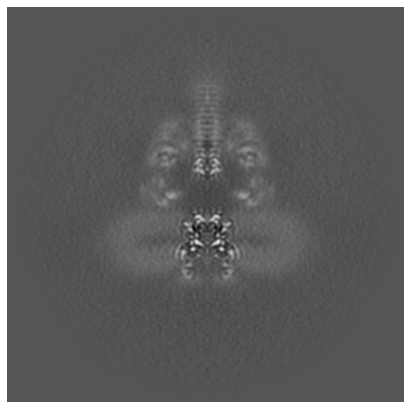


Z

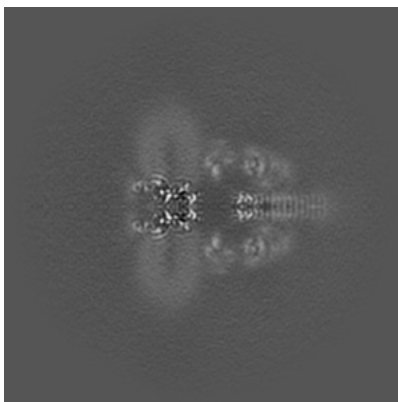
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

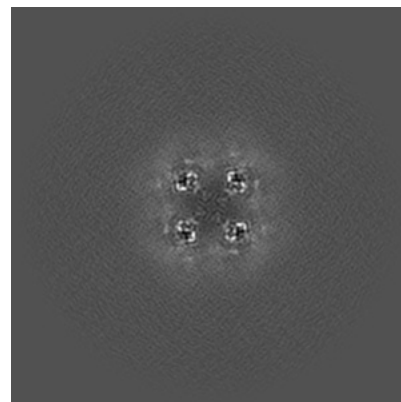
6.2.1 Primary map



X Index: 260

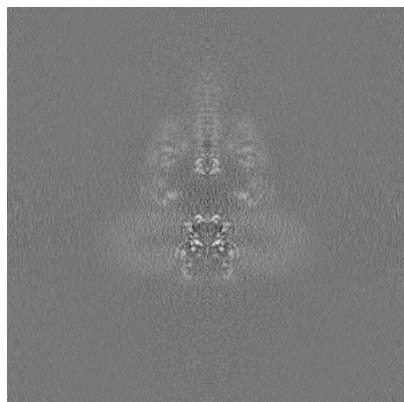


Y Index: 260

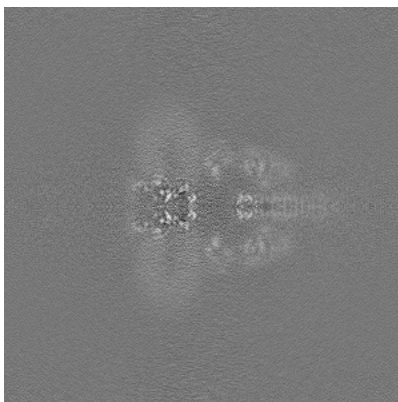


Z Index: 260

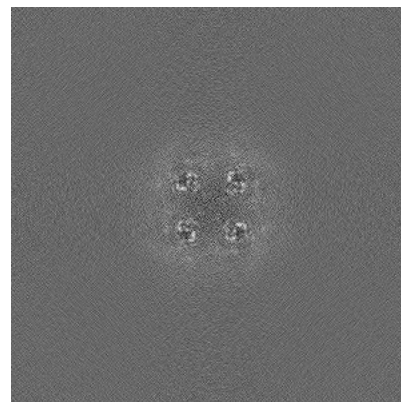
6.2.2 Raw map



X Index: 260



Y Index: 260

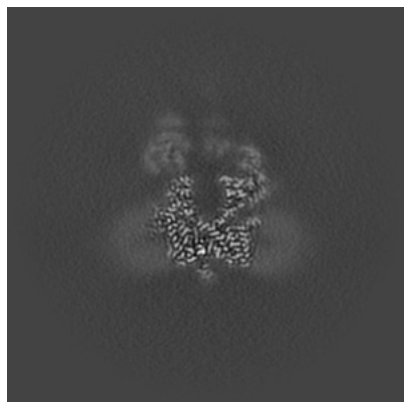


Z Index: 260

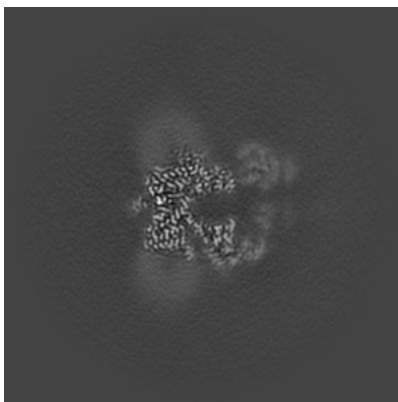
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

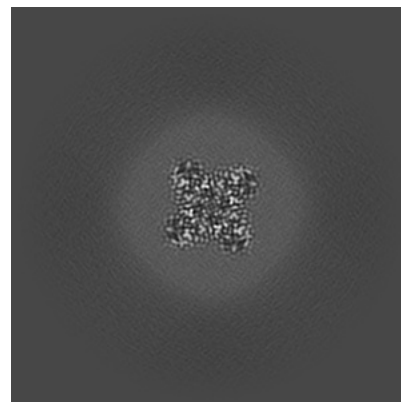
6.3.1 Primary map



X Index: 234

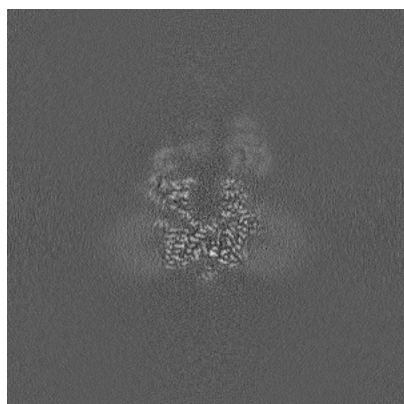


Y Index: 234

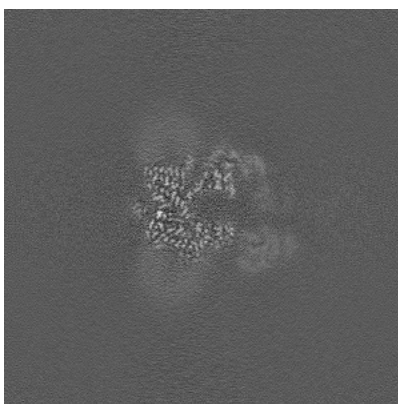


Z Index: 200

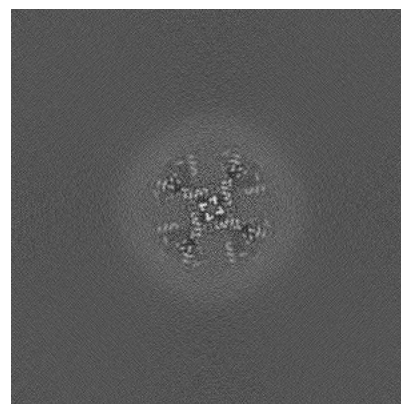
6.3.2 Raw map



X Index: 286



Y Index: 286

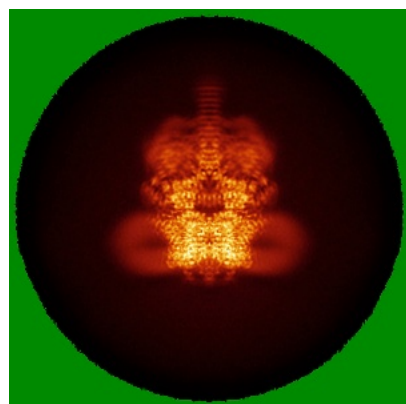


Z Index: 240

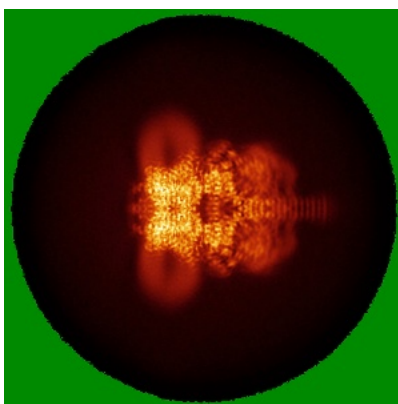
The images above show the largest variance slices of the map in three orthogonal directions.

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

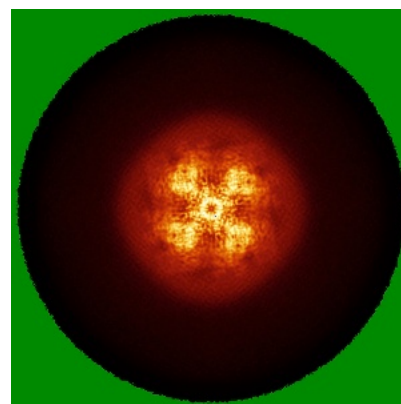
6.4.1 Primary map



X

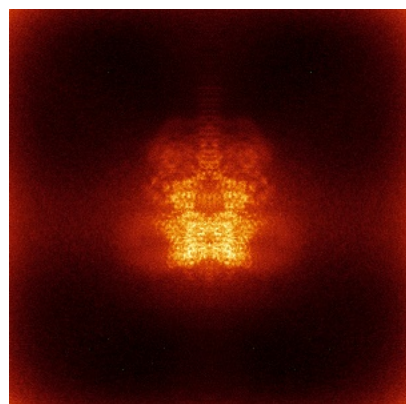


Y

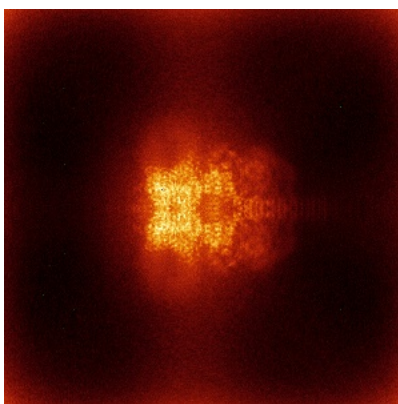


Z

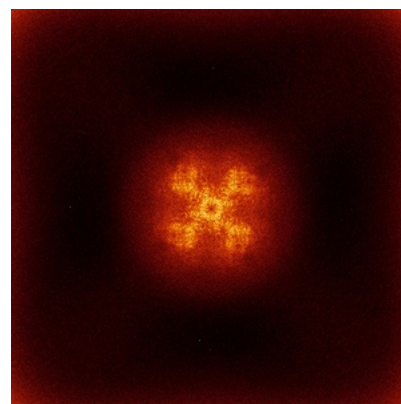
6.4.2 Raw map



X



Y

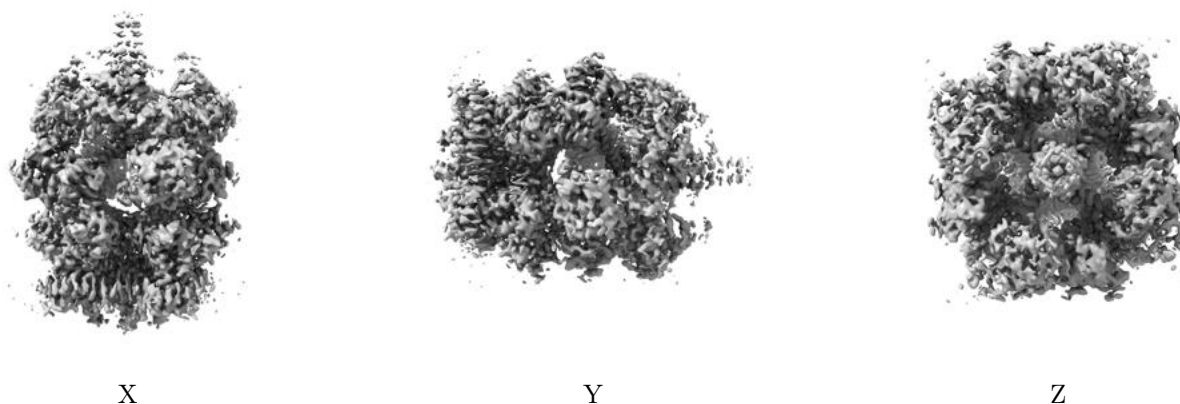


Z

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.

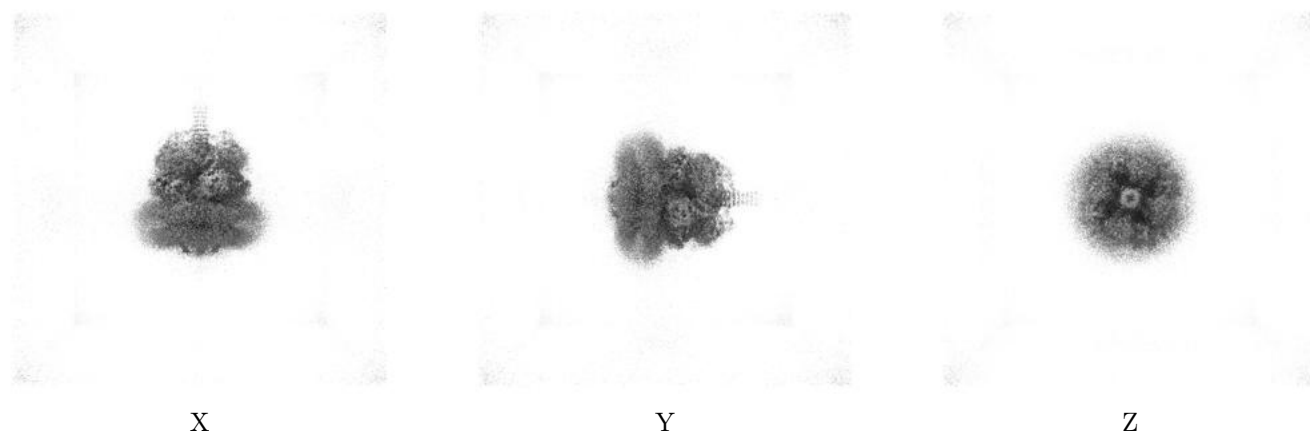
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0551. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

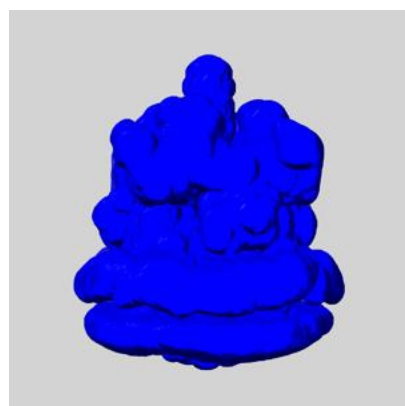
6.6 Mask visualisation [i](#)

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

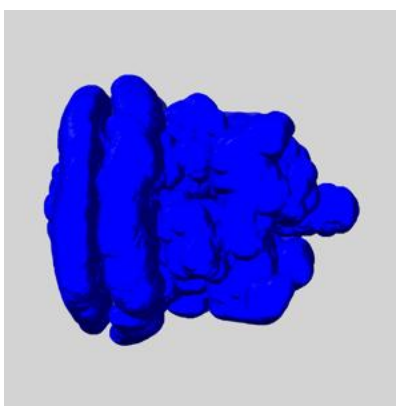
A mask typically either:

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

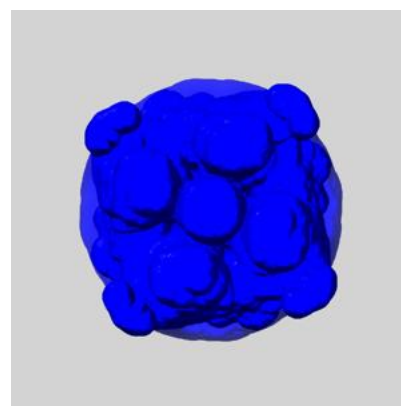
6.6.1 emd_53177_msk_1.map [i](#)



X



Y

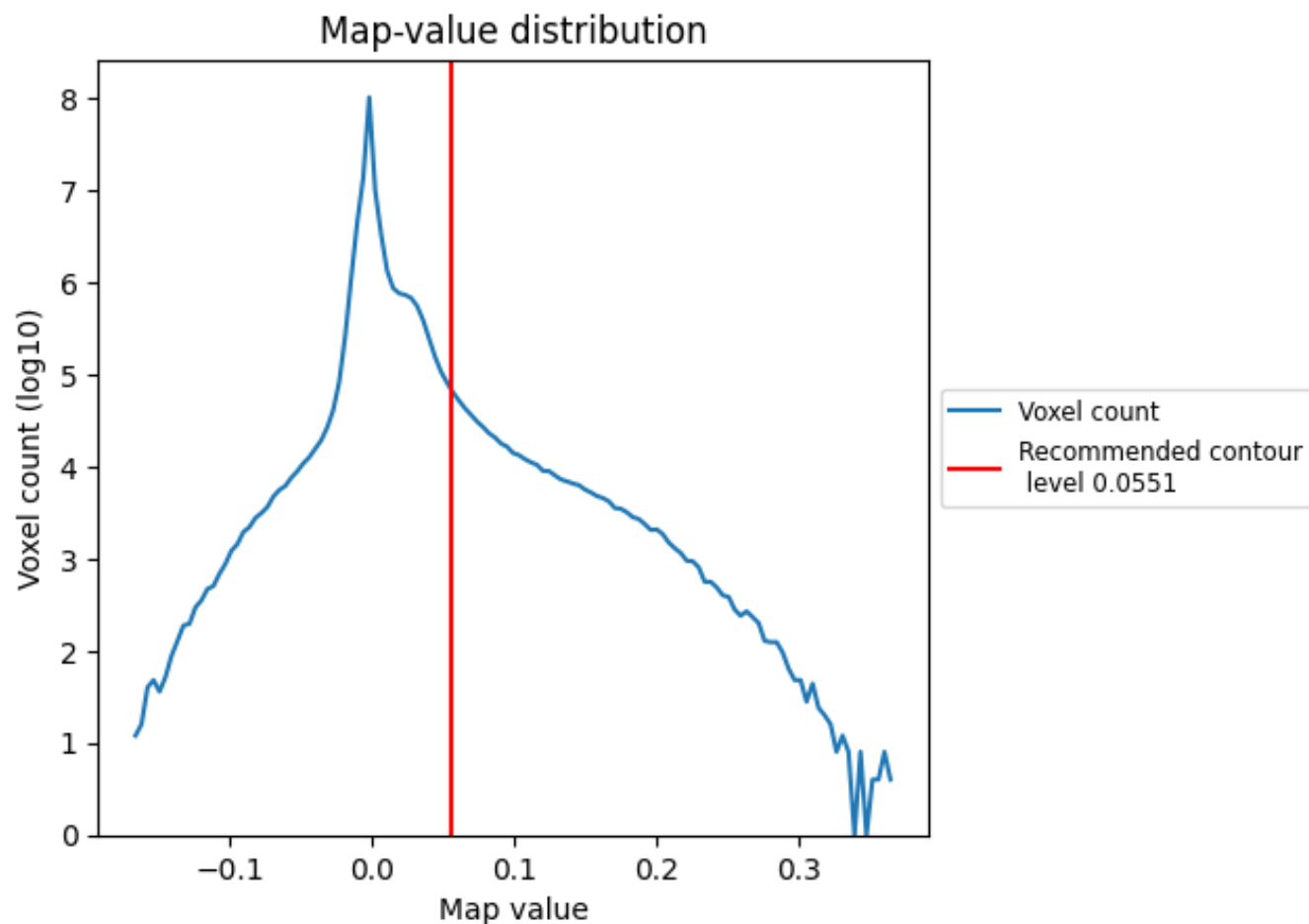


Z

7 Map analysis [i](#)

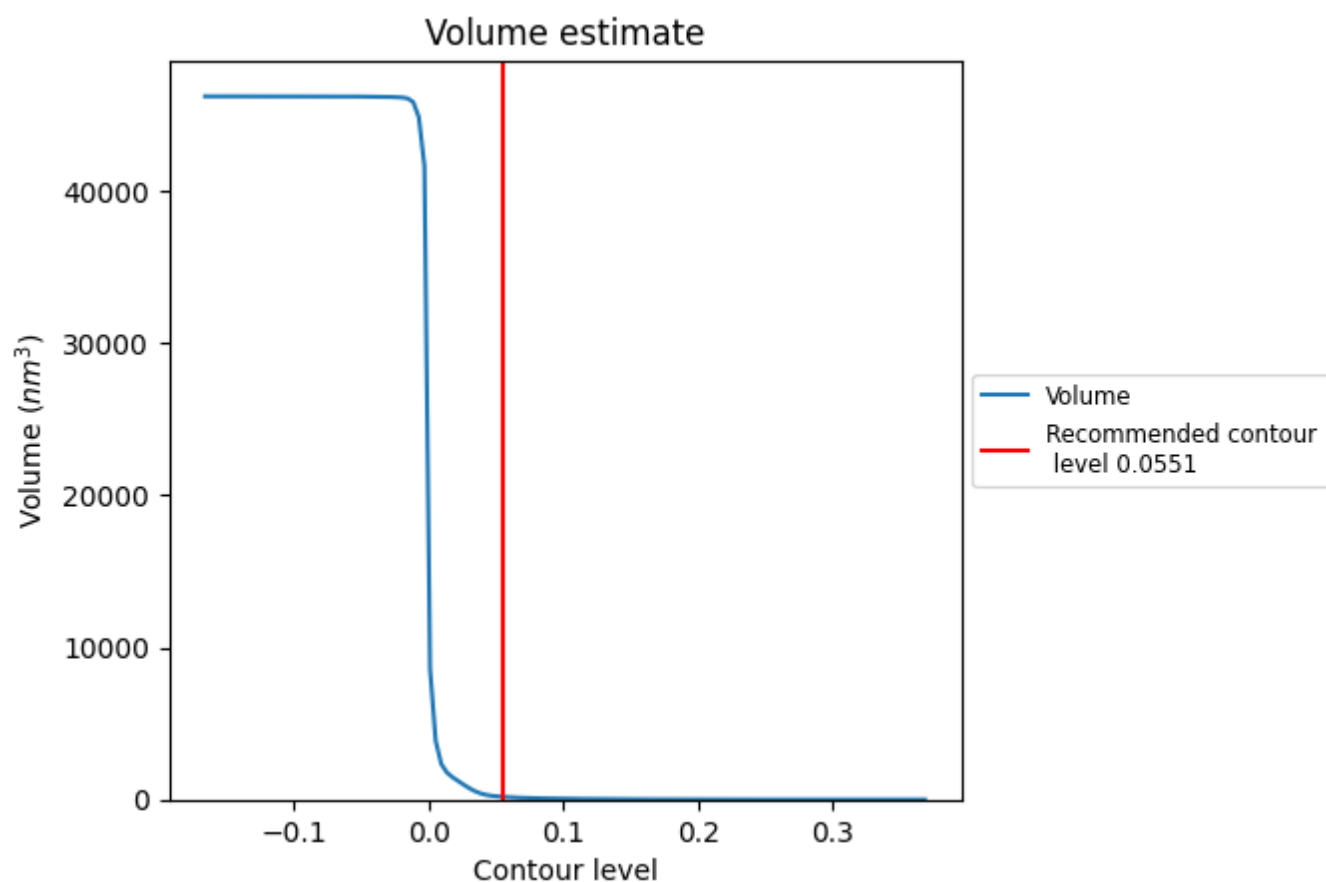
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

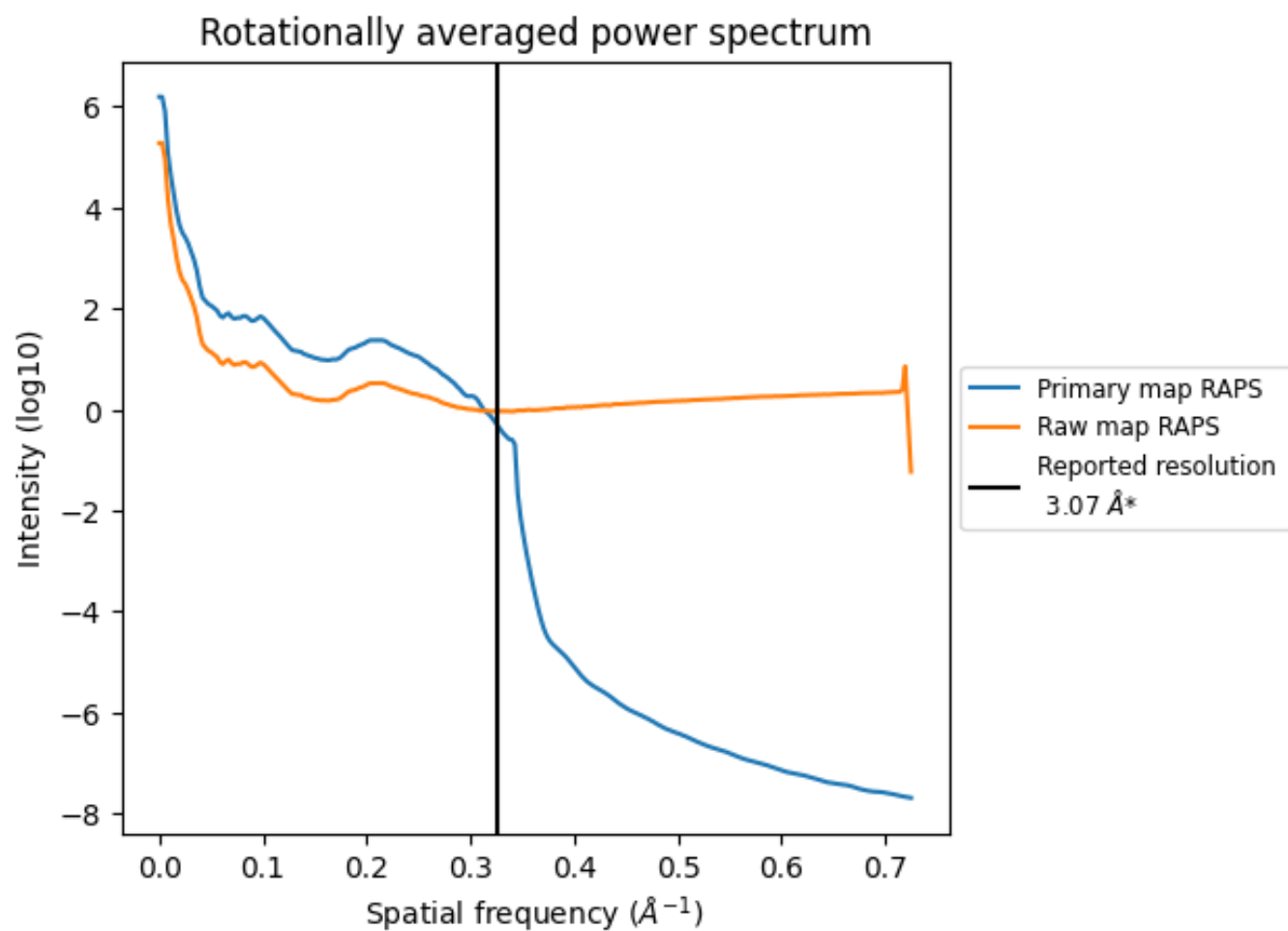
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 176 nm³; this corresponds to an approximate mass of 159 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 ⓘ

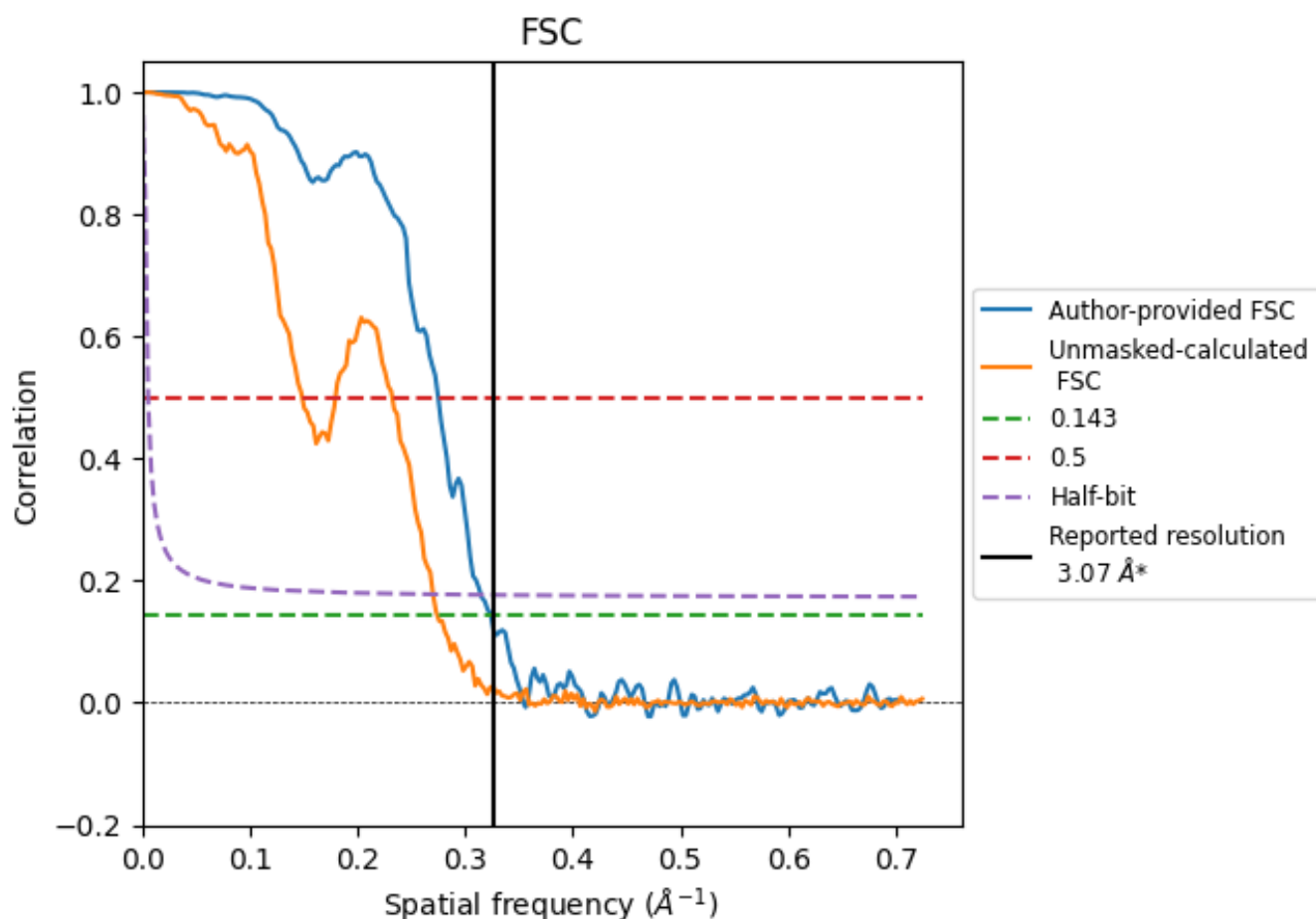


*Reported resolution corresponds to spatial frequency of 0.326 Å⁻¹

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 0.326 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

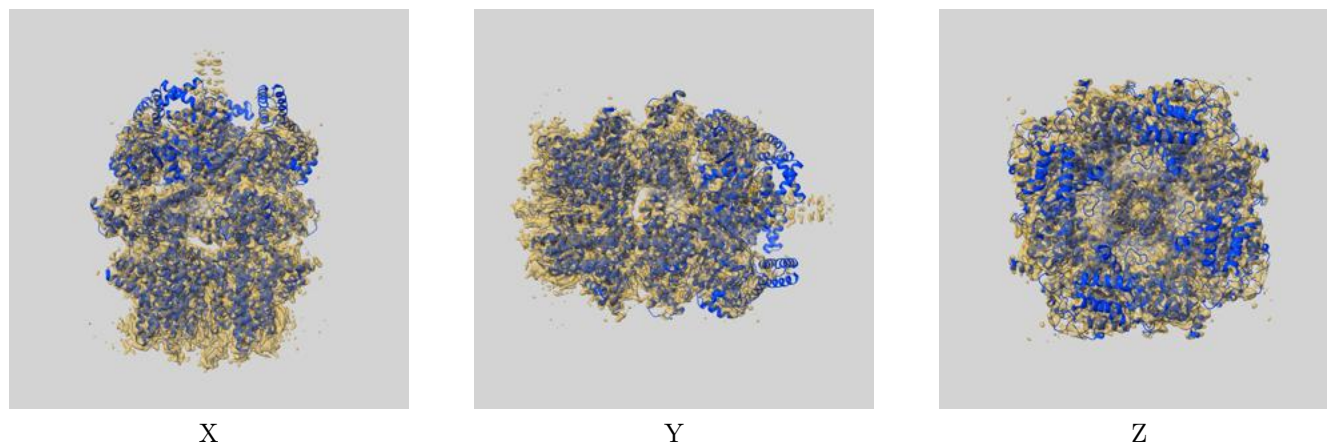
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.07	-	-
Author-provided FSC curve	3.09	3.64	3.18
Unmasked-calculated*	3.65	6.73	3.70

*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 3.65 differs from the reported value 3.07 by more than 10 %

9 Map-model fit [i](#)

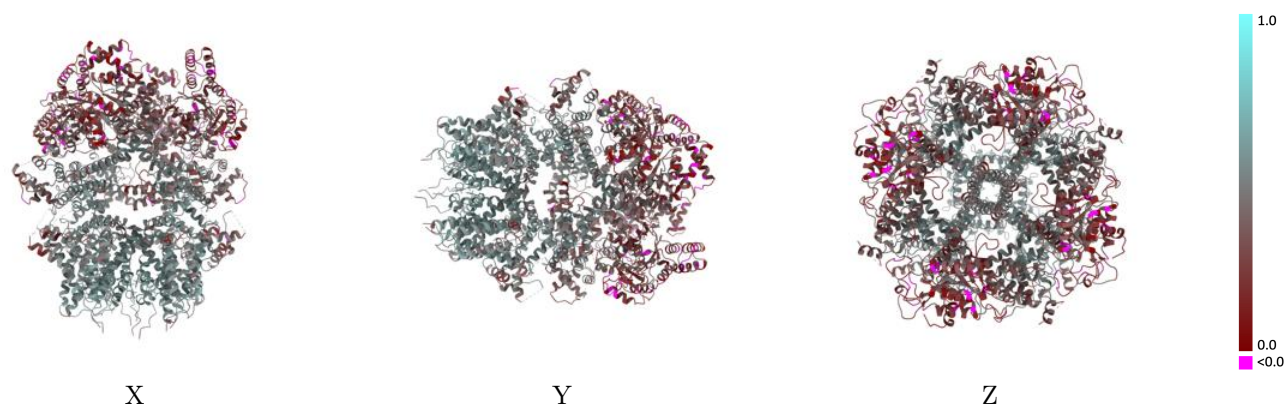
This section contains information regarding the fit between EMDB map EMD-53177 and PDB model 9QHQ. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



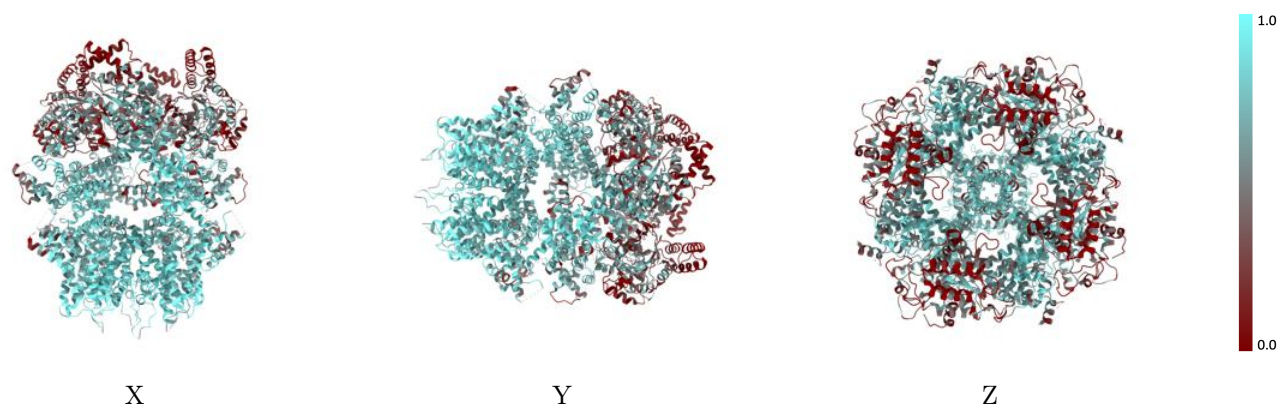
The images above show the 3D surface view of the map at the recommended contour level 0.0551 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



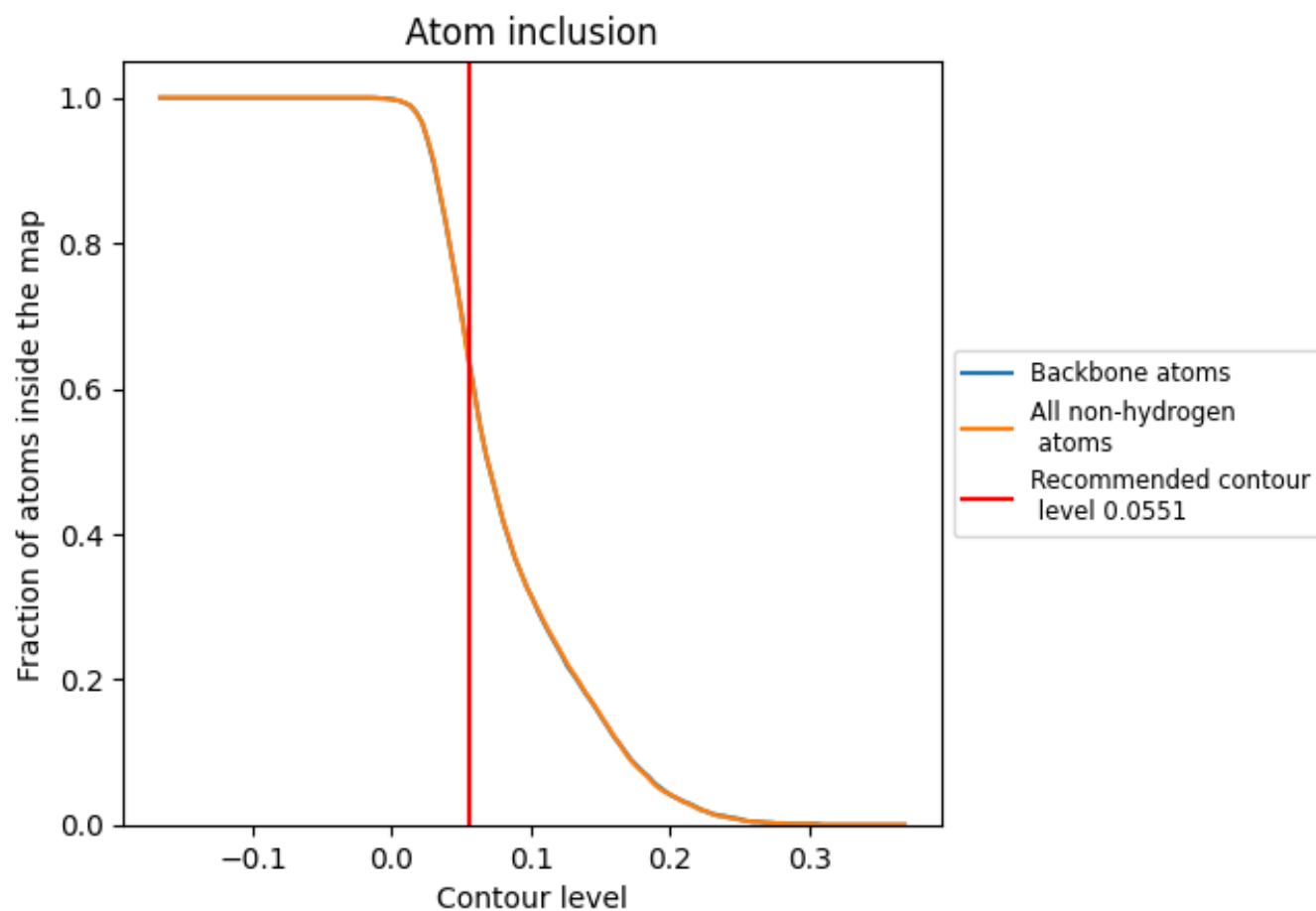
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0551).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 64% 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 (0.0551) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6400	0.4120
A	0.6400	0.4100
B	0.6430	0.4120
C	0.6430	0.4130
D	0.6440	0.4130

