



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 09:32 AM UTC

PDB ID : 9QHP / pdb_00009qhp
EMDB ID : EMD-53176
Title : Cryo-EM structure of mouse TRPM3 alpha 2 in complex with antagonist
Isosakuranetin
Authors : Shkumatov, A.V.; Schenck, S.; Brunner, J.D.
Deposited on : 2025-03-16
Resolution : 2.35 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:

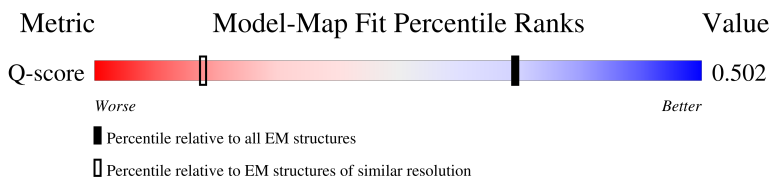
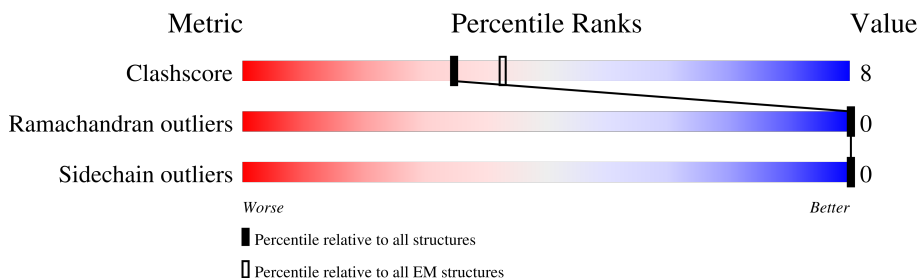
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.35 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	4607 (1.85 - 2.85)

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	10% 55% 11% 34%
1	B	1409	10% 54% 11% 34%
1	C	1409	10% 53% 13% 34%
1	D	1409	10% 53% 13% 34%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	YUV	A	1502	X	-	-	-
3	YUV	B	1503	X	-	-	-
3	YUV	C	1503	X	-	-	-
3	YUV	D	1503	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 61152 atoms, of which 30804 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	925	Total	C	H	N	O	S	0	0
			15109	4878	7603	1264	1308	56		
1	B	925	Total	C	H	N	O	S	0	0
			15109	4878	7603	1264	1308	56		
1	C	925	Total	C	H	N	O	S	0	0
			15109	4878	7603	1264	1308	56		
1	D	925	Total	C	H	N	O	S	0	0
			15109	4878	7603	1264	1308	56		

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

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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

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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

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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

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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

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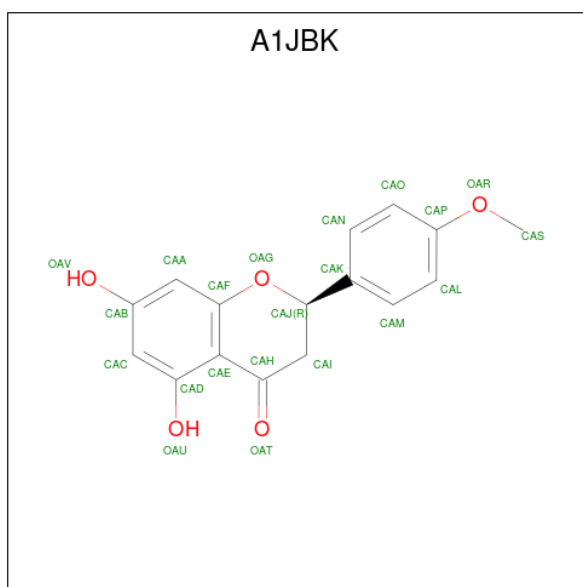
Chain	Residue	Modelled	Actual	Comment	Reference
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C	1402	PRO	-	expression tag	UNP Q69ZE8
C	1403	GLN	-	expression tag	UNP Q69ZE8
C	1404	GLY	-	expression tag	UNP Q69ZE8
C	1405	GLN	-	expression tag	UNP Q69ZE8
C	1406	ARG	-	expression tag	UNP Q69ZE8
C	1407	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

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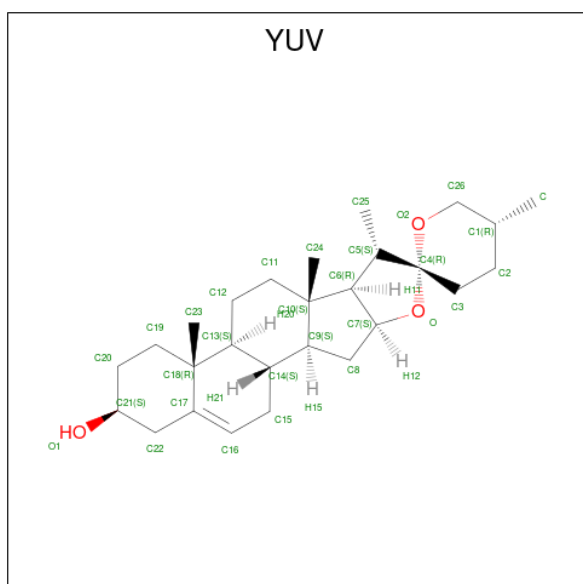
Chain	Residue	Modelled	Actual	Comment	Reference
D	1377	GLY	-	expression tag	UNP Q69ZE8
D	1378	TRP	-	expression tag	UNP Q69ZE8
D	1379	ARG	-	expression tag	UNP Q69ZE8
D	1380	GLY	-	expression tag	UNP Q69ZE8
D	1381	GLY	-	expression tag	UNP Q69ZE8
D	1382	HIS	-	expression tag	UNP Q69ZE8
D	1383	VAL	-	expression 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-(4-methoxyphenyl)-5,7-bis(oxidanyl)-2,3-dihydrochromen-4-one (CCD ID: A1JBK) (formula: C₁₆H₁₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	H	O	0
			35	16	14	5	
2	B	1	Total	C	H	O	0
			35	16	14	5	
2	C	1	Total	C	H	O	0
			35	16	14	5	
2	D	1	Total	C	H	O	0
			35	16	14	5	

- Molecule 3 is (25R)-14beta,17beta-spirost-5-en-3beta-ol (CCD ID: YUV) (formula: $C_{27}H_{42}O_3$).

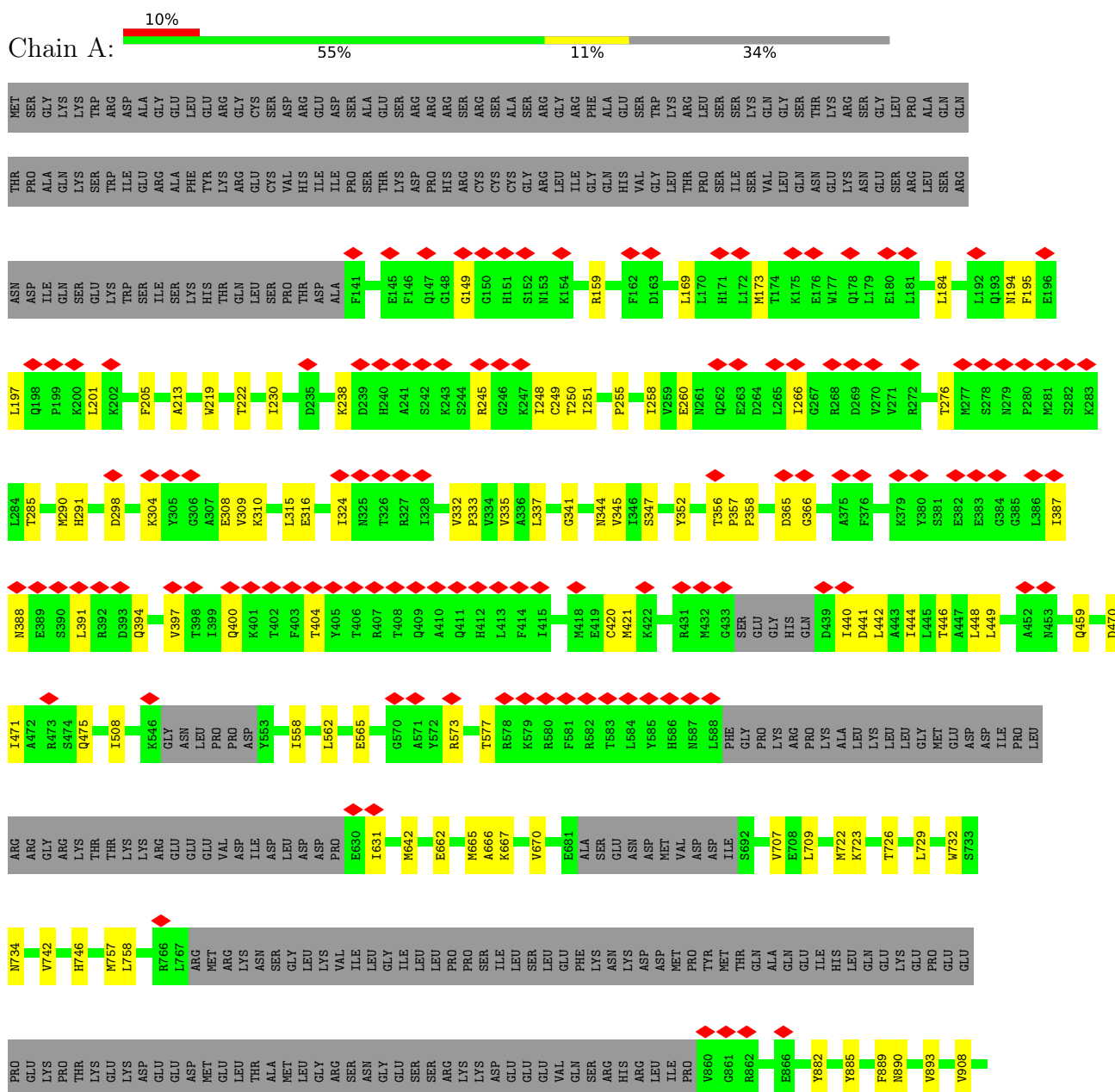


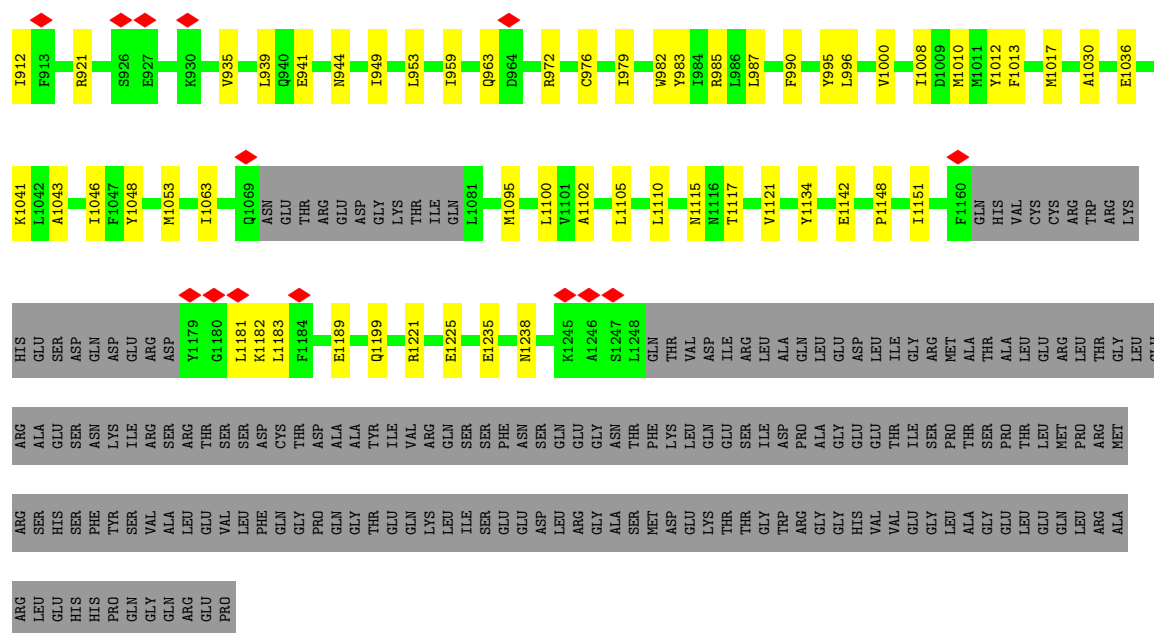
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	H	O	0
			72	27	42	3	
3	A	1	Total	C	H	O	0
			72	27	42	3	
3	B	1	Total	C	H	O	0
			72	27	42	3	
3	B	1	Total	C	H	O	0
			72	27	42	3	
3	C	1	Total	C	H	O	0
			72	27	42	3	
3	C	1	Total	C	H	O	0
			72	27	42	3	
3	D	1	Total	C	H	O	0
			72	27	42	3	
3	D	1	Total	C	H	O	0
			72	27	42	3	

3 Residue-property plots

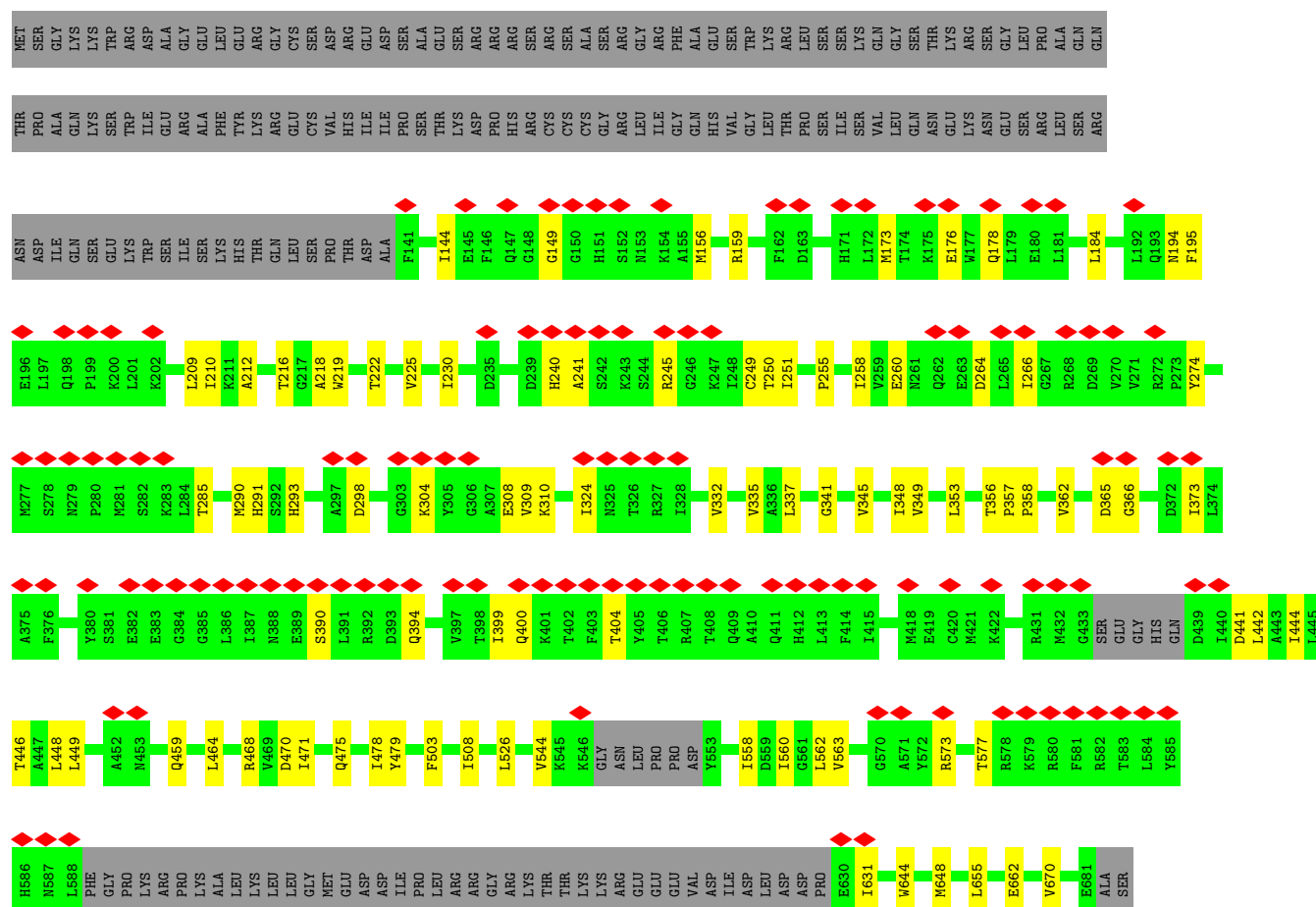
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

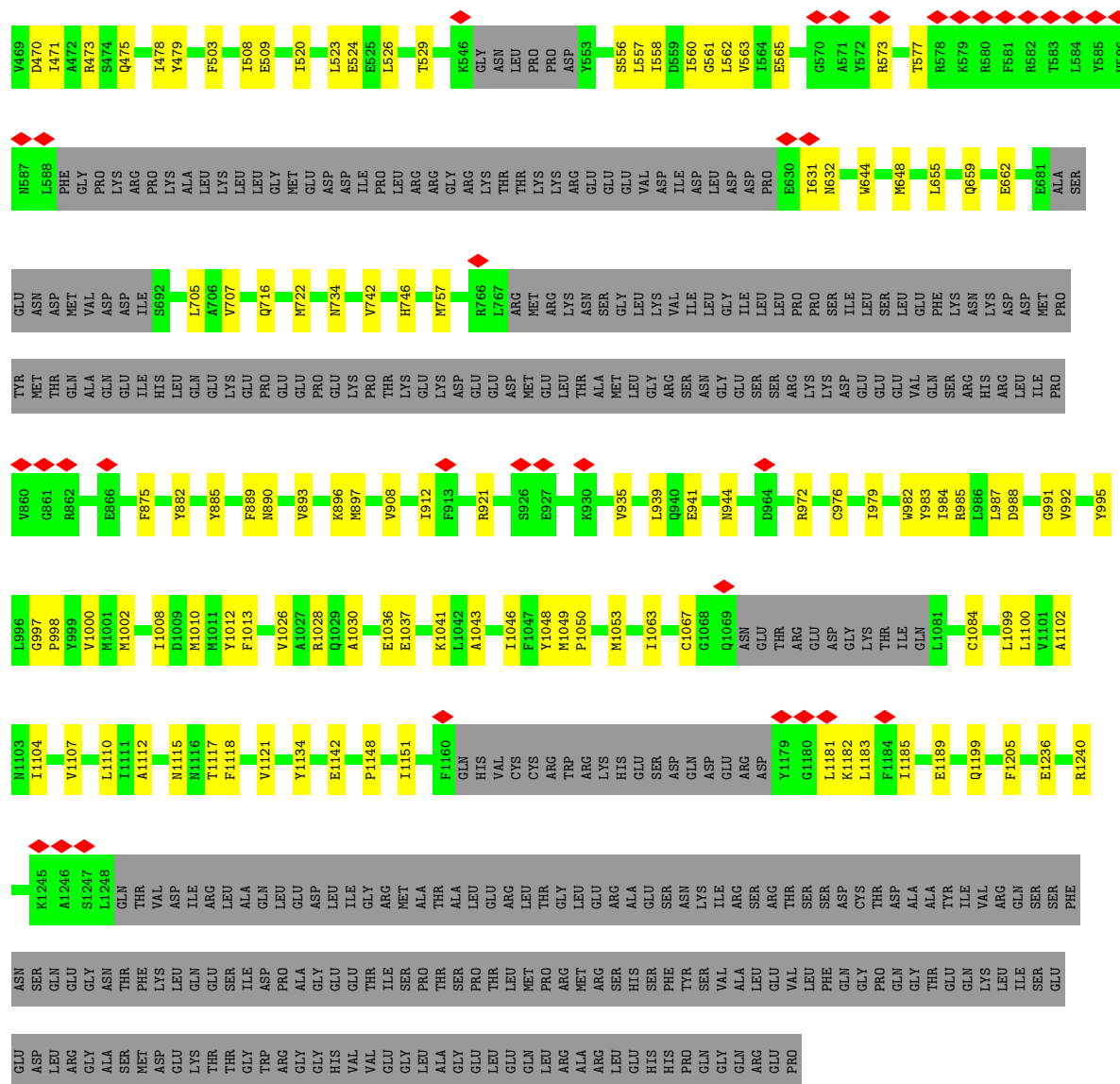
• Molecule 1: MKIAA1616 protein



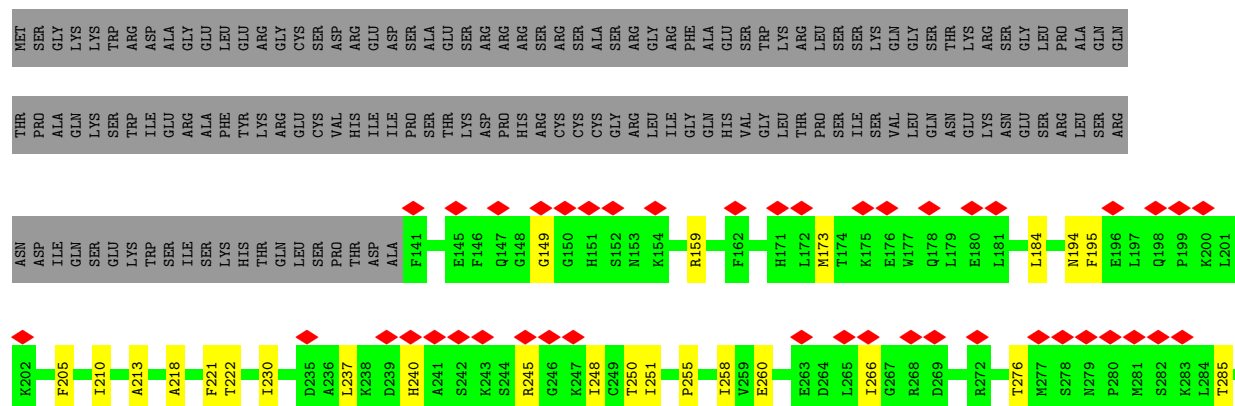


• Molecule 1: MKIAA1616 protein





• 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	281282	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)	700	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.108	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	347.0, 347.0, 347.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.694, 0.694, 0.694	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: YUV, A1JBK

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	0.13	0/7677	0.30	0/10374
1	B	0.13	0/7677	0.31	0/10374
1	C	0.13	0/7677	0.31	0/10374
1	D	0.15	0/7677	0.32	0/10374
All	All	0.14	0/30708	0.31	0/41496

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	7506	7603	7628	128	0
1	B	7506	7603	7628	122	0
1	C	7506	7603	7628	132	0
1	D	7506	7603	7628	142	0
2	A	21	14	0	0	0
2	B	21	14	0	0	0
2	C	21	14	0	0	0
2	D	21	14	0	0	0
3	A	60	84	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	60	84	0	0	0
3	C	60	84	0	0	0
3	D	60	84	0	1	0
All	All	30348	30804	30512	485	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 (485) 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:D:576:TYR:OH	1:D:640:GLU:OE1	1.84	0.95
1:A:173:MET:HE3	1:A:251:ILE:HD13	1.55	0.88
1:A:1221:ARG:NH1	1:A:1225:GLU:OE2	2.11	0.82
1:B:212:ALA:O	1:B:216:THR:OG1	1.98	0.81
1:C:573:ARG:NH2	1:C:577:THR:O	2.16	0.79
1:C:523:LEU:HD22	1:C:557:LEU:HD21	1.67	0.77
1:B:260:GLU:N	1:B:285:THR:O	2.18	0.77
1:A:388:ASN:OD1	1:A:391:LEU:HD23	1.85	0.76
1:B:526:LEU:O	1:B:648:MET:HE1	1.86	0.75
1:A:213:ALA:HB1	1:A:248:ILE:HD11	1.69	0.74
1:D:573:ARG:NH2	1:D:577:THR:O	2.21	0.74
1:B:1221:ARG:NH1	1:B:1225:GLU:OE2	2.21	0.74
1:D:213:ALA:HB1	1:D:248:ILE:HD11	1.69	0.73
1:C:523:LEU:CD2	1:C:557:LEU:HD21	2.19	0.73
1:D:523:LEU:HD22	1:D:557:LEU:HD21	1.70	0.73
1:C:260:GLU:N	1:C:285:THR:O	2.22	0.72
1:C:734:ASN:O	1:C:1182:LYS:NZ	2.22	0.71
1:A:245:ARG:NH2	1:D:1199:GLN:O	2.24	0.70
1:D:662:GLU:OE1	1:D:662:GLU:N	2.24	0.70
1:A:222:THR:HG22	1:A:230:ILE:HD12	1.73	0.70
1:A:889:PHE:HD1	1:A:908:VAL:HG11	1.56	0.70
1:B:889:PHE:CD1	1:B:908:VAL:HG11	2.27	0.70
1:B:889:PHE:HD1	1:B:908:VAL:HG11	1.57	0.70
1:A:260:GLU:N	1:A:285:THR:O	2.23	0.69
1:B:173:MET:HE3	1:B:219:TRP:CZ3	2.26	0.69
1:C:889:PHE:HD1	1:C:908:VAL:HG11	1.59	0.68
1:A:889:PHE:CD1	1:A:908:VAL:HG11	2.28	0.68
1:B:921:ARG:NH2	1:B:1142:GLU:OE1	2.27	0.68
1:A:400:GLN:O	1:A:404:THR:N	2.27	0.67
1:C:890:ASN:HD22	1:D:1026:VAL:HG11	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:921:ARG:NH2	1:C:1142:GLU:OE1	2.28	0.67
1:D:501:VAL:HG21	1:D:652:LYS:HB3	1.77	0.67
1:A:316:GLU:OE1	1:A:352:TYR:OH	2.12	0.67
1:D:400:GLN:O	1:D:404:THR:N	2.27	0.67
1:C:358:PRO:HB2	1:C:426:LEU:HD21	1.75	0.66
1:A:987:LEU:HD11	1:A:1000:VAL:HG22	1.76	0.66
1:D:921:ARG:NH2	1:D:1142:GLU:OE1	2.29	0.66
1:D:987:LEU:HD11	1:D:1000:VAL:HG22	1.77	0.66
1:C:889:PHE:CD1	1:C:908:VAL:HG11	2.31	0.66
1:A:1148:PRO:O	1:A:1151:ILE:HG22	1.96	0.66
1:B:890:ASN:HD22	1:C:1026:VAL:HG11	1.61	0.66
1:B:885:TYR:OH	1:B:912:ILE:HD11	1.97	0.65
1:D:885:TYR:OH	1:D:912:ILE:HD11	1.96	0.65
1:D:889:PHE:CD1	1:D:908:VAL:HG11	2.30	0.65
1:A:573:ARG:NH2	1:A:577:THR:O	2.29	0.65
1:B:987:LEU:HD11	1:B:1000:VAL:HG22	1.77	0.65
1:D:260:GLU:N	1:D:285:THR:O	2.29	0.65
1:D:523:LEU:CD2	1:D:557:LEU:HD21	2.27	0.64
1:D:734:ASN:O	1:D:1182:LYS:NZ	2.28	0.64
1:B:144:ILE:HD11	1:B:274:TYR:CG	2.32	0.64
1:B:194:ASN:OD1	1:B:195:PHE:N	2.30	0.64
1:C:400:GLN:O	1:C:404:THR:N	2.30	0.64
1:D:1148:PRO:O	1:D:1151:ILE:HG22	1.98	0.64
1:A:391:LEU:HD13	1:A:394:GLN:NE2	2.13	0.64
1:C:885:TYR:OH	1:C:912:ILE:HD11	1.98	0.64
1:C:1199:GLN:O	1:D:245:ARG:NH2	2.30	0.63
1:B:442:LEU:O	1:B:446:THR:HG23	1.99	0.63
1:A:1199:GLN:O	1:B:245:ARG:NH2	2.32	0.63
1:D:665:MET:HB2	1:D:709:LEU:HD23	1.81	0.63
1:A:921:ARG:NH2	1:A:1142:GLU:OE1	2.32	0.63
1:A:885:TYR:OH	1:A:912:ILE:HD11	1.98	0.63
1:C:987:LEU:HD11	1:C:1000:VAL:HG22	1.79	0.62
1:A:194:ASN:OD1	1:A:195:PHE:N	2.32	0.62
1:B:885:TYR:HE1	1:B:908:VAL:HG13	1.64	0.62
1:B:717:ASP:OD1	1:B:718:GLU:N	2.33	0.62
1:C:194:ASN:OD1	1:C:195:PHE:N	2.32	0.62
1:A:421:MET:N	1:A:421:MET:HE2	2.15	0.62
1:A:885:TYR:HE1	1:A:908:VAL:HG13	1.64	0.62
1:B:644:TRP:NE1	1:B:648:MET:SD	2.73	0.61
1:B:1148:PRO:O	1:B:1151:ILE:HG22	2.00	0.61
1:B:734:ASN:O	1:B:1182:LYS:NZ	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1117:THR:O	1:A:1121:VAL:HG23	2.01	0.61
1:B:400:GLN:O	1:B:404:THR:N	2.33	0.61
1:A:959:ILE:O	1:A:963:GLN:NE2	2.31	0.60
1:B:144:ILE:HD11	1:B:274:TYR:CB	2.31	0.60
1:C:885:TYR:HE1	1:C:908:VAL:HG13	1.65	0.60
1:A:446:THR:OG1	1:A:475:GLN:NE2	2.34	0.60
1:C:716:GLN:NE2	1:C:1199:GLN:OE1	2.33	0.60
1:B:335:VAL:HG11	1:B:444:ILE:HG23	1.84	0.60
1:C:473:ARG:NH1	1:C:509:GLU:OE2	2.35	0.60
1:C:1117:THR:O	1:C:1121:VAL:HG23	2.02	0.60
1:D:449:LEU:HD11	1:D:471:ILE:CG2	2.32	0.59
1:D:501:VAL:HG22	1:D:653:MET:HE2	1.83	0.59
1:D:722:MET:HE2	1:D:757:MET:HE3	1.84	0.59
1:B:662:GLU:OE1	1:B:662:GLU:N	2.35	0.59
1:D:173:MET:SD	1:D:251:ILE:HD13	2.43	0.59
1:B:890:ASN:HD21	1:B:983:TYR:HE2	1.51	0.59
1:C:1148:PRO:O	1:C:1151:ILE:HG22	2.02	0.59
1:D:421:MET:HE2	1:D:421:MET:N	2.18	0.59
1:C:1048:TYR:OH	1:D:1063:ILE:O	2.19	0.59
1:D:356:THR:OG1	1:D:357:PRO:HD3	2.03	0.59
1:A:149:GLY:HA2	1:D:508:ILE:O	2.03	0.58
1:B:337:LEU:HD23	1:B:362:VAL:HB	1.86	0.58
1:D:194:ASN:OD1	1:D:195:PHE:N	2.36	0.58
1:D:1117:THR:O	1:D:1121:VAL:HG23	2.02	0.58
1:D:1043:ALA:HA	1:D:1046:ILE:HD12	1.86	0.58
1:B:558:ILE:O	1:B:562:LEU:HD23	2.03	0.58
1:B:470:ASP:OD1	1:B:471:ILE:N	2.37	0.58
1:C:1043:ALA:HA	1:C:1046:ILE:HD12	1.86	0.57
1:B:1183:LEU:HD12	1:B:1183:LEU:O	2.04	0.57
1:A:734:ASN:O	1:A:1182:LYS:NZ	2.31	0.57
1:C:631:ILE:HD12	1:C:631:ILE:H	1.69	0.57
1:B:1199:GLN:O	1:C:245:ARG:NH2	2.37	0.57
1:D:642:MET:HE1	1:D:667:LYS:HB3	1.86	0.57
1:D:714:TYR:CE1	1:D:757:MET:HE1	2.40	0.57
1:C:890:ASN:HD21	1:C:983:TYR:HE2	1.52	0.57
1:A:631:ILE:HD12	1:A:631:ILE:H	1.70	0.57
1:C:1028:ARG:NH1	1:C:1049:MET:SD	2.77	0.57
1:D:889:PHE:HD1	1:D:908:VAL:HG11	1.68	0.57
1:B:631:ILE:HD12	1:B:631:ILE:H	1.71	0.56
1:C:558:ILE:O	1:C:562:LEU:HD23	2.05	0.56
1:D:716:GLN:NE2	1:D:1199:GLN:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ASP:OD1	1:A:471:ILE:N	2.38	0.56
1:C:395:LEU:HD11	1:C:417:LEU:HD23	1.86	0.56
1:A:722:MET:CE	1:A:757:MET:HE3	2.34	0.56
1:A:890:ASN:HD21	1:A:983:TYR:HE2	1.54	0.56
1:D:159:ARG:NH1	1:D:298:ASP:OD2	2.38	0.56
1:A:642:MET:HE1	1:A:667:LYS:HB3	1.87	0.56
1:C:1010:MET:HG3	1:D:1105:LEU:HD13	1.86	0.56
1:A:250:THR:HG22	1:A:291:HIS:CD2	2.40	0.56
1:A:1010:MET:HG3	1:B:1105:LEU:HD13	1.88	0.56
1:D:631:ILE:HD12	1:D:631:ILE:H	1.70	0.56
1:A:987:LEU:CD1	1:A:1000:VAL:HG22	2.36	0.56
1:A:1063:ILE:HD11	1:A:1095:MET:HE1	1.88	0.56
1:C:335:VAL:HG11	1:C:444:ILE:HG23	1.89	0.55
1:A:356:THR:HB	1:A:357:PRO:HD3	1.88	0.55
1:B:324:ILE:CG2	1:B:332:VAL:HG22	2.36	0.55
1:A:558:ILE:O	1:A:562:LEU:HD23	2.06	0.55
1:D:885:TYR:HE1	1:D:908:VAL:HG13	1.70	0.55
1:A:238:LYS:HA	1:A:290:MET:HE2	1.89	0.55
1:D:987:LEU:CD1	1:D:1000:VAL:HG22	2.36	0.55
1:C:1185:ILE:HD11	1:C:1189:GLU:OE1	2.07	0.55
1:B:562:LEU:HD22	1:B:577:THR:CG2	2.37	0.54
1:A:308:GLU:N	1:A:308:GLU:OE1	2.41	0.54
1:B:897:MET:HE3	1:B:972:ARG:HG3	1.90	0.54
1:A:1063:ILE:O	1:D:1048:TYR:OH	2.25	0.54
1:C:324:ILE:CG2	1:C:332:VAL:HG22	2.36	0.54
1:D:258:ILE:HD11	1:D:304:LYS:O	2.08	0.54
1:D:558:ILE:O	1:D:562:LEU:HD23	2.07	0.54
1:B:987:LEU:CD1	1:B:1000:VAL:HG22	2.38	0.54
1:A:391:LEU:O	1:A:394:GLN:HG2	2.07	0.54
1:C:356:THR:HB	1:C:357:PRO:HD3	1.89	0.54
1:D:993:ASN:OD1	1:D:994:LYS:N	2.41	0.54
1:B:544:VAL:HG11	1:B:562:LEU:HB3	1.88	0.54
1:B:1048:TYR:OH	1:C:1063:ILE:O	2.25	0.54
1:B:308:GLU:N	1:B:308:GLU:OE1	2.40	0.54
1:A:324:ILE:CG2	1:A:332:VAL:HG22	2.38	0.54
1:C:255:PRO:CG	1:C:258:ILE:HD13	2.38	0.54
1:A:665:MET:HB2	1:A:709:LEU:HD23	1.89	0.53
1:A:1235:GLU:OE2	1:D:1233:ARG:NE	2.41	0.53
1:C:308:GLU:N	1:C:308:GLU:OE1	2.41	0.53
1:A:890:ASN:HD22	1:B:1026:VAL:HG11	1.73	0.53
1:A:1048:TYR:OH	1:B:1063:ILE:O	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:MET:CE	1:A:251:ILE:HD13	2.33	0.53
1:A:508:ILE:O	1:B:149:GLY:HA2	2.09	0.53
1:C:222:THR:HG22	1:C:230:ILE:HD12	1.91	0.53
1:D:308:GLU:N	1:D:308:GLU:OE1	2.41	0.53
1:C:446:THR:OG1	1:C:475:GLN:NE2	2.42	0.53
1:C:1115:ASN:ND2	1:D:1115:ASN:OD1	2.41	0.53
1:A:258:ILE:HD11	1:A:304:LYS:O	2.09	0.53
1:B:1115:ASN:OD1	1:C:1112:ALA:HA	2.09	0.53
1:D:707:VAL:HG23	1:D:746:HIS:CE1	2.44	0.53
1:A:1105:LEU:HD13	1:D:1010:MET:HG3	1.90	0.53
1:B:1010:MET:HE1	1:C:1104:ILE:HG21	1.89	0.53
1:B:255:PRO:CG	1:B:258:ILE:HD13	2.39	0.52
1:D:649:LYS:O	1:D:649:LYS:HG2	2.09	0.52
1:B:893:VAL:O	1:B:972:ARG:NH2	2.42	0.52
1:D:358:PRO:CB	1:D:426:LEU:HD21	2.40	0.52
1:D:442:LEU:O	1:D:446:THR:HG23	2.09	0.52
1:A:893:VAL:O	1:A:972:ARG:NH2	2.42	0.52
1:B:573:ARG:NH2	1:B:577:THR:O	2.43	0.52
1:B:222:THR:HG22	1:B:230:ILE:HD12	1.91	0.52
1:B:356:THR:HB	1:B:357:PRO:HD3	1.92	0.52
1:C:987:LEU:CD1	1:C:1000:VAL:HG22	2.39	0.52
1:D:324:ILE:CG2	1:D:332:VAL:HG22	2.39	0.52
1:A:1017:MET:HE1	1:A:1102:ALA:HB2	1.92	0.52
1:D:222:THR:HG22	1:D:230:ILE:HD12	1.92	0.52
1:A:255:PRO:CG	1:A:258:ILE:HD13	2.39	0.52
1:A:882:TYR:OH	1:A:982:TRP:O	2.24	0.51
1:B:1010:MET:CE	1:C:1100:LEU:HD11	2.40	0.51
1:C:258:ILE:HD11	1:C:304:LYS:O	2.11	0.51
1:B:159:ARG:NH2	1:B:298:ASP:OD2	2.37	0.51
1:B:882:TYR:OH	1:B:982:TRP:O	2.21	0.51
1:C:520:ILE:HD12	1:C:632:ASN:O	2.10	0.51
1:A:159:ARG:NH2	1:A:298:ASP:OD2	2.41	0.51
1:D:255:PRO:CG	1:D:258:ILE:HD13	2.41	0.51
1:D:365:ASP:OD1	1:D:366:GLY:N	2.44	0.51
1:A:1030:ALA:O	1:D:972:ARG:NH1	2.41	0.50
1:A:255:PRO:HG2	1:A:258:ILE:HD13	1.93	0.50
1:D:250:THR:HG22	1:D:291:HIS:CD2	2.45	0.50
1:D:258:ILE:HD11	1:D:304:LYS:C	2.36	0.50
1:D:644:TRP:NE1	1:D:648:MET:SD	2.84	0.50
1:A:885:TYR:CE1	1:A:908:VAL:HG13	2.45	0.50
1:A:1043:ALA:HA	1:A:1046:ILE:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1100:LEU:CD1	1:D:1010:MET:HE1	2.42	0.50
1:D:255:PRO:HG2	1:D:258:ILE:HD13	1.92	0.50
1:D:373:ILE:HD12	1:D:399:ILE:HD13	1.93	0.50
1:A:365:ASP:OD1	1:A:366:GLY:N	2.44	0.50
1:B:935:VAL:O	1:B:939:LEU:HD23	2.11	0.50
1:C:337:LEU:HD11	1:C:440:ILE:HD11	1.93	0.50
1:A:173:MET:HE2	1:A:219:TRP:CZ3	2.47	0.50
1:A:238:LYS:CA	1:A:290:MET:HE2	2.41	0.50
1:B:1043:ALA:HA	1:B:1046:ILE:HD12	1.93	0.50
1:A:1017:MET:HE1	1:A:1102:ALA:CB	2.42	0.50
1:C:159:ARG:NH2	1:C:298:ASP:OD2	2.38	0.50
1:C:707:VAL:HG23	1:C:746:HIS:CE1	2.47	0.50
1:B:562:LEU:HD22	1:B:577:THR:HG22	1.94	0.50
1:D:520:ILE:HG23	1:D:557:LEU:HD12	1.93	0.50
1:D:520:ILE:HD12	1:D:632:ASN:O	2.12	0.50
1:D:420:CYS:C	1:D:421:MET:HE2	2.37	0.50
1:B:365:ASP:OD1	1:B:366:GLY:N	2.45	0.49
1:C:373:ILE:HD12	1:C:399:ILE:HD13	1.94	0.49
1:D:344:ASN:ND2	1:D:344:ASN:O	2.44	0.49
1:A:1238:ASN:ND2	1:D:1236:GLU:OE1	2.44	0.49
1:D:276:THR:HG22	1:D:276:THR:O	2.11	0.49
1:A:337:LEU:HD11	1:A:440:ILE:HD11	1.94	0.49
1:A:341:GLY:CA	1:A:345:VAL:HG21	2.42	0.49
1:A:1036:GLU:OE1	1:A:1041:LYS:NZ	2.30	0.49
1:A:1100:LEU:HD11	1:D:1010:MET:HE1	1.95	0.49
1:B:941:GLU:OE1	1:B:944:ASN:N	2.45	0.49
1:A:249:CYS:SG	1:A:251:ILE:HD11	2.53	0.49
1:A:276:THR:O	1:A:276:THR:HG22	2.11	0.49
1:C:508:ILE:O	1:D:149:GLY:HA2	2.13	0.49
1:D:1181:LEU:HD11	1:D:1182:LYS:HE3	1.94	0.49
1:A:258:ILE:HD11	1:A:304:LYS:C	2.38	0.49
1:A:976:CYS:O	1:A:979:ILE:HG22	2.13	0.48
1:C:896:LYS:NZ	1:D:1037:GLU:OE1	2.39	0.48
1:C:1002:MET:HE1	1:C:1118:PHE:CE1	2.47	0.48
1:D:893:VAL:O	1:D:972:ARG:NH2	2.46	0.48
1:B:896:LYS:NZ	1:C:1037:GLU:OE1	2.39	0.48
1:C:893:VAL:O	1:C:972:ARG:NH2	2.47	0.48
1:A:344:ASN:O	1:A:347:SER:OG	2.22	0.48
1:B:508:ILE:O	1:C:149:GLY:HA2	2.13	0.48
1:C:341:GLY:CA	1:C:345:VAL:HG21	2.43	0.48
1:B:373:ILE:HD12	1:B:399:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:GLY:CA	1:D:345:VAL:HG21	2.44	0.48
1:D:642:MET:HE1	1:D:667:LYS:CB	2.44	0.48
1:A:344:ASN:O	1:A:344:ASN:ND2	2.46	0.48
1:C:941:GLU:OE1	1:C:944:ASN:N	2.44	0.48
1:D:1026:VAL:HG22	1:D:1046:ILE:HG12	1.95	0.48
1:A:1012:TYR:CD2	1:D:995:TYR:CD2	3.02	0.48
1:B:885:TYR:CE1	1:B:908:VAL:HG13	2.46	0.48
1:C:169:LEU:HD22	1:C:315:LEU:HD22	1.95	0.48
1:D:357:PRO:O	1:D:358:PRO:C	2.56	0.48
1:C:885:TYR:CE1	1:C:908:VAL:HG13	2.45	0.47
1:D:935:VAL:O	1:D:939:LEU:HD23	2.14	0.47
1:A:670:VAL:HG11	1:A:732:TRP:CZ3	2.50	0.47
1:A:723:LYS:NZ	1:A:1189:GLU:OE2	2.43	0.47
1:B:356:THR:O	1:B:358:PRO:HD3	2.15	0.47
1:A:388:ASN:OD1	1:A:391:LEU:HB2	2.15	0.47
1:B:241:ALA:HB3	1:B:290:MET:HE2	1.97	0.47
1:C:935:VAL:O	1:C:939:LEU:HD23	2.15	0.47
1:A:642:MET:HE1	1:A:667:LYS:CB	2.44	0.47
1:C:258:ILE:HD11	1:C:304:LYS:C	2.40	0.47
1:C:344:ASN:O	1:C:347:SER:OG	2.24	0.47
1:D:1008:ILE:HD12	1:D:1008:ILE:H	1.79	0.47
1:D:1018:LEU:O	1:D:1022:MET:HG3	2.15	0.47
1:A:1053:MET:HE2	1:A:1095:MET:HE3	1.96	0.47
1:B:258:ILE:HD11	1:B:304:LYS:O	2.15	0.47
1:B:1018:LEU:O	1:B:1022:MET:HG3	2.15	0.47
1:C:341:GLY:HA3	1:C:345:VAL:HG21	1.97	0.47
1:D:677:ALA:O	1:D:681:GLU:OE1	2.32	0.47
1:B:1067:CYS:HB3	1:B:1084:CYS:HB2	1.78	0.47
1:C:991:GLY:HA2	1:C:997:GLY:HA2	1.97	0.47
1:A:995:TYR:CD2	1:B:1012:TYR:CD2	3.03	0.47
1:B:225:VAL:O	1:B:230:ILE:HG21	2.15	0.47
1:C:255:PRO:HG2	1:C:258:ILE:HD13	1.96	0.47
1:D:720:LEU:HD22	1:D:1196:PHE:CG	2.50	0.47
1:D:726:THR:CG2	1:D:758:LEU:HD21	2.45	0.47
1:D:890:ASN:HD22	3:D:1503:YUV:C3	2.28	0.47
1:D:897:MET:HE2	1:D:972:ARG:HG3	1.96	0.47
1:C:897:MET:HE2	1:C:972:ARG:HG3	1.96	0.46
1:A:726:THR:CG2	1:A:758:LEU:HD21	2.45	0.46
1:B:258:ILE:HG22	1:B:258:ILE:O	2.16	0.46
1:C:662:GLU:N	1:C:662:GLU:OE1	2.48	0.46
1:C:722:MET:CE	1:C:757:MET:HE2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1036:GLU:OE1	1:C:1041:LYS:NZ	2.31	0.46
1:D:213:ALA:CB	1:D:248:ILE:HD11	2.43	0.46
1:A:213:ALA:CB	1:A:248:ILE:HD11	2.43	0.46
1:B:255:PRO:HG2	1:B:258:ILE:HD13	1.97	0.46
1:D:344:ASN:ND2	1:D:347:SER:OG	2.46	0.46
1:A:935:VAL:O	1:A:939:LEU:HD23	2.15	0.46
1:C:562:LEU:HD22	1:C:577:THR:CG2	2.46	0.46
1:C:976:CYS:O	1:C:979:ILE:HG22	2.16	0.46
1:C:250:THR:HG22	1:C:291:HIS:CD2	2.50	0.46
1:C:276:THR:O	1:C:276:THR:HG22	2.16	0.46
1:D:486:GLY:O	1:D:490:GLN:OE1	2.33	0.46
1:C:998:PRO:O	1:C:1002:MET:HG3	2.15	0.46
1:D:560:ILE:HA	1:D:563:VAL:HG12	1.97	0.46
1:B:1017:MET:HE1	1:B:1102:ALA:CB	2.46	0.46
1:C:1026:VAL:HG22	1:C:1046:ILE:HG12	1.98	0.46
1:C:995:TYR:CD2	1:D:1012:TYR:CD2	3.03	0.46
1:D:373:ILE:HG23	1:D:399:ILE:HD11	1.98	0.46
1:A:666:ALA:HB2	1:A:729:LEU:HD11	1.97	0.46
1:C:258:ILE:O	1:C:258:ILE:HG22	2.16	0.46
1:C:145:GLU:HG3	1:C:147:GLN:NE2	2.31	0.45
1:C:644:TRP:O	1:C:648:MET:HG2	2.16	0.45
1:D:885:TYR:CE1	1:D:908:VAL:HG13	2.48	0.45
1:A:726:THR:HG21	1:A:758:LEU:HD11	1.97	0.45
1:C:224:GLY:O	1:C:288:ASN:OD1	2.34	0.45
1:B:441:ASP:OD1	1:B:442:LEU:N	2.49	0.45
1:D:1183:LEU:HD12	1:D:1183:LEU:O	2.16	0.45
1:B:249:CYS:SG	1:B:251:ILE:HD11	2.56	0.45
1:A:205:PHE:CE2	1:A:337:LEU:HD21	2.52	0.45
1:D:875:PHE:CE1	1:D:992:VAL:HG21	2.51	0.45
1:A:387:ILE:HG23	1:A:391:LEU:CB	2.47	0.45
1:D:344:ASN:O	1:D:347:SER:OG	2.23	0.45
1:D:890:ASN:OD1	1:D:979:ILE:HD11	2.16	0.45
1:C:468:ARG:NH2	1:C:470:ASP:OD1	2.50	0.45
1:D:221:PHE:HE1	1:D:251:ILE:HD12	1.82	0.45
1:D:335:VAL:HG11	1:D:444:ILE:CG2	2.45	0.45
1:A:449:LEU:HD11	1:A:471:ILE:CG2	2.47	0.45
1:A:197:LEU:HD22	1:A:201:LEU:HD23	1.99	0.45
1:B:1002:MET:HE1	1:B:1118:PHE:CE1	2.52	0.45
1:C:707:VAL:HG23	1:C:746:HIS:HE1	1.81	0.45
1:A:420:CYS:C	1:A:421:MET:HE2	2.41	0.44
1:B:341:GLY:HA3	1:B:345:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:972:ARG:NH1	1:D:1030:ALA:O	2.42	0.44
1:D:1221:ARG:NH1	1:D:1225:GLU:OE2	2.50	0.44
1:C:526:LEU:O	1:C:529:THR:HG22	2.17	0.44
1:A:662:GLU:N	1:A:662:GLU:OE1	2.51	0.44
1:C:1067:CYS:HB3	1:C:1084:CYS:HB2	1.85	0.44
1:D:335:VAL:HG11	1:D:444:ILE:HG23	1.99	0.44
1:D:527:TYR:HA	1:D:648:MET:CE	2.47	0.44
1:A:356:THR:O	1:A:358:PRO:HD3	2.18	0.44
1:A:707:VAL:HG23	1:A:746:HIS:CE1	2.53	0.44
1:B:264:ASP:C	1:B:264:ASP:OD2	2.61	0.44
1:B:357:PRO:O	1:B:358:PRO:C	2.61	0.44
1:B:877:PHE:CE2	1:B:1147:PRO:HD3	2.53	0.44
1:C:1102:ALA:O	1:C:1107:VAL:HG23	2.17	0.44
1:A:258:ILE:HG22	1:A:258:ILE:O	2.17	0.44
1:A:441:ASP:OD1	1:A:442:LEU:N	2.49	0.44
1:C:449:LEU:HD22	1:C:459:GLN:HG3	1.99	0.44
1:B:173:MET:HE3	1:B:219:TRP:CH2	2.52	0.44
1:C:230:ILE:CG2	1:C:288:ASN:OD1	2.66	0.44
1:A:1115:ASN:ND2	1:B:1115:ASN:HD22	2.16	0.44
1:C:655:LEU:CD2	1:C:705:LEU:HD11	2.48	0.44
1:C:882:TYR:OH	1:C:982:TRP:O	2.33	0.44
1:A:266:ILE:HG22	1:A:266:ILE:O	2.18	0.43
1:B:258:ILE:HG22	1:B:285:THR:HG22	2.00	0.43
1:B:324:ILE:HG22	1:B:332:VAL:HG22	2.00	0.43
1:B:446:THR:HG22	1:B:475:GLN:NE2	2.33	0.43
1:C:882:TYR:OH	1:C:985:ARG:HB3	2.18	0.43
1:D:882:TYR:OH	1:D:985:ARG:HB3	2.18	0.43
1:A:1053:MET:CE	1:A:1095:MET:HE3	2.48	0.43
1:C:210:ILE:HG21	1:C:240:HIS:CG	2.53	0.43
1:D:210:ILE:HG21	1:D:240:HIS:CG	2.53	0.43
1:B:309:VAL:HG13	1:B:310:LYS:N	2.34	0.43
1:B:478:ILE:HG22	1:B:479:TYR:N	2.33	0.43
1:C:449:LEU:HD11	1:C:471:ILE:CG2	2.49	0.43
1:C:659:GLN:HG2	1:C:1205:PHE:CZ	2.53	0.43
1:D:358:PRO:HB3	1:D:426:LEU:HD21	1.98	0.43
1:A:670:VAL:HG21	1:A:732:TRP:CE3	2.53	0.43
1:C:1236:GLU:OE2	1:C:1240:ARG:HD2	2.19	0.43
1:D:337:LEU:HD11	1:D:440:ILE:HD11	2.01	0.43
1:A:449:LEU:HD22	1:A:459:GLN:HG3	2.00	0.43
1:B:707:VAL:HG23	1:B:746:HIS:NE2	2.33	0.43
1:B:882:TYR:OH	1:B:985:ARG:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:ASP:OD1	1:C:366:GLY:N	2.52	0.43
1:C:560:ILE:HA	1:C:563:VAL:HG12	2.00	0.43
1:A:344:ASN:C	1:A:344:ASN:HD22	2.26	0.43
1:B:250:THR:HG22	1:B:291:HIS:CD2	2.52	0.43
1:B:449:LEU:HD22	1:B:459:GLN:HG3	2.01	0.43
1:C:875:PHE:CE1	1:C:992:VAL:HG21	2.53	0.43
1:C:1008:ILE:HD12	1:C:1008:ILE:H	1.83	0.43
1:D:258:ILE:O	1:D:258:ILE:HG22	2.19	0.43
1:D:1120:GLU:O	1:D:1124:ILE:HD12	2.18	0.43
1:A:309:VAL:HG13	1:A:310:LYS:N	2.34	0.43
1:A:1046:ILE:HD11	1:D:894:LEU:HD11	2.01	0.43
1:A:335:VAL:HG11	1:A:444:ILE:HG23	2.00	0.43
1:B:210:ILE:HG21	1:B:240:HIS:CG	2.54	0.43
1:B:345:VAL:HA	1:B:348:ILE:HG22	2.01	0.43
1:B:373:ILE:HG23	1:B:399:ILE:HD11	2.01	0.43
1:B:390:SER:O	1:B:394:GLN:HG3	2.19	0.43
1:D:309:VAL:HG13	1:D:310:LYS:N	2.34	0.43
1:B:335:VAL:HG11	1:B:444:ILE:CG2	2.47	0.43
1:D:468:ARG:NH2	1:D:470:ASP:OD1	2.52	0.43
1:A:562:LEU:HD22	1:A:577:THR:CG2	2.49	0.43
1:B:995:TYR:CD2	1:C:1012:TYR:CD2	3.07	0.43
1:D:324:ILE:HG22	1:D:332:VAL:HG22	2.00	0.43
1:B:1203:GLU:OE1	1:C:245:ARG:NH1	2.53	0.42
1:C:143:THR:HG22	1:C:144:ILE:N	2.34	0.42
1:C:441:ASP:OD1	1:C:442:LEU:N	2.50	0.42
1:C:742:VAL:HG21	1:C:1134:TYR:CD1	2.54	0.42
1:A:1181:LEU:HD11	1:A:1182:LYS:HE3	2.00	0.42
1:B:258:ILE:HD11	1:B:304:LYS:C	2.45	0.42
1:D:205:PHE:CE2	1:D:337:LEU:HD21	2.53	0.42
1:B:449:LEU:HD11	1:B:471:ILE:CG2	2.49	0.42
1:D:527:TYR:HA	1:D:648:MET:HE1	2.01	0.42
1:D:1109:LEU:O	1:D:1113:VAL:HG23	2.20	0.42
1:B:464:LEU:HD23	1:B:503:PHE:CD2	2.54	0.42
1:C:464:LEU:HD23	1:C:503:PHE:CD2	2.54	0.42
1:C:478:ILE:HG22	1:C:479:TYR:N	2.34	0.42
1:D:184:LEU:HB3	1:D:218:ALA:HB2	2.01	0.42
1:A:882:TYR:OH	1:A:985:ARG:HB3	2.19	0.42
1:B:222:THR:CG2	1:B:230:ILE:HD12	2.49	0.42
1:B:722:MET:HE2	1:B:757:MET:HE3	2.01	0.42
1:A:941:GLU:OE1	1:A:944:ASN:N	2.53	0.42
1:B:184:LEU:HB3	1:B:218:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:520:ILE:HD12	1:C:520:ILE:H	1.85	0.42
1:D:941:GLU:OE1	1:D:944:ASN:N	2.53	0.42
1:B:1117:THR:O	1:B:1121:VAL:HG23	2.19	0.42
1:C:291:HIS:HB2	1:C:294:PHE:CZ	2.55	0.42
1:D:358:PRO:HB2	1:D:426:LEU:HD21	2.02	0.42
1:D:670:VAL:HG11	1:D:732:TRP:CZ3	2.54	0.42
1:C:373:ILE:HG23	1:C:399:ILE:HD11	2.01	0.42
1:B:869:ASN:OD1	1:B:869:ASN:O	2.38	0.42
1:A:565:GLU:OE2	1:A:577:THR:OG1	2.27	0.42
1:B:875:PHE:CE1	1:B:992:VAL:HG21	2.55	0.42
1:C:309:VAL:HG13	1:C:310:LYS:N	2.34	0.42
1:C:524:GLU:OE2	1:C:556:SER:HA	2.19	0.42
1:D:341:GLY:HA2	1:D:345:VAL:HG21	2.02	0.42
1:D:464:LEU:HD23	1:D:503:PHE:CD2	2.54	0.42
1:D:492:MET:HE3	1:D:514:MET:CE	2.50	0.42
1:D:492:MET:HE2	1:D:507:LEU:HB2	2.00	0.42
1:A:341:GLY:HA2	1:A:345:VAL:HG21	2.01	0.41
1:A:357:PRO:O	1:A:358:PRO:C	2.61	0.41
1:A:449:LEU:HD22	1:A:459:GLN:CG	2.50	0.41
1:C:561:GLY:O	1:C:565:GLU:HG3	2.20	0.41
1:C:988:ASP:OD1	1:C:988:ASP:C	2.63	0.41
1:C:1183:LEU:O	1:C:1183:LEU:HD12	2.20	0.41
1:D:446:THR:HG22	1:D:475:GLN:CD	2.45	0.41
1:D:714:TYR:OH	1:D:757:MET:HE1	2.20	0.41
1:A:324:ILE:HG22	1:A:332:VAL:HG22	2.01	0.41
1:A:1008:ILE:HD12	1:A:1008:ILE:H	1.85	0.41
1:A:949:ILE:O	1:A:953:LEU:HD23	2.20	0.41
1:B:655:LEU:CD2	1:B:705:LEU:HD11	2.50	0.41
1:D:520:ILE:HD12	1:D:520:ILE:H	1.84	0.41
1:B:156:MET:HE2	1:B:293:HIS:CD2	2.55	0.41
1:B:266:ILE:O	1:B:266:ILE:HG22	2.20	0.41
1:B:560:ILE:HA	1:B:563:VAL:HG12	2.02	0.41
1:C:324:ILE:HG22	1:C:332:VAL:HG22	2.02	0.41
1:D:440:ILE:O	1:D:444:ILE:HG13	2.21	0.41
1:C:266:ILE:O	1:C:266:ILE:HG22	2.19	0.41
1:C:449:LEU:HD22	1:C:459:GLN:CG	2.50	0.41
1:D:441:ASP:OD1	1:D:442:LEU:N	2.50	0.41
1:D:562:LEU:HD22	1:D:577:THR:CG2	2.51	0.41
1:A:387:ILE:HG23	1:A:391:LEU:HB3	2.01	0.41
1:A:742:VAL:HG21	1:A:1134:TYR:CD1	2.56	0.41
1:C:222:THR:HG22	1:C:223:GLY:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:707:VAL:HG23	1:D:746:HIS:HE1	1.85	0.41
1:A:184:LEU:HD11	1:A:448:LEU:HD11	2.03	0.41
1:B:209:LEU:HD13	1:B:337:LEU:HD11	2.01	0.41
1:B:349:VAL:O	1:B:353:LEU:HD13	2.21	0.41
1:B:1053:MET:HB3	1:B:1099:LEU:HD21	2.02	0.41
1:D:266:ILE:O	1:D:266:ILE:HG22	2.20	0.41
1:D:333:PRO:HB2	1:D:448:LEU:HD22	2.02	0.41
1:D:565:GLU:OE1	1:D:573:ARG:HA	2.20	0.41
1:A:990:PHE:HB3	1:A:996:LEU:HD13	2.03	0.41
1:B:991:GLY:HA2	1:B:997:GLY:HA2	2.03	0.41
1:B:1124:ILE:O	1:B:1128:VAL:HG23	2.21	0.41
1:C:335:VAL:HB	1:C:448:LEU:HD21	2.03	0.41
1:C:1013:PHE:HB2	1:C:1110:LEU:HD13	2.02	0.41
1:A:341:GLY:HA3	1:A:345:VAL:HG21	2.02	0.41
1:A:972:ARG:NH1	1:B:1030:ALA:O	2.47	0.41
1:A:1013:PHE:HB2	1:A:1110:LEU:HD13	2.03	0.41
1:B:670:VAL:HG21	1:B:732:TRP:CE3	2.55	0.41
1:B:670:VAL:HG11	1:B:732:TRP:CZ3	2.56	0.41
1:C:390:SER:O	1:C:394:GLN:HG3	2.20	0.41
1:D:991:GLY:HA2	1:D:997:GLY:HA2	2.03	0.41
1:B:176:GLU:O	1:B:178:GLN:NE2	2.54	0.41
1:D:959:ILE:O	1:D:963:GLN:OE1	2.38	0.41
1:D:1013:PHE:HB2	1:D:1110:LEU:HD13	2.03	0.41
1:B:468:ARG:NH2	1:B:470:ASP:OD2	2.53	0.40
1:D:1002:MET:O	1:D:1006:MET:HG2	2.21	0.40
1:D:1013:PHE:CZ	1:D:1017:MET:HE3	2.56	0.40
1:B:972:ARG:NH1	1:C:1030:ALA:O	2.46	0.40
1:C:1049:MET:HB2	1:C:1050:PRO:HD3	2.03	0.40
1:C:1053:MET:HB3	1:C:1099:LEU:HD21	2.03	0.40
1:C:1181:LEU:HD11	1:C:1182:LYS:HE3	2.02	0.40
1:A:169:LEU:HD23	1:A:315:LEU:HD22	2.04	0.40
1:C:230:ILE:HG22	1:C:288:ASN:OD1	2.21	0.40
1:C:258:ILE:HG22	1:C:285:THR:HG22	2.03	0.40
1:C:984:ILE:O	1:C:987:LEU:HB3	2.22	0.40
1:C:1240:ARG:HG2	1:C:1240:ARG:HH11	1.87	0.40
1:D:237:LEU:CD2	1:D:248:ILE:HG21	2.52	0.40
1:D:666:ALA:HB2	1:D:729:LEU:HD11	2.03	0.40
1:A:1183:LEU:HD12	1:A:1183:LEU:O	2.21	0.40
1:C:145:GLU:HG3	1:C:147:GLN:HE21	1.86	0.40
1:C:1183:LEU:HD13	1:C:1185:ILE:HD13	2.01	0.40
1:A:333:PRO:HB2	1:A:448:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:GLN:HA	1:A:397:VAL:HG12	2.04	0.40
1:B:335:VAL:HB	1:B:448:LEU:HD21	2.04	0.40
1:B:746:HIS:CD2	1:B:749:PHE:HB2	2.57	0.40
1:D:742:VAL:HG21	1:D:1134:TYR:CD1	2.57	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	909/1409 (64%)	891 (98%)	18 (2%)	0	100	100
1	B	909/1409 (64%)	892 (98%)	17 (2%)	0	100	100
1	C	909/1409 (64%)	888 (98%)	21 (2%)	0	100	100
1	D	909/1409 (64%)	888 (98%)	21 (2%)	0	100	100
All	All	3636/5636 (64%)	3559 (98%)	77 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	818/1247 (66%)	818 (100%)	0	100	100
1	B	818/1247 (66%)	818 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	818/1247 (66%)	818 (100%)	0	100	100
1	D	818/1247 (66%)	818 (100%)	0	100	100
All	All	3272/4988 (66%)	3272 (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 (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	HIS
1	A	232	HIS
1	A	240	HIS
1	A	378	HIS
1	A	409	GLN
1	A	475	GLN
1	A	531	HIS
1	A	633	HIS
1	A	712	GLN
1	A	890	ASN
1	A	965	GLN
1	A	1062	GLN
1	A	1103	ASN
1	A	1194	HIS
1	A	1213	ASN
1	B	147	GLN
1	B	232	HIS
1	B	240	HIS
1	B	318	HIS
1	B	378	HIS
1	B	409	GLN
1	B	459	GLN
1	B	475	GLN
1	B	531	HIS
1	B	890	ASN
1	B	965	GLN
1	B	1103	ASN
1	B	1115	ASN
1	B	1116	ASN
1	B	1126	ASN
1	B	1194	HIS
1	B	1213	ASN

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Mol	Chain	Res	Type
1	B	1238	ASN
1	C	232	HIS
1	C	293	HIS
1	C	318	HIS
1	C	344	ASN
1	C	378	HIS
1	C	475	GLN
1	C	515	HIS
1	C	531	HIS
1	C	633	HIS
1	C	746	HIS
1	C	890	ASN
1	C	1126	ASN
1	C	1127	GLN
1	C	1132	GLN
1	C	1194	HIS
1	C	1213	ASN
1	C	1229	ASN
1	C	1238	ASN
1	D	232	HIS
1	D	240	HIS
1	D	262	GLN
1	D	378	HIS
1	D	409	GLN
1	D	510	ASN
1	D	515	HIS
1	D	531	HIS
1	D	731	ASN
1	D	746	HIS
1	D	978	ASN
1	D	1213	ASN
1	D	1216	ASN
1	D	1238	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](#)

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	YUV	A	1503	-	35,35,35	4.26	23 (65%)	58,58,58	3.00	20 (34%)
3	YUV	D	1501	-	35,35,35	4.26	23 (65%)	58,58,58	3.00	20 (34%)
2	A1JBK	B	1502	-	23,23,23	1.42	3 (13%)	33,33,33	1.74	3 (9%)
2	A1JBK	D	1502	-	23,23,23	1.44	4 (17%)	33,33,33	1.75	3 (9%)
3	YUV	A	1502	-	35,35,35	4.24	22 (62%)	58,58,58	2.91	22 (37%)
3	YUV	D	1503	-	35,35,35	4.25	22 (62%)	58,58,58	2.95	22 (37%)
3	YUV	B	1501	-	35,35,35	4.27	22 (62%)	58,58,58	2.97	20 (34%)
3	YUV	C	1503	-	35,35,35	4.25	22 (62%)	58,58,58	2.90	21 (36%)
3	YUV	B	1503	-	35,35,35	4.24	22 (62%)	58,58,58	2.94	22 (37%)
2	A1JBK	A	1501	-	23,23,23	1.44	4 (17%)	33,33,33	1.74	3 (9%)
3	YUV	C	1501	-	35,35,35	4.26	22 (62%)	58,58,58	2.98	20 (34%)
2	A1JBK	C	1502	-	23,23,23	1.44	4 (17%)	33,33,33	1.72	3 (9%)

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	YUV	A	1503	-	-	-	0/6/6/6
3	YUV	D	1501	-	-	-	0/6/6/6
2	A1JBK	B	1502	-	-	4/6/18/18	0/3/3/3
3	YUV	A	1502	-	1/1/13/13	-	0/6/6/6
2	A1JBK	C	1502	-	-	4/6/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1JBK	D	1502	-	-	4/6/18/18	0/3/3/3
3	YUV	B	1501	-	-	-	0/6/6/6
3	YUV	C	1503	-	1/1/13/13	-	0/6/6/6
3	YUV	B	1503	-	1/1/13/13	-	0/6/6/6
2	A1JBK	A	1501	-	-	4/6/18/18	0/3/3/3
3	YUV	C	1501	-	-	-	0/6/6/6
3	YUV	D	1503	-	1/1/13/13	-	0/6/6/6

All (193) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1502	YUV	C12-C13	11.98	1.73	1.53
3	C	1503	YUV	C12-C13	11.98	1.73	1.53
3	B	1503	YUV	C12-C13	11.97	1.73	1.53
3	D	1503	YUV	C12-C13	11.96	1.73	1.53
3	A	1503	YUV	C12-C13	11.83	1.73	1.53
3	C	1501	YUV	C12-C13	11.83	1.73	1.53
3	D	1501	YUV	C12-C13	11.80	1.73	1.53
3	B	1501	YUV	C12-C13	11.79	1.73	1.53
3	B	1501	YUV	C10-C9	-8.88	1.38	1.55
3	A	1503	YUV	C10-C9	-8.82	1.38	1.55
3	D	1501	YUV	C10-C9	-8.79	1.38	1.55
3	C	1501	YUV	C10-C9	-8.78	1.38	1.55
3	B	1503	YUV	C10-C9	-8.76	1.38	1.55
3	C	1503	YUV	C10-C9	-8.72	1.39	1.55
3	D	1503	YUV	C10-C9	-8.71	1.39	1.55
3	A	1502	YUV	C10-C9	-8.69	1.39	1.55
3	D	1501	YUV	C8-C7	8.52	1.70	1.52
3	B	1501	YUV	C8-C7	8.50	1.70	1.52
3	C	1501	YUV	C8-C7	8.50	1.70	1.52
3	A	1503	YUV	C8-C7	8.49	1.70	1.52
3	A	1502	YUV	C8-C7	8.29	1.70	1.52
3	C	1503	YUV	C8-C7	8.28	1.70	1.52
3	D	1503	YUV	C8-C7	8.26	1.70	1.52
3	B	1503	YUV	C8-C7	8.15	1.70	1.52
3	C	1503	YUV	C20-C21	6.38	1.66	1.51
3	D	1503	YUV	C20-C21	6.37	1.66	1.51
3	B	1503	YUV	C20-C21	6.36	1.66	1.51
3	A	1502	YUV	C20-C21	6.35	1.66	1.51
3	C	1501	YUV	C20-C21	6.09	1.65	1.51
3	A	1503	YUV	C20-C21	6.06	1.65	1.51
3	D	1501	YUV	C20-C21	6.05	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1501	YUV	C16-C17	6.03	1.45	1.33
3	B	1501	YUV	C20-C21	6.02	1.65	1.51
3	B	1501	YUV	C8-C9	6.01	1.66	1.54
3	D	1501	YUV	C16-C17	6.01	1.45	1.33
3	A	1503	YUV	C16-C17	6.00	1.45	1.33
3	D	1501	YUV	C8-C9	5.98	1.66	1.54
3	A	1503	YUV	C8-C9	5.98	1.66	1.54
3	C	1501	YUV	C8-C9	5.97	1.66	1.54
3	C	1501	YUV	C16-C17	5.93	1.45	1.33
3	C	1503	YUV	C16-C17	5.87	1.45	1.33
3	B	1503	YUV	C16-C17	5.86	1.45	1.33
3	A	1502	YUV	C16-C17	5.84	1.45	1.33
3	D	1503	YUV	C8-C9	5.83	1.66	1.54
3	D	1503	YUV	C16-C17	5.83	1.45	1.33
3	C	1503	YUV	C8-C9	5.82	1.66	1.54
3	A	1502	YUV	C8-C9	5.82	1.66	1.54
3	B	1503	YUV	C8-C9	5.74	1.66	1.54
3	B	1501	YUV	C6-C7	-5.54	1.44	1.54
3	C	1501	YUV	C6-C7	-5.49	1.44	1.54
3	D	1501	YUV	C6-C7	-5.46	1.44	1.54
3	A	1503	YUV	C6-C7	-5.42	1.44	1.54
3	D	1503	YUV	C22-C17	-5.42	1.40	1.51
3	B	1503	YUV	C22-C17	-5.40	1.40	1.51
3	A	1502	YUV	C22-C17	-5.36	1.40	1.51
3	D	1503	YUV	C19-C20	5.34	1.64	1.53
3	A	1502	YUV	C19-C20	5.33	1.64	1.53
3	C	1503	YUV	C19-C20	5.33	1.64	1.53
3	C	1503	YUV	C22-C17	-5.33	1.41	1.51
3	D	1503	YUV	C6-C7	-5.32	1.44	1.54
3	B	1503	YUV	C19-C20	5.31	1.64	1.53
3	B	1503	YUV	C6-C7	-5.29	1.44	1.54
3	A	1502	YUV	C6-C7	-5.29	1.44	1.54
3	C	1503	YUV	C6-C7	-5.28	1.44	1.54
3	C	1501	YUV	C22-C17	-4.95	1.41	1.51
3	C	1501	YUV	C19-C20	4.93	1.63	1.53
3	D	1501	YUV	C22-C17	-4.92	1.41	1.51
3	D	1501	YUV	C19-C20	4.92	1.63	1.53
3	B	1501	YUV	C22-C17	-4.91	1.41	1.51
3	B	1501	YUV	C19-C20	4.89	1.63	1.53
3	A	1503	YUV	C19-C20	4.87	1.63	1.53
3	A	1503	YUV	C22-C17	-4.86	1.41	1.51
3	C	1503	YUV	C19-C18	-4.58	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1501	YUV	C19-C18	-4.56	1.45	1.54
3	D	1503	YUV	C19-C18	-4.55	1.45	1.54
3	A	1503	YUV	C19-C18	-4.54	1.45	1.54
3	B	1503	YUV	C19-C18	-4.53	1.45	1.54
3	A	1502	YUV	C19-C18	-4.53	1.45	1.54
3	C	1501	YUV	C19-C18	-4.50	1.46	1.54
3	D	1501	YUV	C19-C18	-4.47	1.46	1.54
2	D	1502	A1JBK	CAI-CAH	-4.38	1.42	1.50
2	B	1502	A1JBK	CAI-CAH	-4.34	1.42	1.50
2	A	1501	A1JBK	CAI-CAH	-4.31	1.42	1.50
2	C	1502	A1JBK	CAI-CAH	-4.30	1.42	1.50
3	C	1501	YUV	C18-C17	4.27	1.61	1.52
3	A	1503	YUV	C18-C17	4.24	1.60	1.52
3	D	1501	YUV	C18-C17	4.22	1.60	1.52
3	B	1501	YUV	C18-C17	4.18	1.60	1.52
3	D	1501	YUV	O-C4	4.14	1.51	1.42
3	B	1501	YUV	O-C4	4.10	1.51	1.42
3	C	1501	YUV	O-C4	4.10	1.51	1.42
3	A	1503	YUV	O-C4	4.09	1.51	1.42
3	B	1503	YUV	O1-C21	-4.02	1.31	1.43
3	C	1503	YUV	O1-C21	-4.01	1.31	1.43
3	D	1503	YUV	O1-C21	-4.01	1.31	1.43
3	A	1502	YUV	O1-C21	-4.01	1.31	1.43
3	C	1501	YUV	O1-C21	-4.00	1.31	1.43
3	B	1501	YUV	O1-C21	-3.99	1.31	1.43
3	A	1503	YUV	O1-C21	-3.99	1.31	1.43
3	D	1501	YUV	O1-C21	-3.97	1.31	1.43
3	D	1503	YUV	O-C4	3.96	1.50	1.42
3	C	1503	YUV	O-C4	3.90	1.50	1.42
3	A	1502	YUV	O-C4	3.89	1.50	1.42
3	B	1503	YUV	O-C4	3.87	1.50	1.42
3	B	1503	YUV	C18-C17	3.82	1.60	1.52
3	D	1503	YUV	C18-C17	3.80	1.60	1.52
3	A	1502	YUV	C18-C17	3.78	1.60	1.52
3	C	1503	YUV	C18-C17	3.76	1.60	1.52
3	A	1503	YUV	C11-C10	-3.48	1.48	1.54
3	B	1501	YUV	C11-C10	-3.47	1.48	1.54
3	C	1501	YUV	C11-C10	-3.45	1.48	1.54
3	D	1501	YUV	C11-C10	-3.43	1.48	1.54
3	C	1503	YUV	C11-C10	-3.42	1.48	1.54
3	B	1503	YUV	C18-C13	-3.40	1.50	1.56
3	D	1503	YUV	C18-C13	-3.39	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1503	YUV	C11-C10	-3.38	1.48	1.54
3	D	1503	YUV	C11-C10	-3.38	1.48	1.54
3	B	1501	YUV	C18-C13	-3.36	1.50	1.56
3	D	1501	YUV	C18-C13	-3.33	1.50	1.56
3	A	1502	YUV	C11-C10	-3.33	1.48	1.54
3	C	1501	YUV	C18-C13	-3.33	1.50	1.56
3	C	1503	YUV	C18-C13	-3.30	1.50	1.56
3	A	1503	YUV	C18-C13	-3.30	1.50	1.56
3	A	1502	YUV	C18-C13	-3.26	1.50	1.56
3	B	1501	YUV	C15-C14	-3.21	1.47	1.53
3	A	1503	YUV	C15-C14	-3.18	1.48	1.53
3	D	1501	YUV	C15-C14	-3.17	1.48	1.53
3	C	1501	YUV	C15-C14	-3.15	1.48	1.53
3	B	1503	YUV	C15-C16	-3.13	1.43	1.50
3	B	1503	YUV	C15-C14	-3.11	1.48	1.53
3	C	1501	YUV	C15-C16	-3.11	1.43	1.50
3	C	1503	YUV	C15-C16	-3.10	1.43	1.50
3	D	1503	YUV	C15-C16	-3.09	1.43	1.50
3	C	1503	YUV	C15-C14	-3.07	1.48	1.53
3	A	1502	YUV	C15-C16	-3.06	1.44	1.50
3	D	1503	YUV	C15-C14	-3.06	1.48	1.53
3	B	1501	YUV	C15-C16	-3.05	1.44	1.50
3	A	1503	YUV	C15-C16	-3.02	1.44	1.50
3	D	1501	YUV	C15-C16	-3.02	1.44	1.50
3	A	1502	YUV	C15-C14	-3.00	1.48	1.53
3	B	1501	YUV	C6-C5	-2.79	1.46	1.54
3	A	1503	YUV	C6-C5	-2.77	1.46	1.54
3	D	1501	YUV	C6-C5	-2.76	1.46	1.54
3	C	1501	YUV	C6-C5	-2.75	1.46	1.54
3	D	1501	YUV	C4-C5	-2.66	1.48	1.53
3	B	1501	YUV	C4-C5	-2.64	1.48	1.53
3	A	1503	YUV	C4-C5	-2.63	1.48	1.53
3	D	1503	YUV	C6-C5	-2.61	1.47	1.54
3	C	1503	YUV	C6-C5	-2.59	1.47	1.54
3	C	1501	YUV	C4-C5	-2.58	1.48	1.53
3	A	1502	YUV	C6-C5	-2.55	1.47	1.54
3	B	1503	YUV	C6-C5	-2.55	1.47	1.54
3	D	1503	YUV	C14-C13	-2.47	1.49	1.53
3	C	1503	YUV	C4-C5	-2.45	1.48	1.53
3	B	1503	YUV	C4-C5	-2.45	1.48	1.53
3	A	1502	YUV	C4-C5	-2.44	1.48	1.53
3	A	1502	YUV	C14-C13	-2.44	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1501	YUV	C14-C13	-2.44	1.49	1.53
3	C	1503	YUV	C14-C13	-2.42	1.49	1.53
3	A	1503	YUV	C14-C13	-2.41	1.49	1.53
3	C	1501	YUV	C22-C21	2.41	1.56	1.52
3	B	1503	YUV	C14-C13	-2.40	1.49	1.53
3	D	1501	YUV	C14-C13	-2.39	1.49	1.53
3	B	1501	YUV	C22-C21	2.38	1.56	1.52
3	B	1501	YUV	C14-C13	-2.37	1.49	1.53
3	D	1503	YUV	C4-C5	-2.36	1.49	1.53
3	D	1501	YUV	C22-C21	2.35	1.56	1.52
3	A	1503	YUV	C22-C21	2.34	1.56	1.52
3	D	1501	YUV	C25-C5	2.27	1.57	1.53
3	B	1503	YUV	C25-C5	2.27	1.57	1.53
2	C	1502	A1JBK	OAG-CAF	2.26	1.41	1.38
3	C	1501	YUV	C25-C5	2.25	1.57	1.53
3	D	1503	YUV	C25-C5	2.24	1.57	1.53
3	B	1501	YUV	C25-C5	2.24	1.57	1.53
3	C	1503	YUV	C25-C5	2.23	1.57	1.53
3	A	1502	YUV	C25-C5	2.23	1.57	1.53
3	A	1503	YUV	C25-C5	2.22	1.57	1.53
2	A	1501	A1JBK	OAG-CAF	2.21	1.41	1.38
2	D	1502	A1JBK	OAG-CAF	2.20	1.41	1.38
3	A	1502	YUV	C22-C21	2.19	1.56	1.52
3	C	1503	YUV	C22-C21	2.15	1.56	1.52
3	B	1503	YUV	C22-C21	2.13	1.55	1.52
2	B	1502	A1JBK	OAG-CAF	2.12	1.40	1.38
3	D	1503	YUV	C22-C21	2.11	1.55	1.52
2	A	1501	A1JBK	OAU-CAD	2.08	1.40	1.36
2	C	1502	A1JBK	OAU-CAD	2.07	1.40	1.36
2	D	1502	A1JBK	OAU-CAD	2.06	1.40	1.36
3	D	1501	YUV	C26-C1	2.04	1.55	1.51
2	A	1501	A1JBK	OAT-CAH	-2.04	1.18	1.22
2	C	1502	A1JBK	OAT-CAH	-2.04	1.18	1.22
2	D	1502	A1JBK	OAT-CAH	-2.03	1.18	1.22
2	B	1502	A1JBK	OAU-CAD	2.03	1.40	1.36
3	A	1503	YUV	C26-C1	2.02	1.55	1.51

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1503	YUV	O2-C4-C5	11.31	140.98	107.26
3	B	1501	YUV	O2-C4-C5	11.28	140.90	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1501	YUV	O2-C4-C5	11.27	140.86	107.26
3	D	1501	YUV	O2-C4-C5	11.26	140.82	107.26
3	D	1503	YUV	O2-C4-C5	11.16	140.53	107.26
3	A	1502	YUV	O2-C4-C5	11.05	140.21	107.26
3	C	1503	YUV	O2-C4-C5	11.02	140.12	107.26
3	B	1503	YUV	O2-C4-C5	11.00	140.06	107.26
3	B	1503	YUV	O2-C4-O	-9.98	86.14	109.88
3	A	1502	YUV	O2-C4-O	-9.96	86.19	109.88
3	C	1503	YUV	O2-C4-O	-9.84	86.46	109.88
3	D	1503	YUV	O2-C4-O	-9.66	86.89	109.88
3	C	1501	YUV	O2-C4-O	-8.93	88.63	109.88
3	A	1503	YUV	O2-C4-O	-8.76	89.04	109.88
3	B	1501	YUV	O2-C4-O	-8.74	89.09	109.88
3	D	1501	YUV	O2-C4-O	-8.60	89.42	109.88
2	D	1502	A1JBK	OAG-CAJ-CAK	-8.17	92.26	107.47
3	B	1503	YUV	O-C4-C3	-8.13	92.03	108.54
2	B	1502	A1JBK	OAG-CAJ-CAK	-8.12	92.36	107.47
2	A	1501	A1JBK	OAG-CAJ-CAK	-8.08	92.43	107.47
3	D	1503	YUV	O-C4-C3	-8.08	92.14	108.54
2	C	1502	A1JBK	OAG-CAJ-CAK	-8.03	92.52	107.47
3	C	1503	YUV	O-C4-C3	-7.78	92.74	108.54
3	A	1502	YUV	O-C4-C3	-7.67	92.96	108.54
3	D	1501	YUV	O-C4-C3	-6.86	94.61	108.54
3	C	1501	YUV	O-C4-C3	-6.79	94.75	108.54
3	D	1501	YUV	O2-C4-C3	-6.77	104.86	110.76
3	B	1501	YUV	O-C4-C3	-6.73	94.88	108.54
3	A	1503	YUV	O-C4-C3	-6.66	95.02	108.54
3	A	1503	YUV	O2-C4-C3	-6.64	104.98	110.76
3	B	1501	YUV	O2-C4-C3	-6.44	105.14	110.76
3	C	1501	YUV	O2-C4-C3	-6.42	105.16	110.76
3	A	1503	YUV	C2-C1-C26	6.07	115.95	108.59
3	D	1501	YUV	C2-C1-C26	6.00	115.87	108.59
3	D	1503	YUV	C9-C8-C7	-5.98	91.99	102.40
3	C	1501	YUV	C2-C1-C26	5.92	115.77	108.59
3	B	1503	YUV	C9-C8-C7	-5.89	92.14	102.40
3	C	1503	YUV	C9-C8-C7	-5.82	92.25	102.40
3	A	1502	YUV	C9-C8-C7	-5.69	92.48	102.40
3	B	1501	YUV	C2-C1-C26	5.65	115.45	108.59
3	D	1501	YUV	C9-C8-C7	-4.95	93.77	102.40
3	C	1501	YUV	C9-C8-C7	-4.92	93.83	102.40
3	A	1503	YUV	C9-C8-C7	-4.89	93.88	102.40
3	B	1501	YUV	C9-C8-C7	-4.86	93.94	102.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1501	YUV	C11-C10-C6	-4.42	109.07	115.36
3	D	1501	YUV	C11-C10-C6	-4.41	109.08	115.36
3	C	1501	YUV	C11-C10-C6	-4.35	109.16	115.36
3	A	1503	YUV	C11-C10-C6	-4.35	109.17	115.36
3	D	1503	YUV	C11-C10-C6	-4.29	109.26	115.36
3	D	1503	YUV	O2-C4-C3	-4.12	107.17	110.76
3	C	1503	YUV	C11-C10-C6	-4.04	109.61	115.36
3	B	1503	YUV	C11-C10-C6	-4.00	109.67	115.36
3	A	1502	YUV	C11-C10-C6	-3.95	109.74	115.36
3	B	1503	YUV	O2-C4-C3	-3.85	107.41	110.76
3	A	1503	YUV	C11-C10-C9	3.76	112.87	107.25
3	B	1501	YUV	C11-C10-C9	3.74	112.85	107.25
3	D	1501	YUV	C11-C10-C9	3.70	112.78	107.25
3	B	1503	YUV	C8-C9-C14	-3.68	112.41	119.53
3	A	1502	YUV	O2-C4-C3	-3.65	107.58	110.76
3	C	1501	YUV	C11-C10-C9	3.64	112.70	107.25
3	C	1503	YUV	C8-C9-C14	-3.59	112.58	119.53
3	A	1502	YUV	C8-C9-C14	-3.54	112.67	119.53
3	D	1501	YUV	C25-C5-C4	-3.48	109.33	114.94
3	A	1503	YUV	C25-C5-C4	-3.46	109.36	114.94
3	C	1503	YUV	O2-C4-C3	-3.43	107.77	110.76
3	B	1501	YUV	C25-C5-C4	-3.42	109.42	114.94
3	C	1501	YUV	C25-C5-C4	-3.41	109.44	114.94
3	D	1503	YUV	C8-C9-C14	-3.37	113.00	119.53
3	B	1501	YUV	C22-C17-C18	3.35	120.71	116.42
3	A	1503	YUV	C22-C17-C18	3.34	120.70	116.42
3	A	1503	YUV	O2-C26-C1	3.33	116.44	112.17
3	C	1503	YUV	C19-C20-C21	3.32	114.88	110.48
3	C	1501	YUV	C22-C17-C18	3.31	120.66	116.42
3	D	1501	YUV	O2-C26-C1	3.31	116.42	112.17
3	C	1503	YUV	C25-C5-C4	-3.30	109.61	114.94
3	A	1502	YUV	C19-C20-C21	3.29	114.85	110.48
3	B	1503	YUV	C19-C20-C21	3.29	114.84	110.48
3	D	1501	YUV	C22-C17-C18	3.28	120.62	116.42
3	A	1502	YUV	C25-C5-C4	-3.27	109.66	114.94
3	B	1503	YUV	C25-C5-C4	-3.27	109.67	114.94
3	D	1503	YUV	C19-C20-C21	3.20	114.72	110.48
3	C	1501	YUV	C8-C9-C14	-3.14	113.44	119.53
3	C	1501	YUV	O2-C26-C1	3.13	116.19	112.17
3	D	1503	YUV	C12-C13-C14	-3.12	107.42	111.78
3	D	1503	YUV	C15-C14-C9	-3.11	106.53	110.93
3	B	1501	YUV	C8-C9-C14	-3.10	113.52	119.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1503	YUV	C8-C9-C14	-3.09	113.55	119.53
2	A	1501	A1JBK	CAD-CAE-CAF	3.08	120.35	117.41
3	B	1503	YUV	C15-C14-C9	-3.08	106.57	110.93
3	A	1502	YUV	C12-C13-C14	-3.08	107.48	111.78
3	B	1501	YUV	O2-C26-C1	3.08	116.12	112.17
3	D	1501	YUV	C8-C9-C14	-3.07	113.58	119.53
2	C	1502	A1JBK	CAD-CAE-CAF	3.07	120.34	117.41
3	B	1501	YUV	C3-C4-C5	-3.05	110.13	115.66
2	B	1502	A1JBK	CAD-CAE-CAF	3.02	120.29	117.41
3	A	1502	YUV	C15-C14-C9	-3.01	106.67	110.93
3	C	1503	YUV	C15-C14-C9	-3.01	106.68	110.93
3	B	1503	YUV	C12-C13-C14	-2.99	107.60	111.78
2	D	1502	A1JBK	CAD-CAE-CAF	2.97	120.25	117.41
2	B	1502	A1JBK	CAI-CAJ-CAK	2.94	123.71	114.22
3	A	1503	YUV	C3-C4-C5	-2.94	110.34	115.66
3	C	1503	YUV	C12-C13-C14	-2.92	107.70	111.78
3	D	1501	YUV	C3-C4-C5	-2.90	110.41	115.66
3	A	1502	YUV	C21-C22-C17	-2.90	107.44	112.05
2	D	1502	A1JBK	CAI-CAJ-CAK	2.89	123.52	114.22
3	D	1503	YUV	C21-C22-C17	-2.87	107.48	112.05
3	D	1503	YUV	C25-C5-C4	-2.85	110.35	114.94
3	D	1503	YUV	C11-C10-C9	2.84	111.50	107.25
3	C	1501	YUV	C3-C4-C5	-2.80	110.58	115.66
2	A	1501	A1JBK	CAI-CAJ-CAK	2.79	123.22	114.22
2	C	1502	A1JBK	CAI-CAJ-CAK	2.78	123.19	114.22
3	D	1501	YUV	C25-C5-C6	-2.75	109.00	114.50
3	C	1503	YUV	C21-C22-C17	-2.72	107.72	112.05
3	B	1501	YUV	C25-C5-C6	-2.71	109.07	114.50
3	B	1503	YUV	O-C7-C6	2.70	108.79	105.12
3	C	1503	YUV	C3-C4-C5	-2.70	110.78	115.66
3	B	1503	YUV	C21-C22-C17	-2.69	107.77	112.05
3	C	1503	YUV	C11-C10-C9	2.68	111.26	107.25
3	C	1501	YUV	C25-C5-C6	-2.65	109.19	114.50
3	A	1503	YUV	C25-C5-C6	-2.64	109.23	114.50
3	A	1503	YUV	C15-C14-C9	-2.62	107.22	110.93
3	A	1502	YUV	C11-C10-C9	2.62	111.16	107.25
3	B	1503	YUV	C11-C10-C9	2.61	111.16	107.25
3	D	1503	YUV	C3-C4-C5	-2.61	110.92	115.66
3	D	1503	YUV	O-C7-C6	2.61	108.66	105.12
3	A	1502	YUV	C3-C4-C5	-2.59	110.97	115.66
3	D	1501	YUV	C15-C14-C9	-2.59	107.27	110.93
3	A	1502	YUV	O-C4-C5	-2.58	101.12	104.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1501	YUV	C15-C14-C9	-2.56	107.30	110.93
3	A	1502	YUV	C4-O-C7	-2.55	101.09	108.14
3	D	1503	YUV	C15-C14-C13	2.55	112.67	109.72
3	C	1503	YUV	O-C7-C6	2.54	108.57	105.12
3	B	1501	YUV	C15-C14-C9	-2.53	107.34	110.93
3	C	1503	YUV	C4-O-C7	-2.53	101.15	108.14
3	D	1503	YUV	C10-C6-C7	2.52	106.92	104.20
3	D	1503	YUV	C25-C5-C6	-2.51	109.48	114.50
3	A	1502	YUV	O-C7-C6	2.48	108.48	105.12
3	B	1503	YUV	C4-O-C7	-2.44	101.39	108.14
3	B	1503	YUV	C25-C5-C6	-2.44	109.62	114.50
3	B	1503	YUV	C3-C4-C5	-2.39	111.33	115.66
3	C	1503	YUV	O-C4-C5	-2.38	101.39	104.56
3	A	1503	YUV	C4-O-C7	-2.38	101.56	108.14
3	A	1502	YUV	C25-C5-C6	-2.38	109.74	114.50
3	B	1501	YUV	C12-C11-C10	-2.37	108.74	112.74
3	C	1501	YUV	C4-O-C7	-2.35	101.66	108.14
3	D	1503	YUV	O-C4-C5	-2.34	101.44	104.56
3	C	1501	YUV	C12-C13-C14	-2.34	108.52	111.78
3	D	1503	YUV	C4-O-C7	-2.33	101.71	108.14
3	C	1503	YUV	C10-C6-C7	2.32	106.71	104.20
3	A	1503	YUV	C12-C11-C10	-2.31	108.84	112.74
3	B	1503	YUV	C10-C6-C7	2.31	106.69	104.20
3	C	1501	YUV	C12-C11-C10	-2.30	108.86	112.74
3	C	1503	YUV	C25-C5-C6	-2.29	109.91	114.50
3	A	1502	YUV	C10-C6-C7	2.29	106.68	104.20
3	D	1501	YUV	C12-C11-C10	-2.29	108.87	112.74
3	B	1501	YUV	C4-O-C7	-2.29	101.82	108.14
3	B	1503	YUV	C10-C9-C14	2.26	117.63	114.41
3	B	1501	YUV	C18-C17-C16	-2.25	119.64	122.93
3	A	1503	YUV	C2-C3-C4	-2.23	108.43	111.93
3	A	1502	YUV	C10-C9-C14	2.23	117.58	114.41
3	D	1501	YUV	C18-C17-C16	-2.22	119.68	122.93
3	C	1503	YUV	C10-C9-C14	2.22	117.56	114.41
3	B	1503	YUV	C15-C14-C13	2.21	112.28	109.72
3	B	1503	YUV	O-C4-C5	-2.21	101.62	104.56
3	A	1502	YUV	C15-C14-C13	2.21	112.27	109.72
3	A	1503	YUV	C18-C17-C16	-2.20	119.71	122.93
3	B	1501	YUV	C2-C3-C4	-2.18	108.51	111.93
3	D	1501	YUV	C4-O-C7	-2.17	102.13	108.14
3	D	1501	YUV	O-C7-C6	2.15	108.04	105.12
3	B	1501	YUV	C12-C13-C14	-2.13	108.81	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1503	YUV	C13-C14-C9	-2.13	106.31	109.09
3	D	1501	YUV	C12-C13-C14	-2.13	108.81	111.78
3	B	1503	YUV	C22-C17-C18	2.11	119.13	116.42
3	A	1503	YUV	C12-C13-C14	-2.11	108.84	111.78
3	D	1503	YUV	C10-C9-C14	2.07	117.36	114.41
3	C	1501	YUV	C18-C17-C16	-2.07	119.91	122.93
3	C	1503	YUV	C22-C17-C18	2.06	119.06	116.42
3	A	1502	YUV	C22-C17-C18	2.02	119.01	116.42
3	C	1501	YUV	O-C7-C6	2.01	107.85	105.12

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1502	YUV	C4
3	B	1503	YUV	C4
3	C	1503	YUV	C4
3	D	1503	YUV	C4

All (16) torsion outliers are listed below:

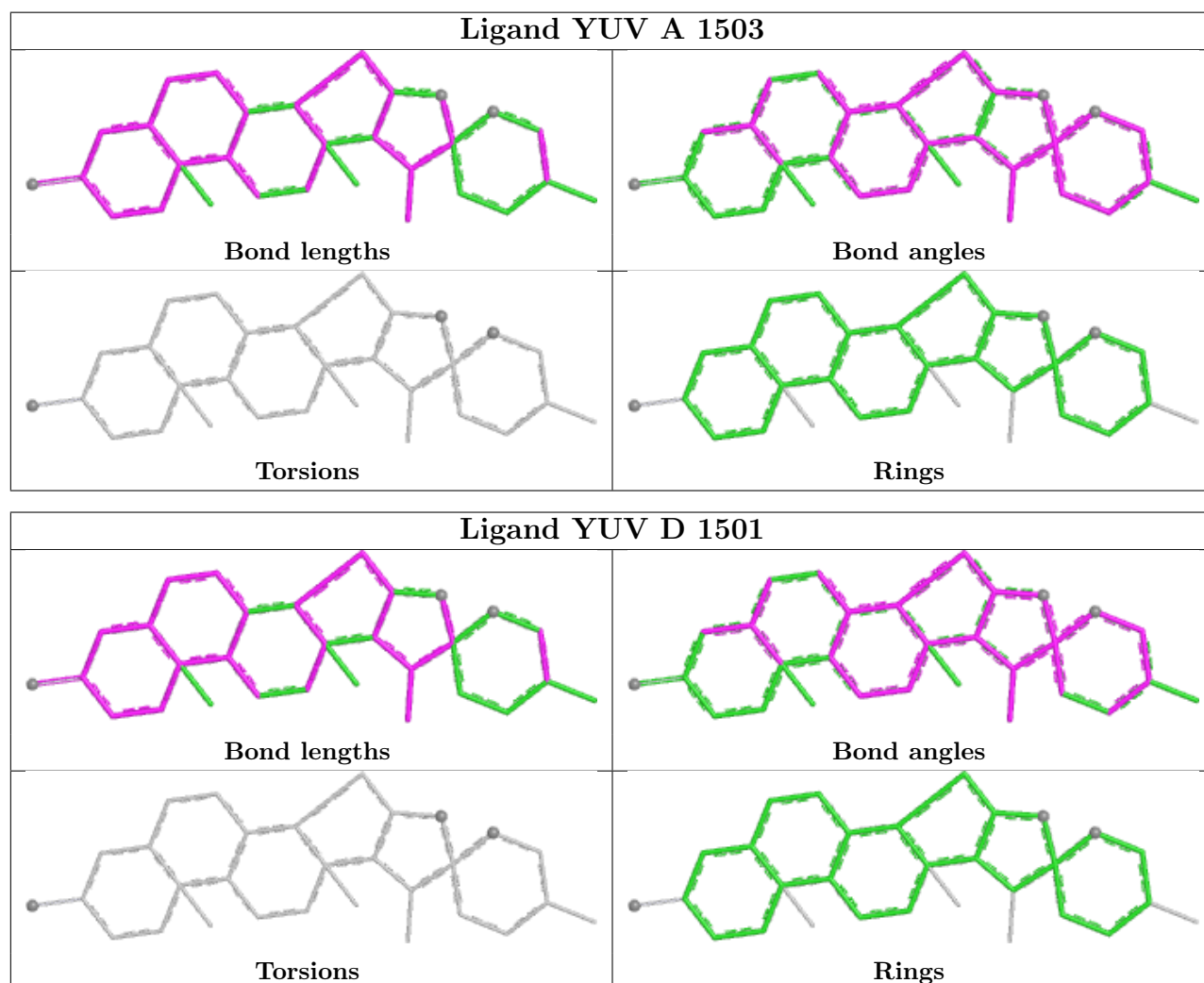
Mol	Chain	Res	Type	Atoms
2	A	1501	A1JBK	CAO-CAP-OAR-CAS
2	B	1502	A1JBK	CAL-CAP-OAR-CAS
2	B	1502	A1JBK	CAO-CAP-OAR-CAS
2	C	1502	A1JBK	CAO-CAP-OAR-CAS
2	D	1502	A1JBK	CAO-CAP-OAR-CAS
2	A	1501	A1JBK	CAL-CAP-OAR-CAS
2	C	1502	A1JBK	CAL-CAP-OAR-CAS
2	D	1502	A1JBK	CAL-CAP-OAR-CAS
2	D	1502	A1JBK	CAI-CAJ-CAK-CAM
2	A	1501	A1JBK	CAI-CAJ-CAK-CAM
2	B	1502	A1JBK	CAI-CAJ-CAK-CAM
2	C	1502	A1JBK	CAI-CAJ-CAK-CAM
2	A	1501	A1JBK	CAI-CAJ-CAK-CAN
2	D	1502	A1JBK	CAI-CAJ-CAK-CAN
2	C	1502	A1JBK	CAI-CAJ-CAK-CAN
2	B	1502	A1JBK	CAI-CAJ-CAK-CAN

There are no ring outliers.

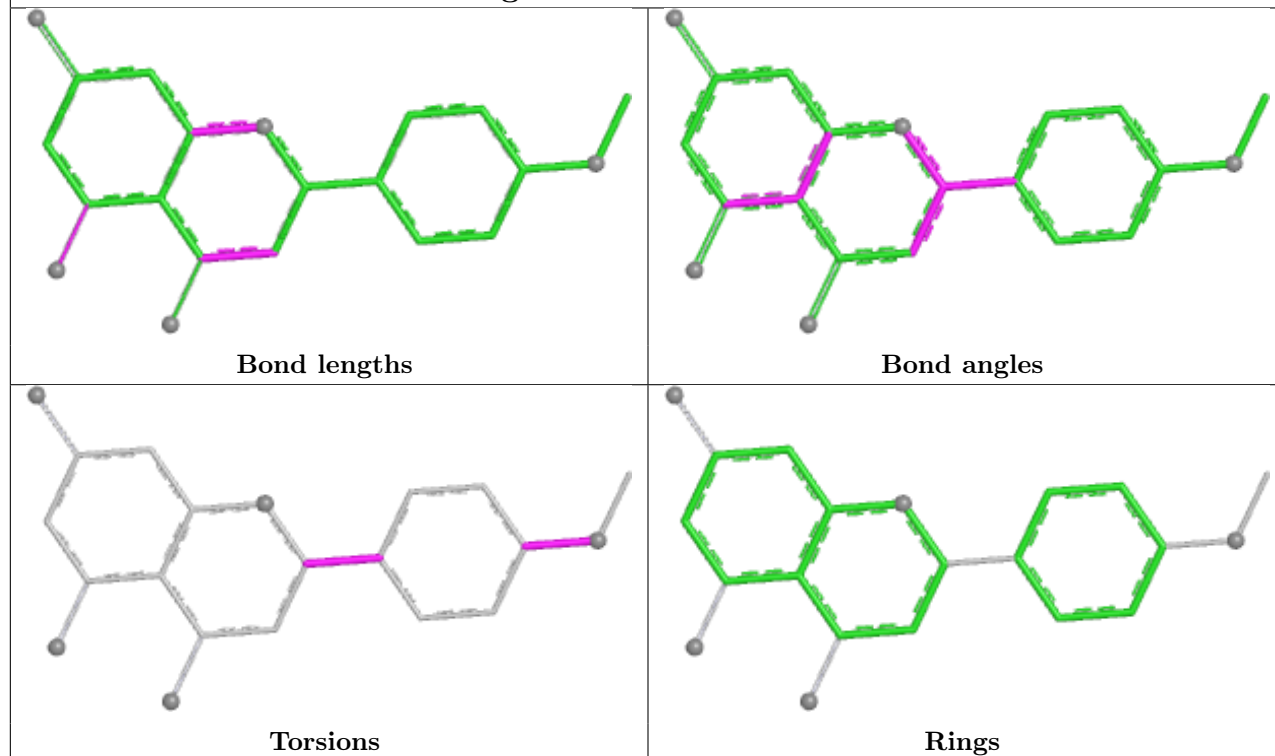
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1503	YUV	1	0

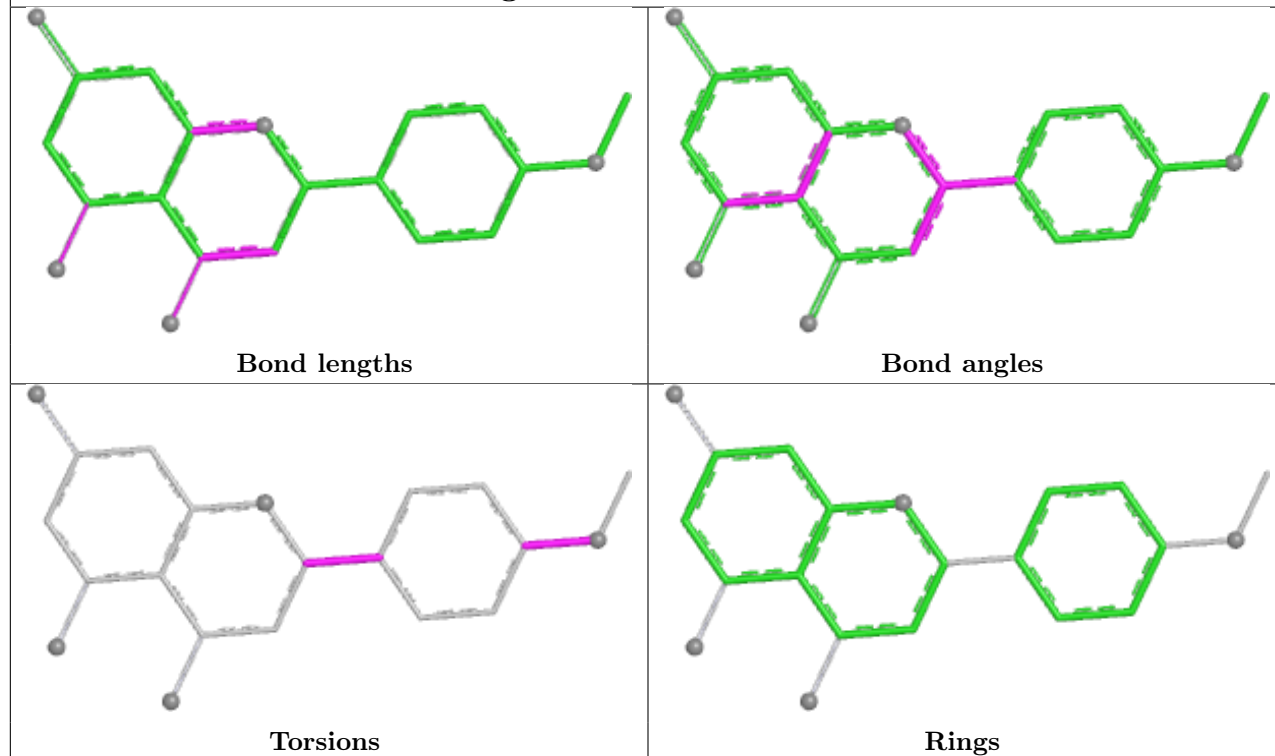
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



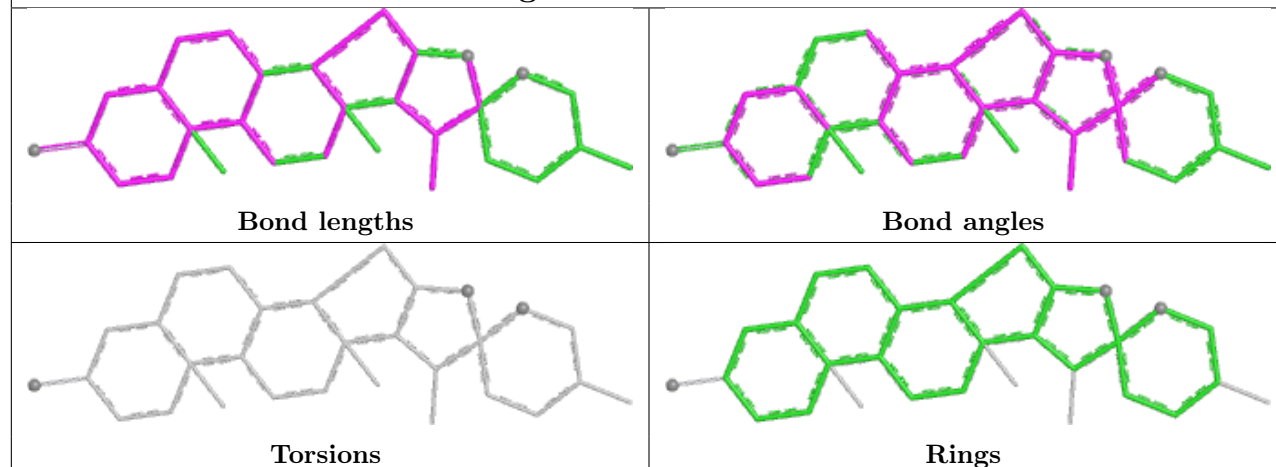
Ligand A1JBK B 1502



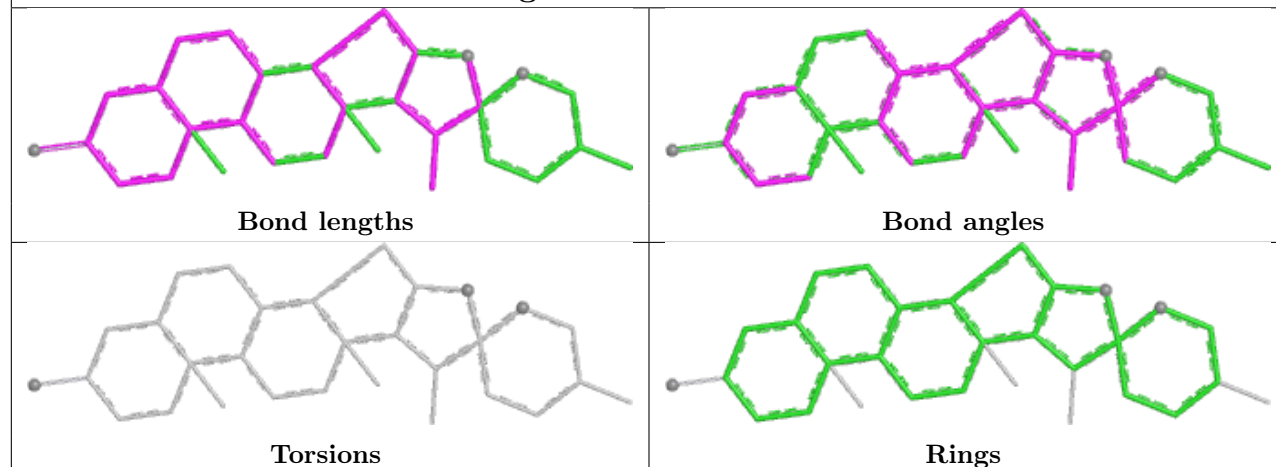
Ligand A1JBK D 1502



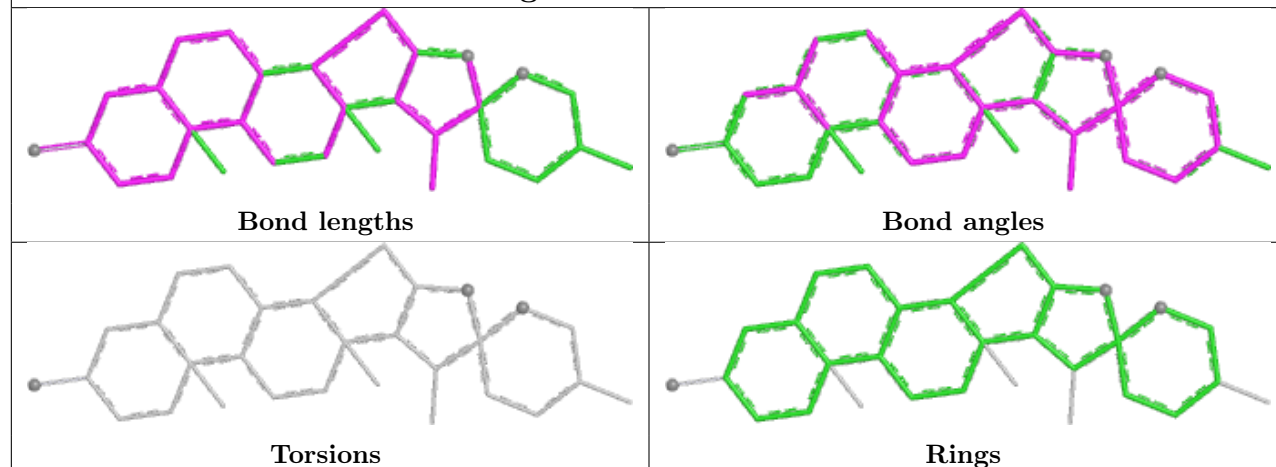
Ligand YUV A 1502

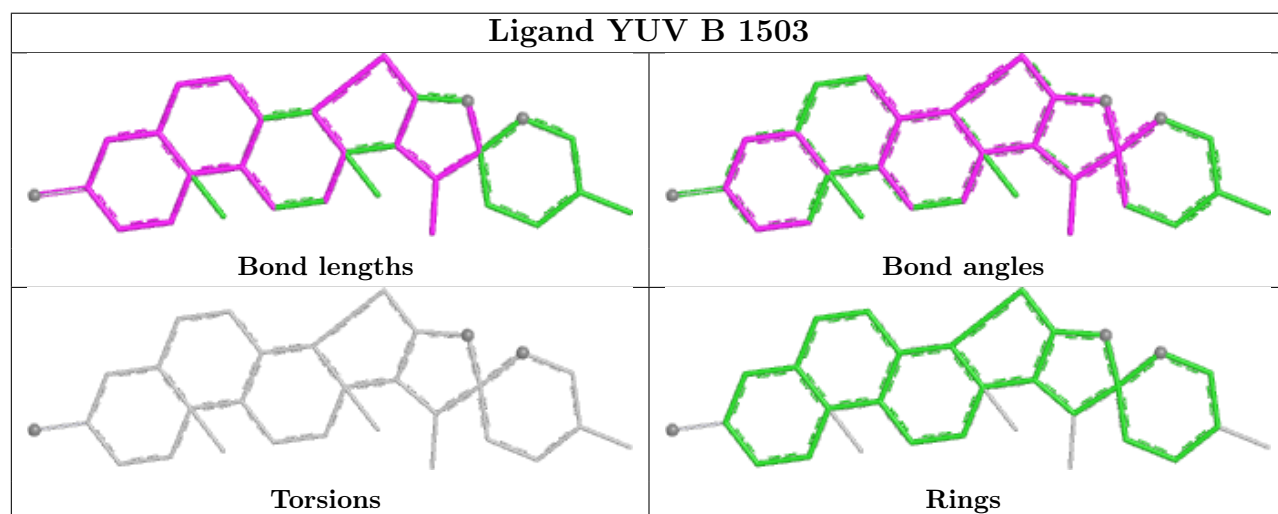
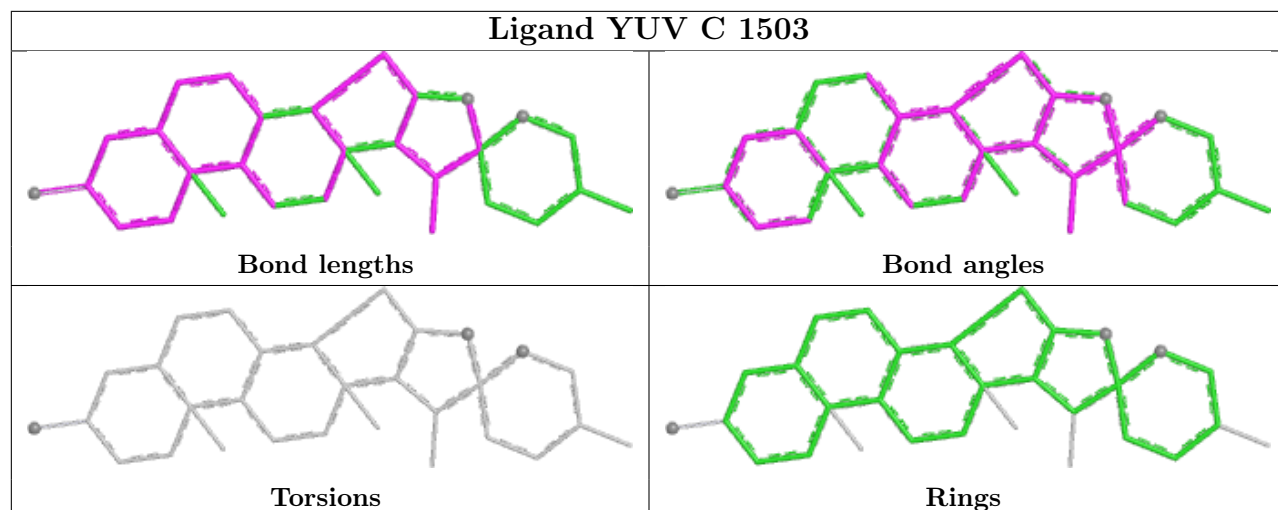


Ligand YUV D 1503

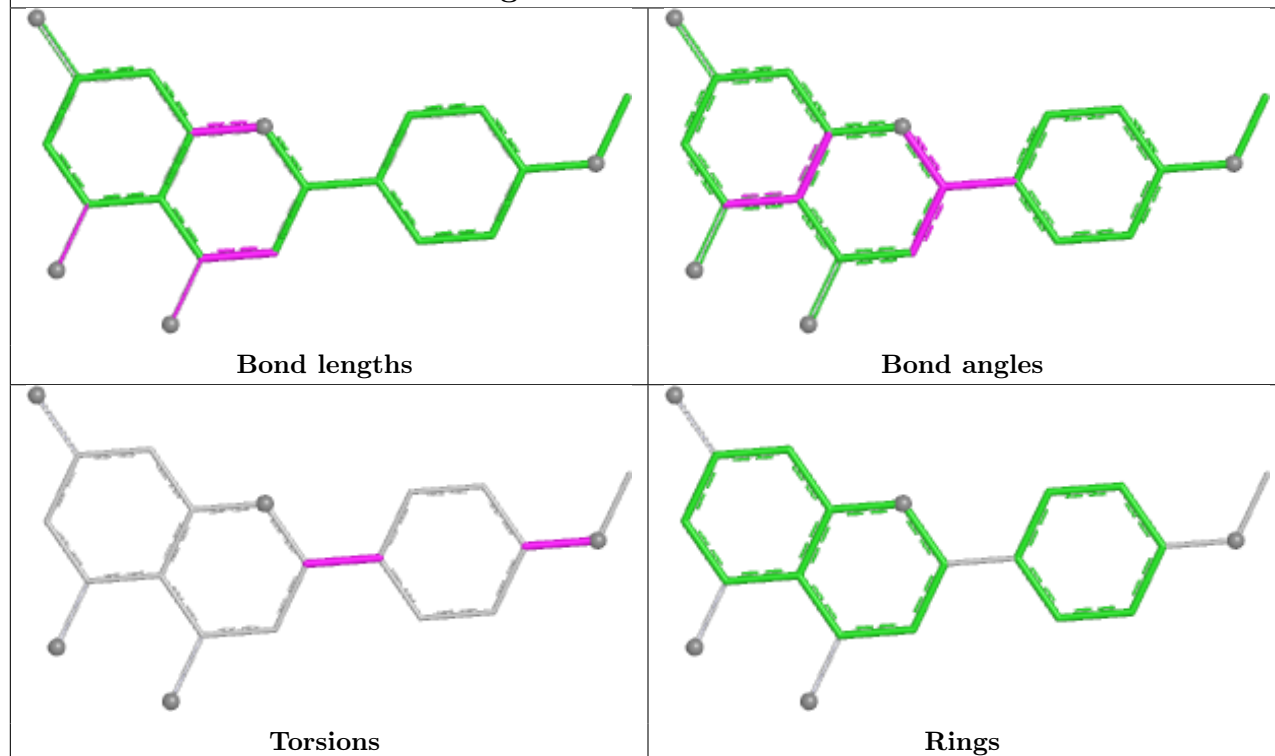


Ligand YUV B 1501

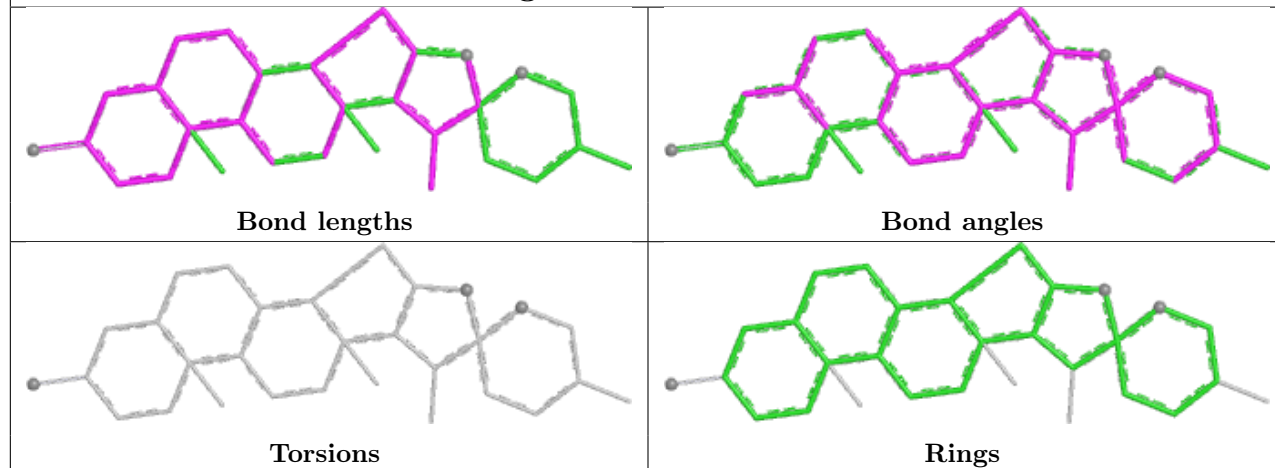


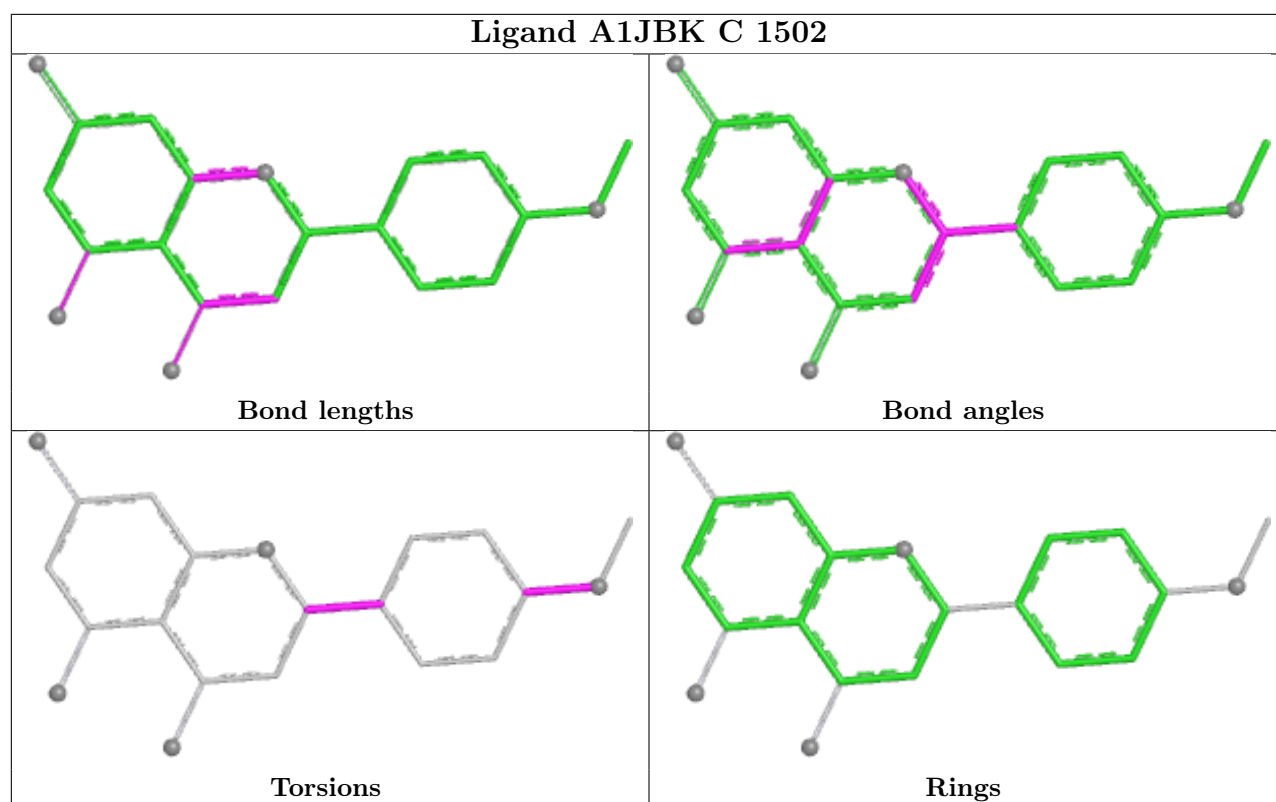


Ligand A1JBK A 1501



Ligand YUV C 1501





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.

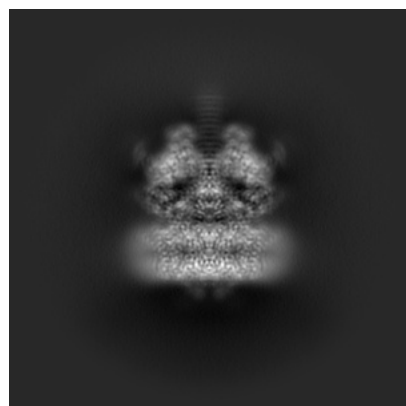
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53176. These allow visual inspection of the internal detail of the map and identification of artifacts.

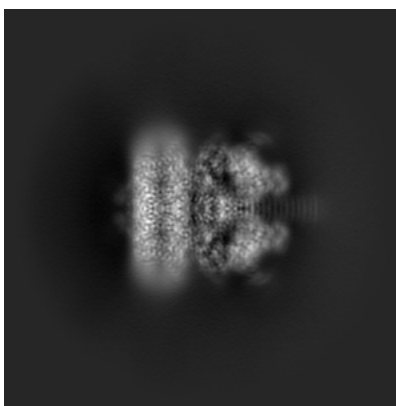
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

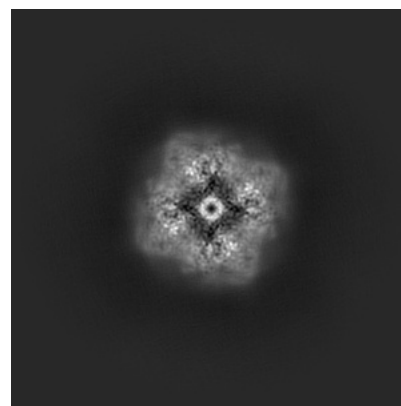
6.1.1 Primary map



X

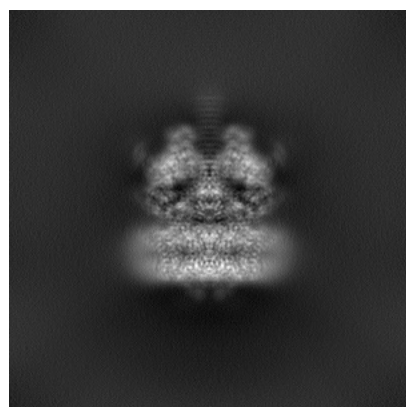


Y

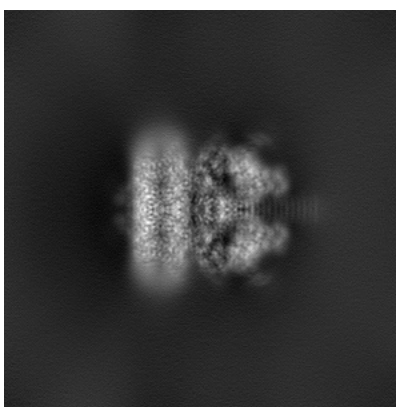


Z

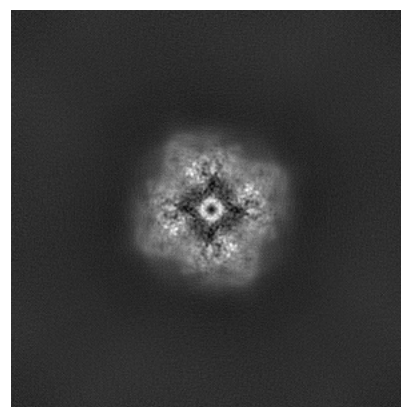
6.1.2 Raw map



X



Y

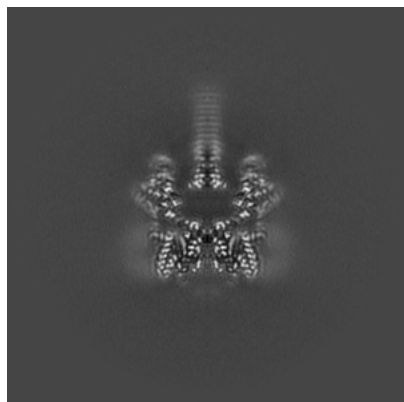


Z

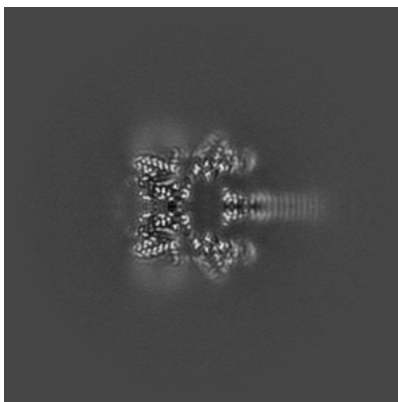
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

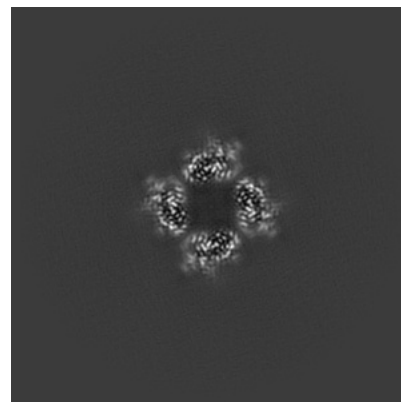
6.2.1 Primary map



X Index: 250

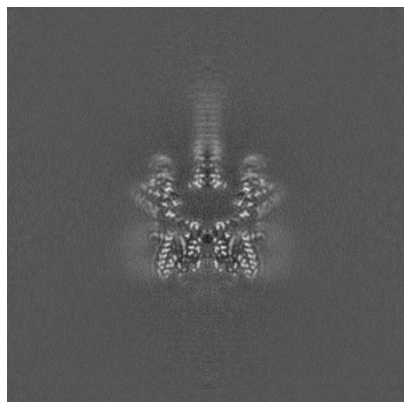


Y Index: 250

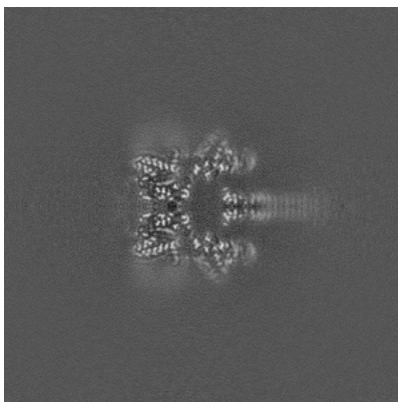


Z Index: 250

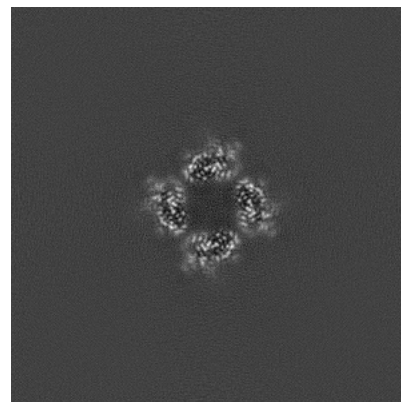
6.2.2 Raw map



X Index: 250



Y Index: 250

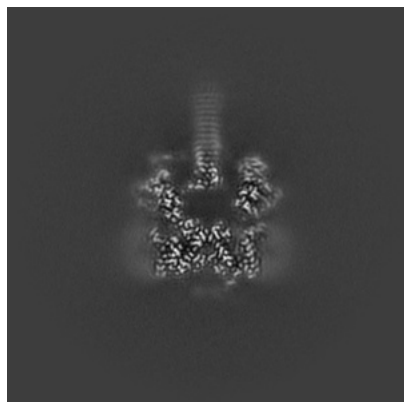


Z Index: 250

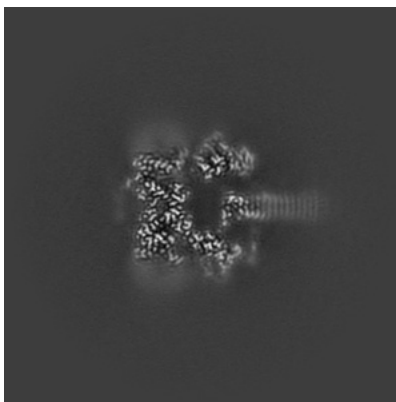
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

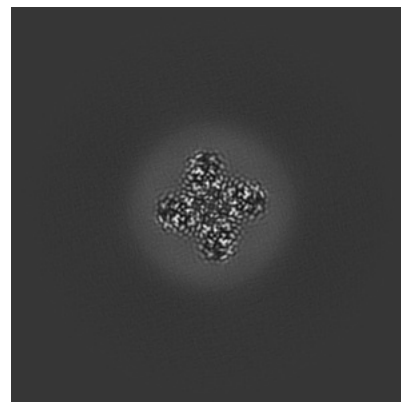
6.3.1 Primary map



X Index: 254

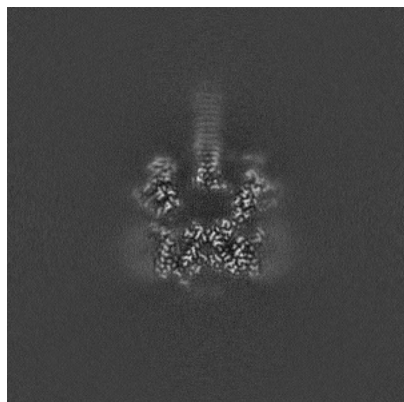


Y Index: 246

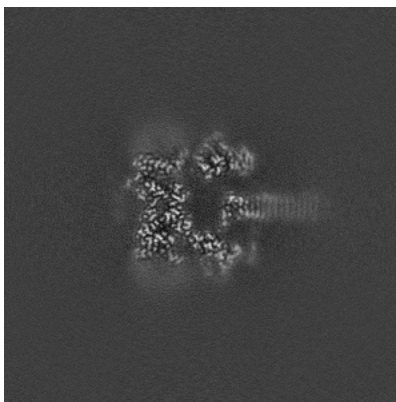


Z Index: 178

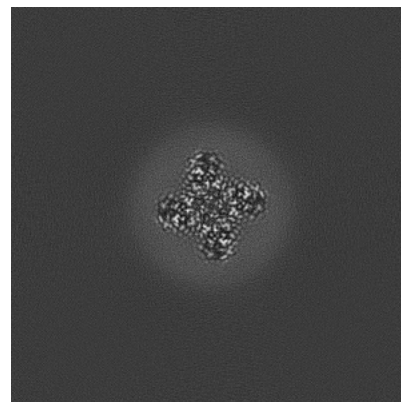
6.3.2 Raw map



X Index: 246



Y Index: 246

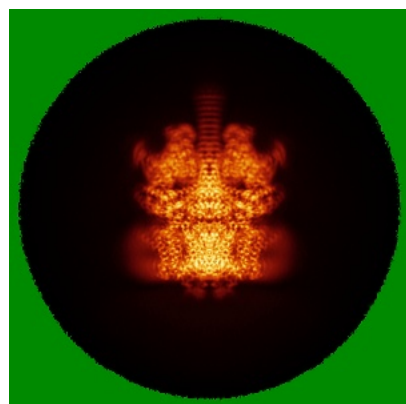


Z Index: 178

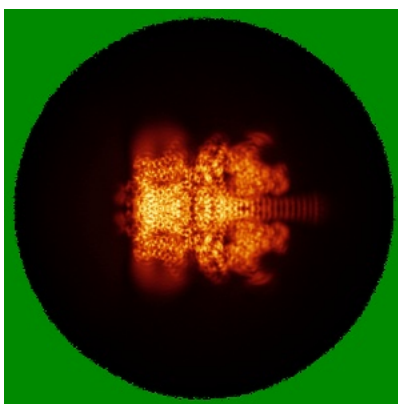
The images above show the largest variance slices of the map in three orthogonal directions.

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

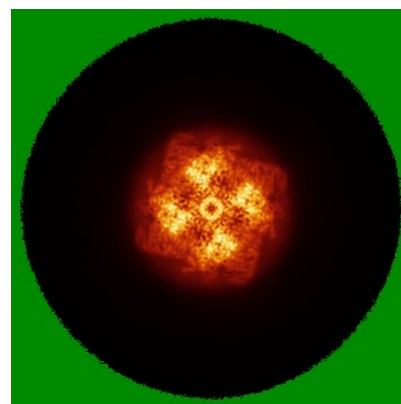
6.4.1 Primary map



X

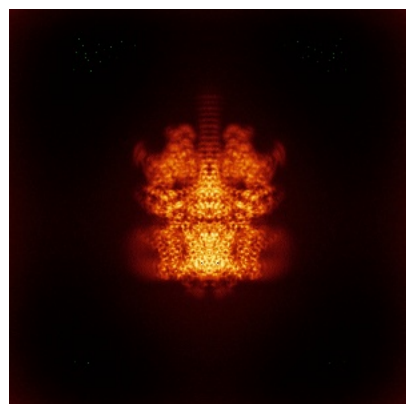


Y

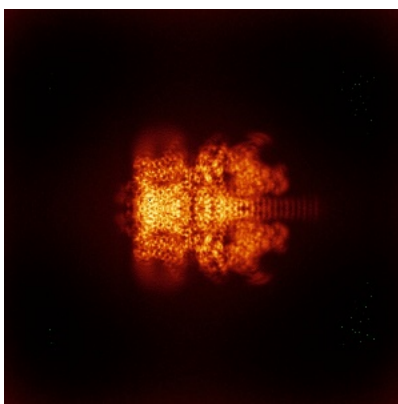


Z

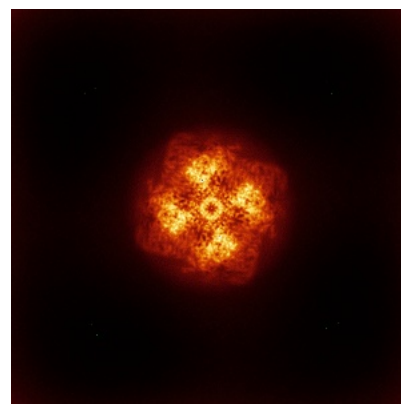
6.4.2 Raw map



X



Y

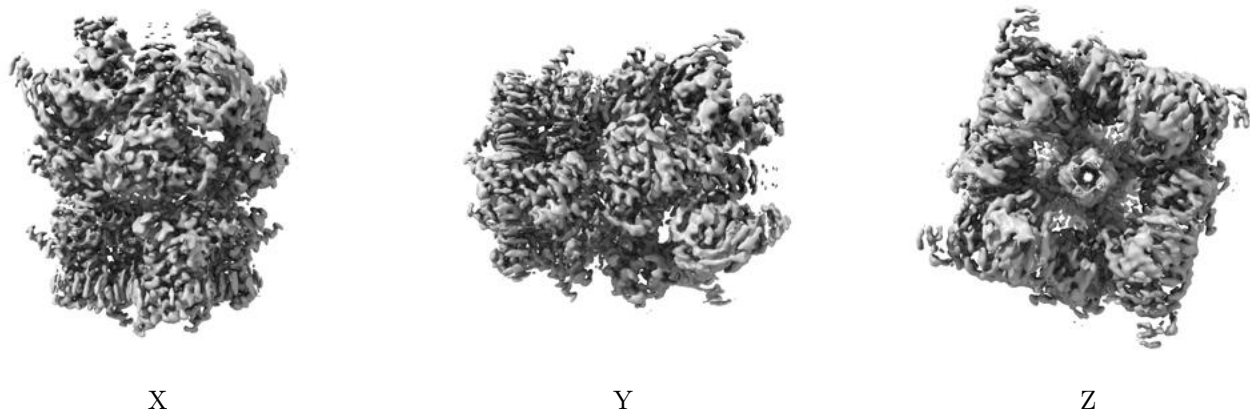


Z

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.

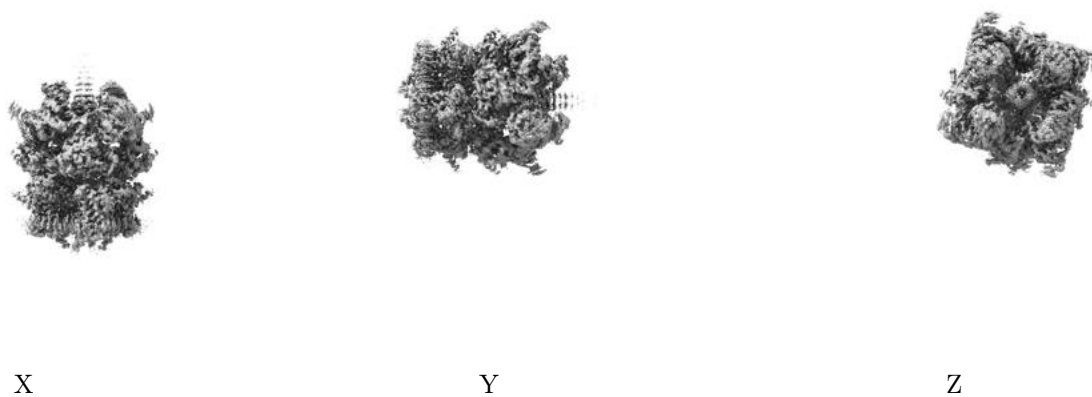
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

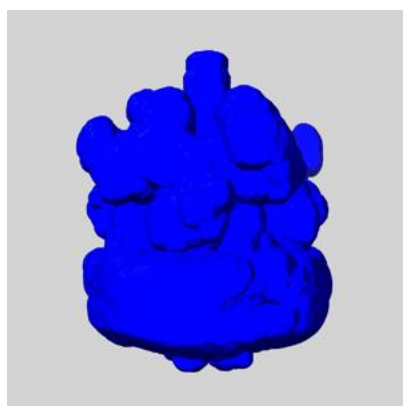
6.6 Mask visualisation [i](#)

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

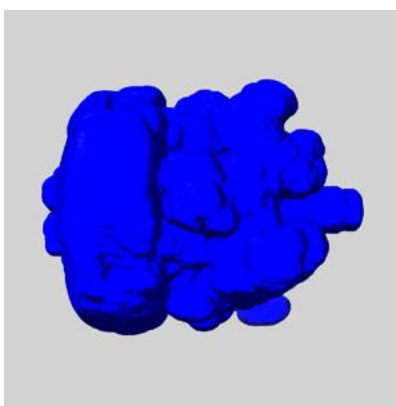
A mask typically either:

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

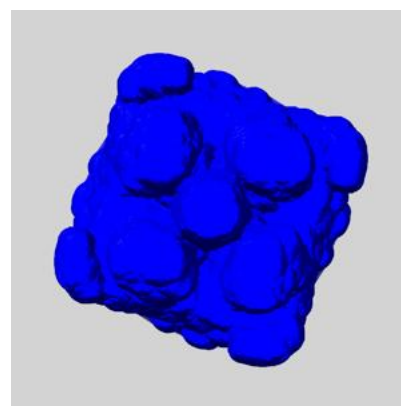
6.6.1 emd_53176_msk_1.map [i](#)



X



Y

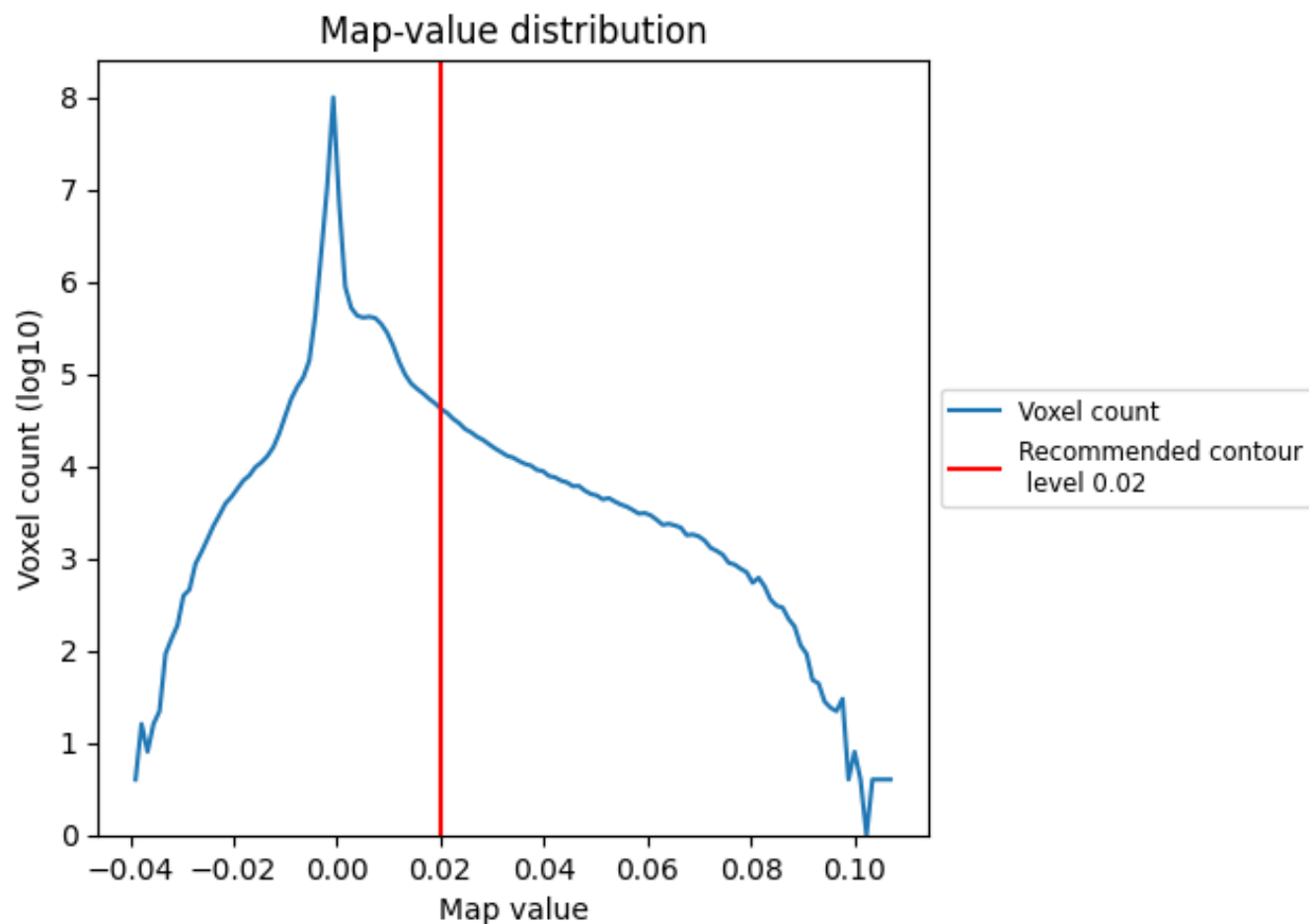


Z

7 Map analysis [i](#)

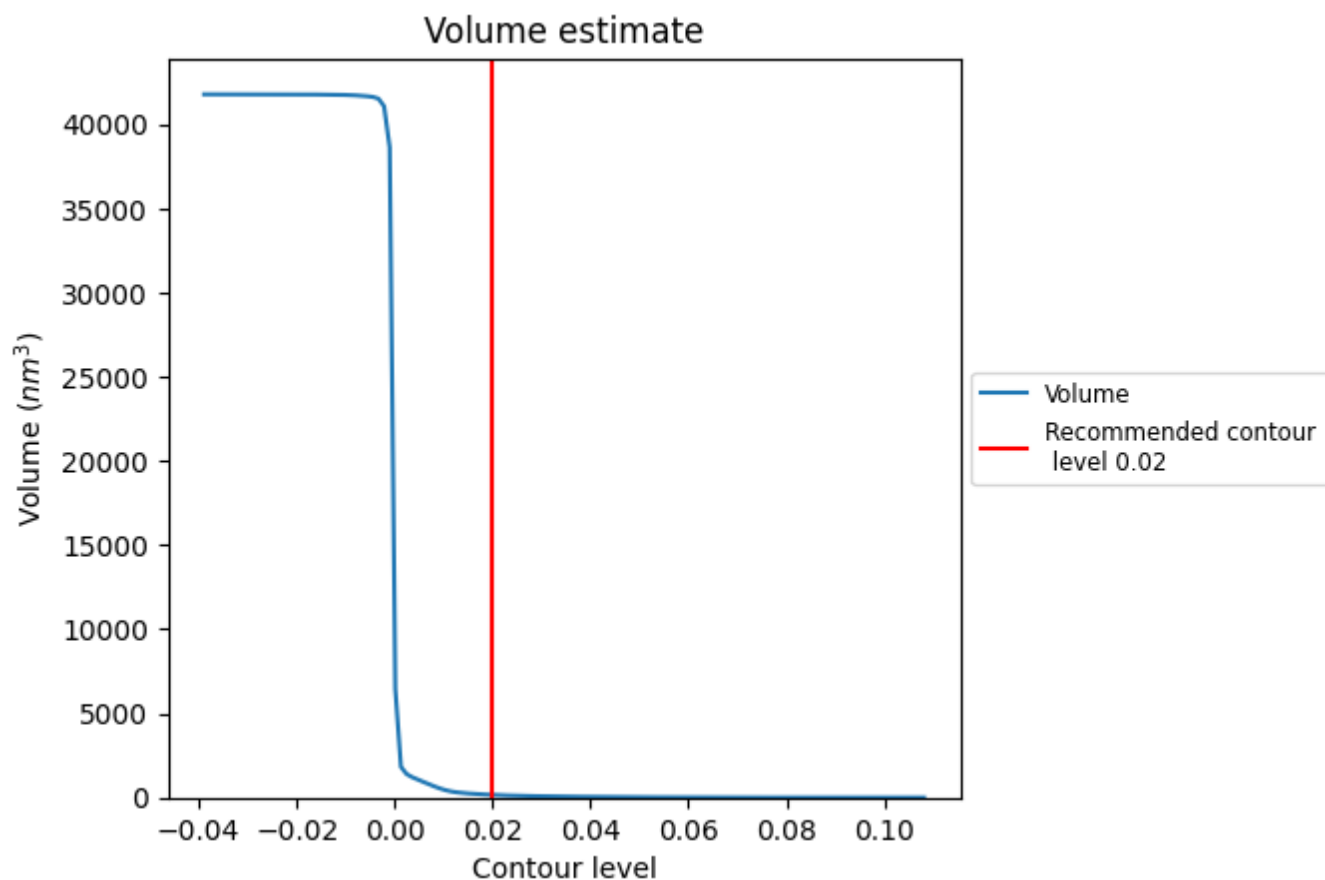
This section contains the results of statistical analysis of the map.

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.

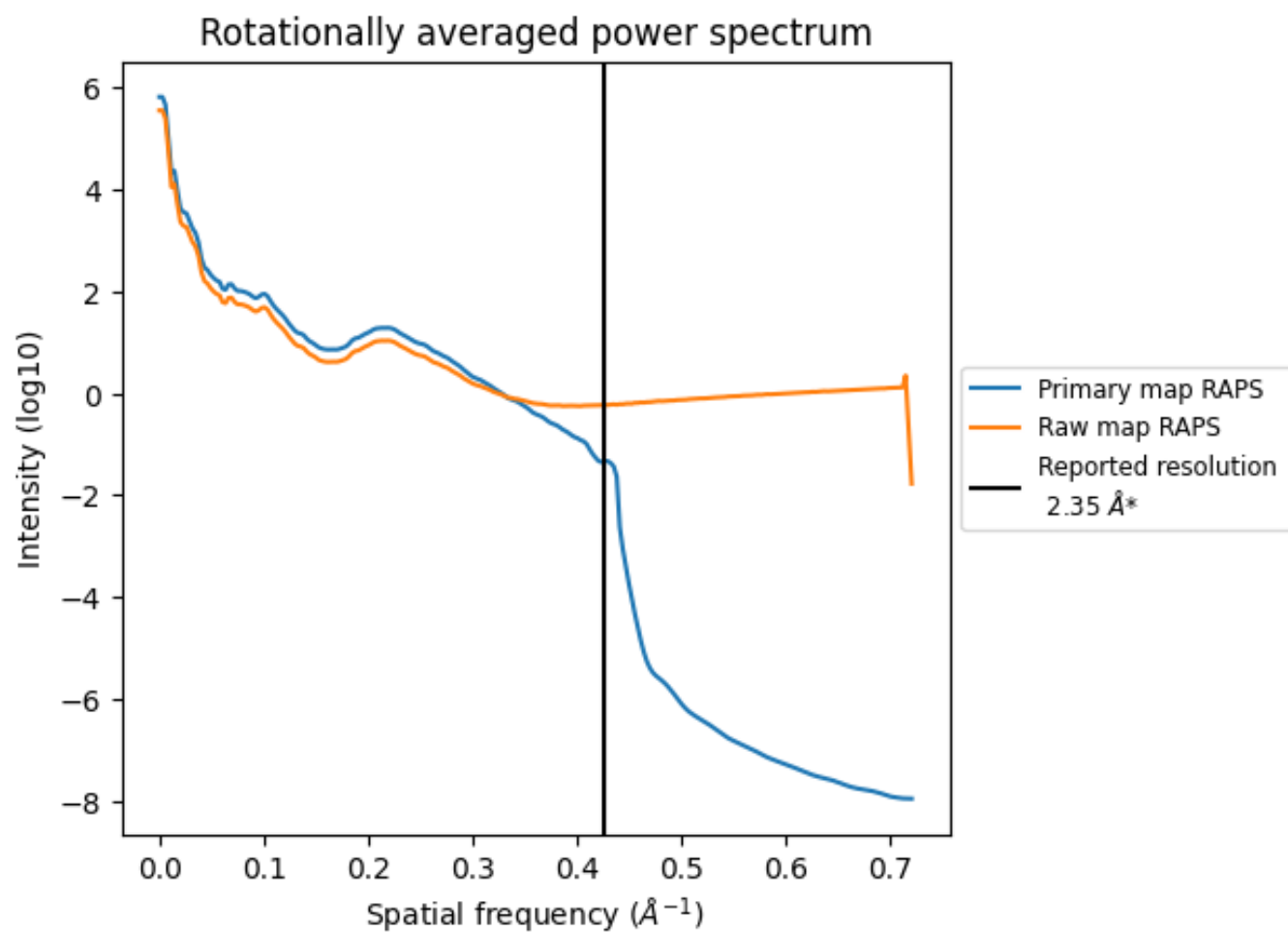
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 159 nm³; this corresponds to an approximate mass of 143 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 ⓘ

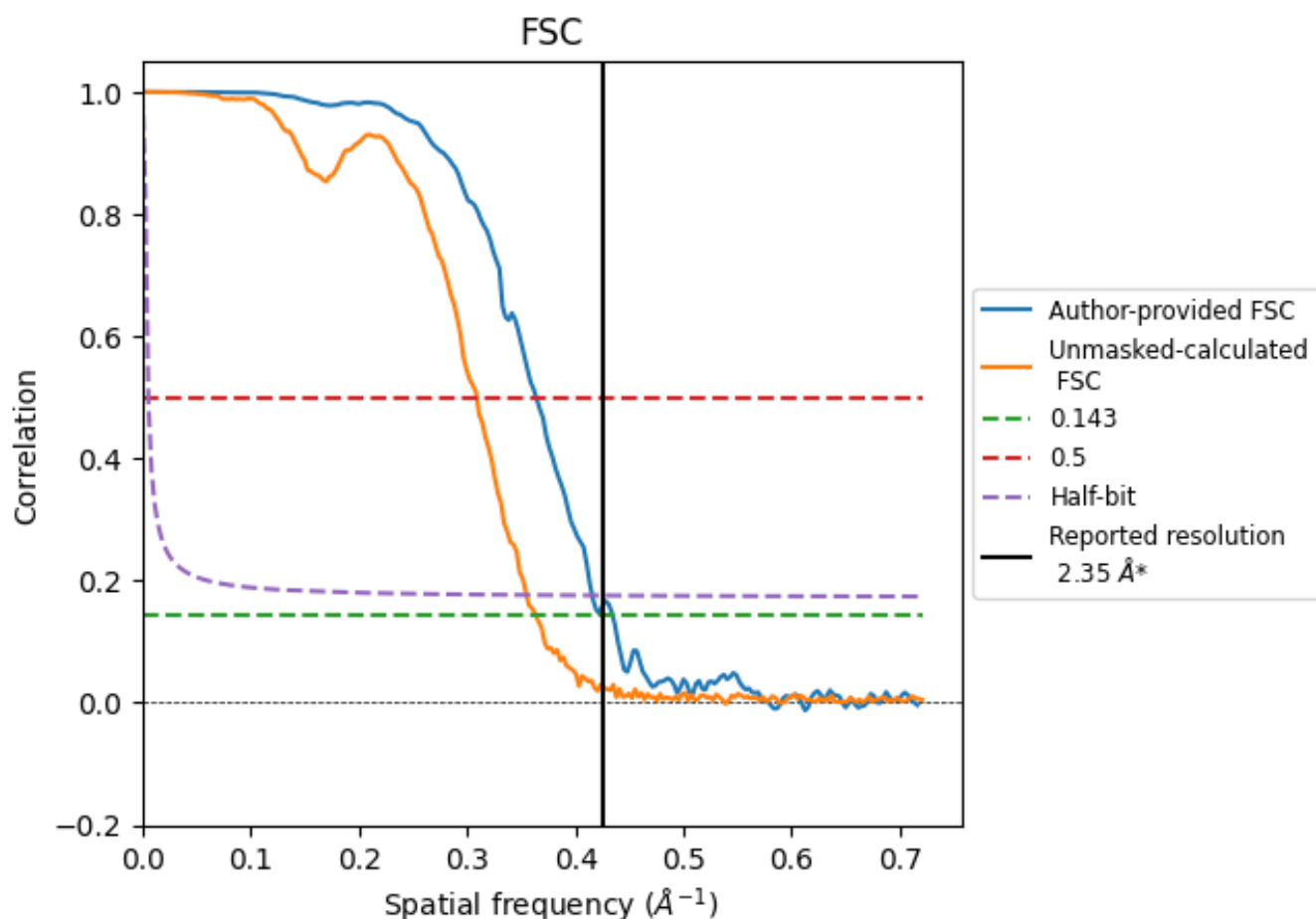


*Reported resolution corresponds to spatial frequency of 0.426 Å⁻¹

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 0.426 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

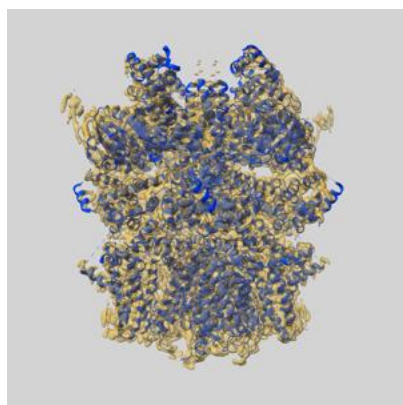
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.35	-	-
Author-provided FSC curve	2.30	2.75	2.41
Unmasked-calculated*	2.75	3.24	2.82

*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 2.75 differs from the reported value 2.35 by more than 10 %

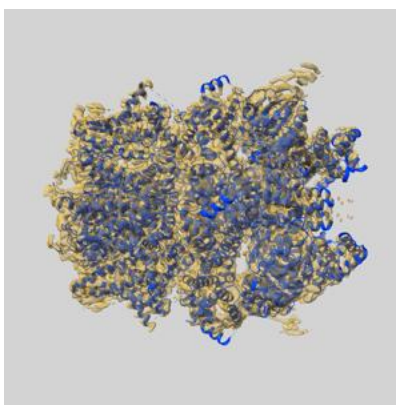
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53176 and PDB model 9QHP. Per-residue inclusion information can be found in section [3](#) on page [13](#).

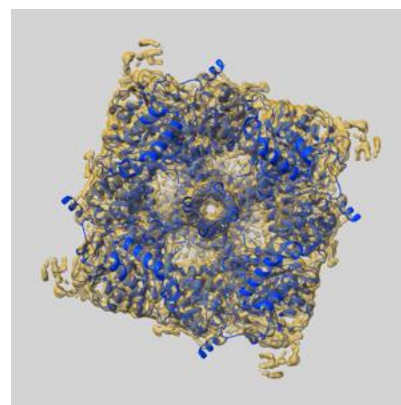
9.1 Map-model overlay [i](#)



X



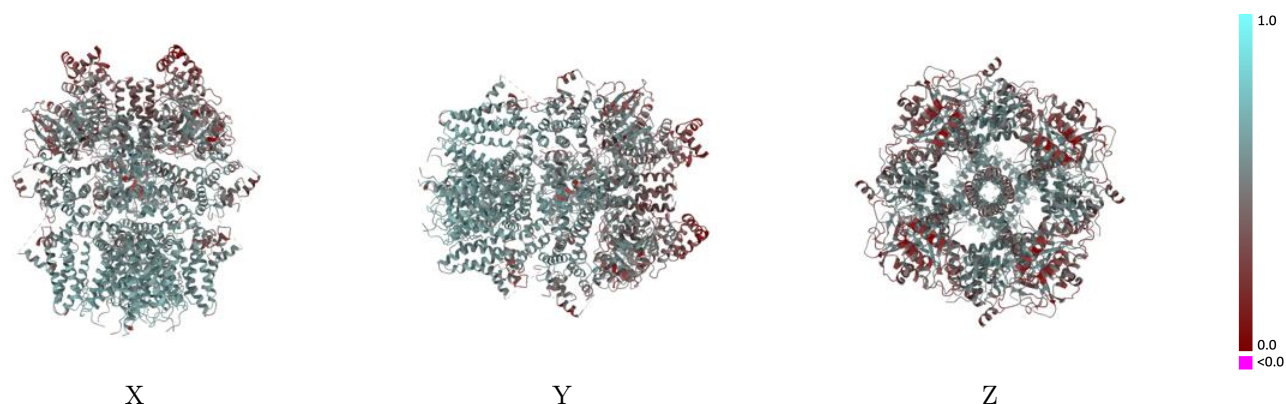
Y



Z

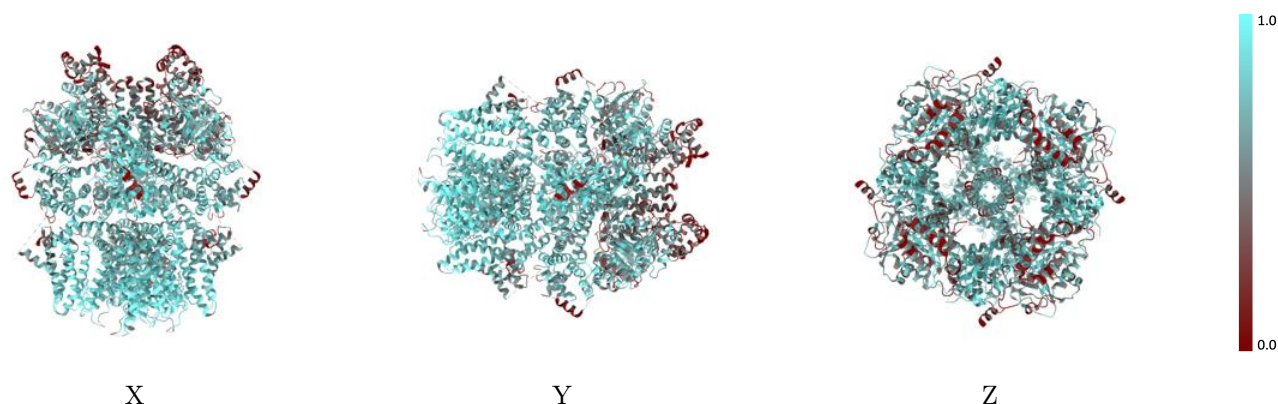
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



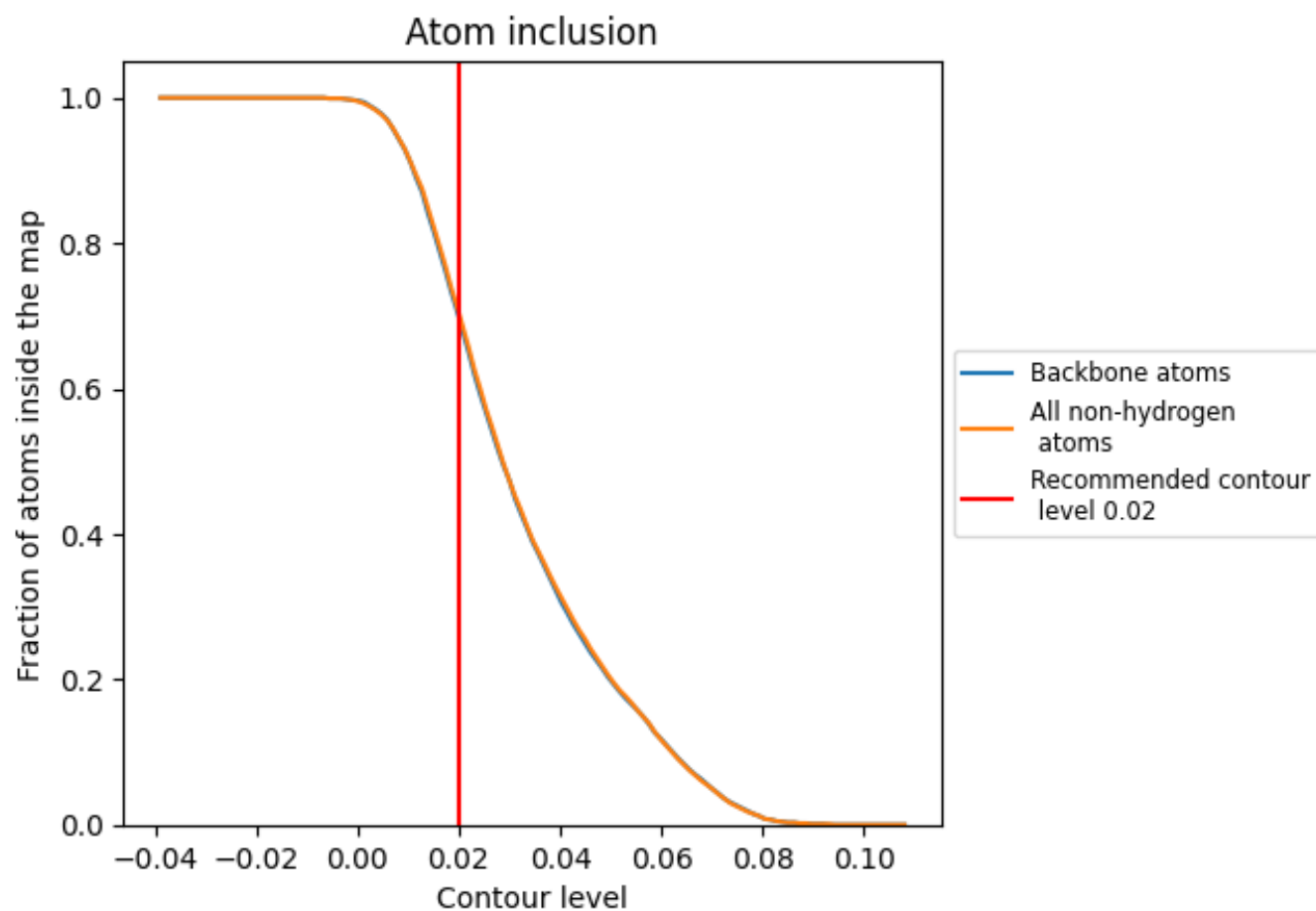
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 70% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7050	0.5020
A	0.7150	0.5030
B	0.7140	0.5000
C	0.7130	0.5020
D	0.7130	0.5020

