



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:44 AM UTC

PDB ID : 8ED9 / pdb_00008ed9
EMDB ID : EMD-28033
Title : cryo-EM structure of TRPM3 ion channel in the presence with PIP2 and PregS, state 2
Authors : Zhao, C.; MacKinnon, R.
Deposited on : 2022-09-03
Resolution : 3.40 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:

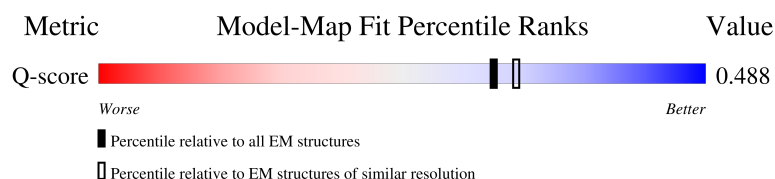
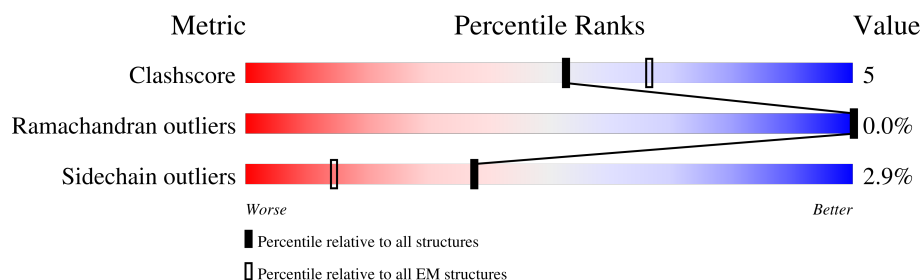
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.40 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	14717 (2.90 - 3.90)

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	1343	6% 62% 10% 28%
1	B	1343	6% 64% 8% 28%
1	C	1343	6% 62% 9% 28%
1	D	1343	6% 63% 8% 28%

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Mol	Chain	Length	Quality of chain
2	E	17	18% 88% 12%
2	F	17	18% 94% 6%
2	G	17	18% 94% 6%
2	H	17	18% 94% 6%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 32229 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

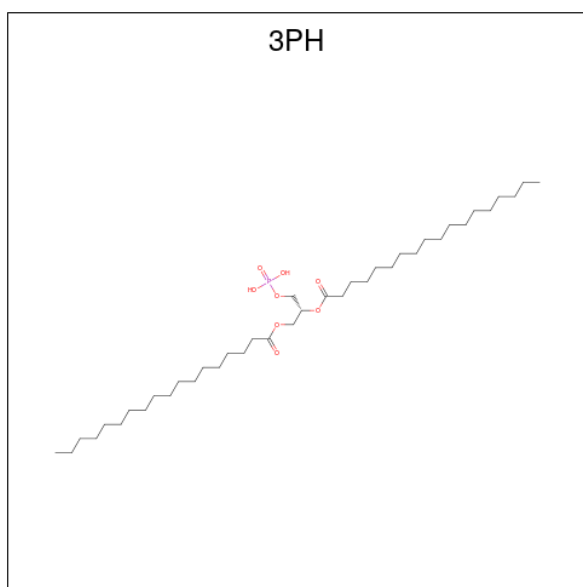
- Molecule 1 is a protein called Transient receptor potential cation channel, subfamily M, member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	968	Total	C	N	O	S	2	0
			7841	5083	1327	1373	58		
1	B	968	Total	C	N	O	S	2	0
			7841	5083	1327	1373	58		
1	C	968	Total	C	N	O	S	2	0
			7841	5083	1327	1373	58		
1	D	968	Total	C	N	O	S	2	0
			7841	5083	1327	1373	58		

- Molecule 2 is a protein called Unidentified segment at the N-terminus of TRPM3.

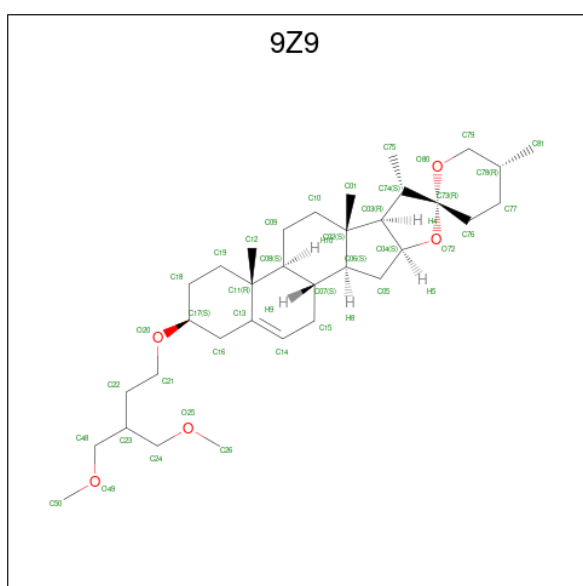
Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	17	Total	C	N	O	0	0
			85	51	17	17		
2	F	17	Total	C	N	O	0	0
			85	51	17	17		
2	G	17	Total	C	N	O	0	0
			85	51	17	17		
2	H	17	Total	C	N	O	0	0
			85	51	17	17		

- Molecule 3 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: C₃₉H₇₇O₈P).



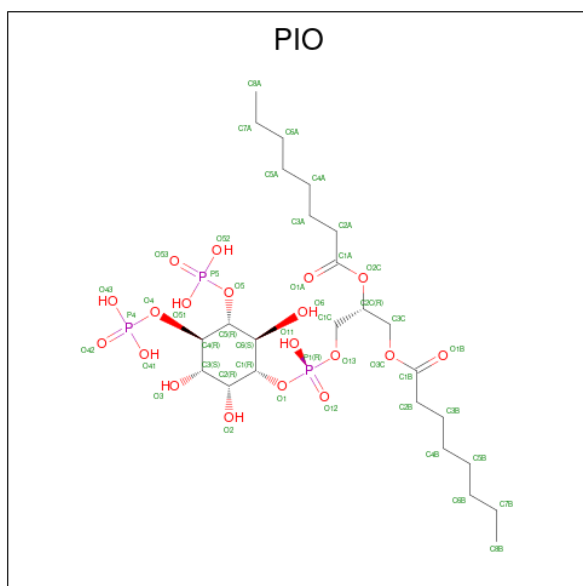
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			45	36	8	1	
3	B	1	Total	C	O	P	0
			45	36	8	1	
3	C	1	Total	C	O	P	0
			45	36	8	1	
3	D	1	Total	C	O	P	0
			45	36	8	1	

- Molecule 4 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (CCD ID: 9Z9) (formula: C₃₄H₅₆O₅).



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

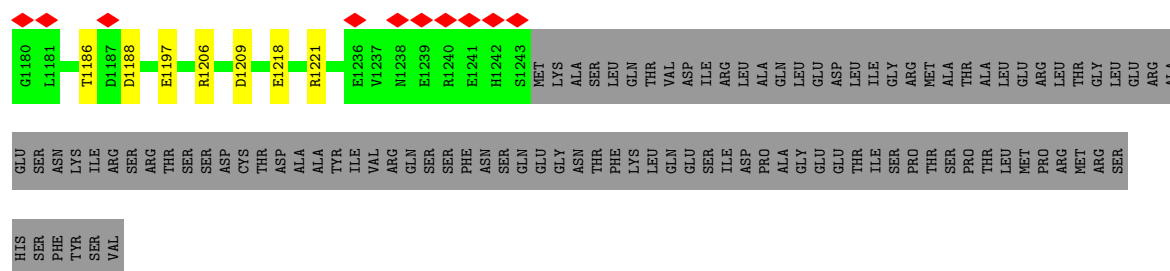
- Molecule 5 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (CCD ID: PIO) (formula: C₂₅H₄₉O₁₉P₃) (labeled as "Ligand of Interest" by depositor).



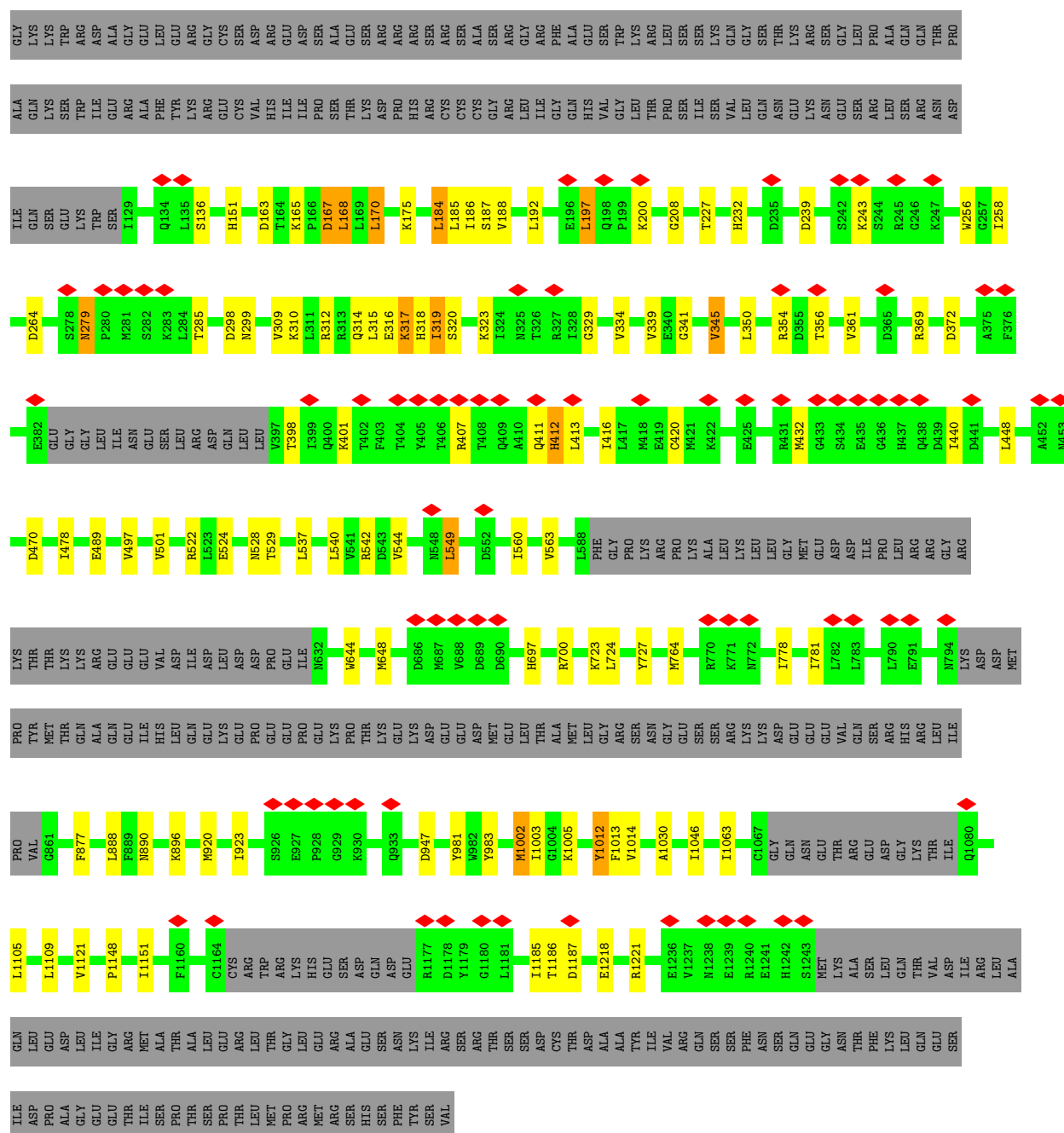
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			47	25	19	3	
5	B	1	Total	C	O	P	0
			47	25	19	3	
5	C	1	Total	C	O	P	0
			47	25	19	3	
5	D	1	Total	C	O	P	0
			47	25	19	3	

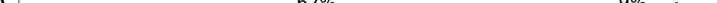
- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Na	0
			1	1	



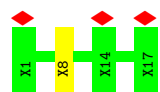
- Molecule 1: Transient receptor potential cation channel, subfamily M, member 3



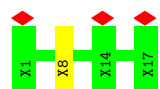
- Chain C:  6% 62% 9% 28%



- Molecule 2: Unidentified segment at the N-terminus of TRPM3



- Molecule 2: Unidentified segment at the N-terminus of TRPM3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	152184	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.865	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.662	Depositor
Minimum map value	-1.595	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	414.72003, 414.72003, 414.72003	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: PIO, 3PH, NA, 9Z9

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	0.14	0/8023	0.28	0/10848
1	B	0.28	0/8023	0.35	1/10848 (0.0%)
1	C	0.28	1/8023 (0.0%)	0.35	1/10848 (0.0%)
1	D	0.15	0/8023	0.30	0/10848
All	All	0.22	1/32092 (0.0%)	0.32	2/43392 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	186	ILE	CA-C	-5.02	1.46	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	319	ILE	N-CA-C	-10.14	103.60	113.53
1	B	319	ILE	N-CA-C	-8.99	104.39	113.47

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	7841	0	7955	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7841	0	7955	71	0
1	C	7841	0	7955	79	0
1	D	7841	0	7955	61	0
2	E	85	0	23	2	0
2	F	85	0	23	1	0
2	G	85	0	23	1	0
2	H	85	0	23	1	0
3	A	45	0	66	1	0
3	B	45	0	66	0	0
3	C	45	0	66	2	0
3	D	45	0	66	1	0
4	A	39	0	0	15	0
4	B	39	0	0	15	0
4	C	39	0	0	15	0
4	D	39	0	0	15	0
5	A	47	0	44	1	0
5	B	47	0	44	0	0
5	C	47	0	44	1	0
5	D	47	0	44	0	0
6	B	1	0	0	0	0
All	All	32229	0	32352	340	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 5.

All (340) 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)
4:A:1402:9Z9:C73	4:A:1402:9Z9:C74	1.81	1.59
4:D:1402:9Z9:C74	4:D:1402:9Z9:C73	1.81	1.56
4:A:1402:9Z9:C06	4:A:1402:9Z9:C07	1.84	1.55
4:C:1402:9Z9:C73	4:C:1402:9Z9:C74	1.81	1.55
4:B:1402:9Z9:C07	4:B:1402:9Z9:C06	1.84	1.55
4:B:1402:9Z9:C73	4:B:1402:9Z9:C74	1.81	1.53
4:C:1402:9Z9:C06	4:C:1402:9Z9:C07	1.84	1.53
4:D:1402:9Z9:C06	4:D:1402:9Z9:C07	1.84	1.53
4:A:1402:9Z9:C74	4:A:1402:9Z9:C75	1.90	1.50
4:B:1402:9Z9:C74	4:B:1402:9Z9:C75	1.90	1.49
4:C:1402:9Z9:C74	4:C:1402:9Z9:C75	1.90	1.47
4:D:1402:9Z9:C74	4:D:1402:9Z9:C75	1.90	1.47
4:B:1402:9Z9:C75	4:B:1402:9Z9:C03	2.32	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1402:9Z9:C75	4:C:1402:9Z9:C03	2.32	1.06
4:D:1402:9Z9:C75	4:D:1402:9Z9:C03	2.32	1.06
4:A:1402:9Z9:C75	4:A:1402:9Z9:C03	2.32	1.04
4:B:1402:9Z9:C06	4:B:1402:9Z9:C02	1.78	1.00
4:D:1402:9Z9:C06	4:D:1402:9Z9:C02	1.78	0.98
4:A:1402:9Z9:C06	4:A:1402:9Z9:C02	1.78	0.97
4:D:1402:9Z9:C74	4:D:1402:9Z9:O80	2.14	0.96
4:B:1402:9Z9:C74	4:B:1402:9Z9:O80	2.14	0.95
4:C:1402:9Z9:C74	4:C:1402:9Z9:O80	2.14	0.95
4:C:1402:9Z9:C06	4:C:1402:9Z9:C02	1.78	0.95
4:A:1402:9Z9:C74	4:A:1402:9Z9:O80	2.14	0.94
4:A:1402:9Z9:C07	4:A:1402:9Z9:C05	2.51	0.86
4:B:1402:9Z9:C07	4:B:1402:9Z9:C05	2.51	0.85
4:D:1402:9Z9:C07	4:D:1402:9Z9:C05	2.51	0.84
4:C:1402:9Z9:C07	4:C:1402:9Z9:C05	2.51	0.82
4:C:1402:9Z9:C06	4:C:1402:9Z9:C15	2.61	0.79
4:B:1402:9Z9:C06	4:B:1402:9Z9:C15	2.61	0.78
4:A:1402:9Z9:C06	4:A:1402:9Z9:C15	2.61	0.78
4:D:1402:9Z9:C06	4:D:1402:9Z9:C15	2.61	0.76
4:D:1402:9Z9:C06	4:D:1402:9Z9:C10	2.64	0.76
4:B:1402:9Z9:C06	4:B:1402:9Z9:C10	2.64	0.76
4:A:1402:9Z9:C06	4:A:1402:9Z9:C10	2.64	0.75
4:C:1402:9Z9:C06	4:C:1402:9Z9:C10	2.64	0.75
1:A:1063:ILE:HD13	1:A:1095:MET:HE1	1.69	0.74
4:A:1402:9Z9:C06	4:A:1402:9Z9:C08	2.69	0.71
4:B:1402:9Z9:C75	4:B:1402:9Z9:O80	2.39	0.71
4:A:1402:9Z9:C75	4:A:1402:9Z9:O80	2.39	0.71
4:B:1402:9Z9:C06	4:B:1402:9Z9:C08	2.69	0.71
4:C:1402:9Z9:C75	4:C:1402:9Z9:O80	2.39	0.71
4:D:1402:9Z9:C75	4:D:1402:9Z9:O80	2.39	0.71
4:C:1402:9Z9:C06	4:C:1402:9Z9:C08	2.69	0.70
4:D:1402:9Z9:C06	4:D:1402:9Z9:C08	2.69	0.70
1:A:893:VAL:HG21	1:A:979:ILE:HD13	1.73	0.69
4:C:1402:9Z9:C06	4:C:1402:9Z9:C01	2.73	0.67
4:A:1402:9Z9:C06	4:A:1402:9Z9:C01	2.73	0.65
4:B:1402:9Z9:C06	4:B:1402:9Z9:C01	2.73	0.65
1:C:981:TYR:HB2	3:C:1401:3PH:H3C2	1.80	0.64
4:D:1402:9Z9:C06	4:D:1402:9Z9:C01	2.73	0.63
1:D:1002:MET:HG2	1:D:1121:VAL:HG12	1.81	0.62
1:B:407:ARG:HB2	1:B:411:GLN:HB3	1.82	0.62
1:B:316:GLU:O	1:B:319:ILE:HG22	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:ILE:HD12	1:A:1064:ASP:H	1.65	0.61
1:C:407:ARG:HB2	1:C:411:GLN:HB3	1.81	0.61
1:C:208:GLY:HA3	1:C:440:ILE:HB	1.82	0.61
1:B:407:ARG:HH21	1:B:411:GLN:HE21	1.50	0.60
1:B:1005:LYS:HD2	1:B:1121:VAL:HG13	1.82	0.59
1:B:1030:ALA:O	1:C:972:ARG:NH1	2.30	0.59
1:B:350:LEU:HD13	1:B:416:ILE:HG23	1.84	0.58
1:C:238:LYS:HG3	1:C:290:MET:HG3	1.84	0.58
1:D:890:ASN:ND2	1:D:983:TYR:OH	2.35	0.58
1:A:1005:LYS:HD2	1:A:1121:VAL:HG13	1.85	0.58
1:C:1005:LYS:HD2	1:C:1121:VAL:HG13	1.84	0.58
1:B:890:ASN:ND2	1:B:983:TYR:OH	2.34	0.58
1:A:350:LEU:HD22	1:A:416:ILE:HG23	1.86	0.58
1:A:768:ARG:NH1	1:A:792:PHE:O	2.37	0.57
1:C:489:GLU:OE2	1:C:522:ARG:NE	2.32	0.57
1:C:256:TRP:HB3	1:C:298:ASP:HB3	1.87	0.57
1:D:256:TRP:HB3	1:D:298:ASP:HB3	1.86	0.57
1:A:1002:MET:HG2	1:A:1121:VAL:HG12	1.87	0.57
1:B:256:TRP:HB3	1:B:298:ASP:HB3	1.87	0.57
1:D:556:SER:OG	1:D:559:ASP:OD1	2.23	0.57
1:A:890:ASN:ND2	1:A:983:TYR:OH	2.37	0.57
1:D:508:ILE:HD11	1:D:514:MET:HE2	1.86	0.57
1:A:972:ARG:NH1	1:D:1030:ALA:O	2.32	0.57
1:A:185:LEU:HB3	1:A:334:VAL:HG12	1.88	0.56
1:B:208:GLY:HA3	1:B:440:ILE:HB	1.87	0.56
1:D:489:GLU:OE2	1:D:522:ARG:NE	2.31	0.55
1:A:1060:ALA:HA	1:A:1063:ILE:HD11	1.89	0.55
1:A:279:ASN:ND2	1:A:281:MET:SD	2.76	0.55
1:C:317:LYS:O	1:C:320:SER:N	2.39	0.55
1:B:398:THR:O	1:B:401:LYS:NZ	2.37	0.55
1:A:524:GLU:O	1:A:528:ASN:ND2	2.38	0.55
1:B:524:GLU:O	1:B:528:ASN:ND2	2.37	0.54
1:C:990:PHE:HE1	5:C:1403:PIO:H5B	1.73	0.54
1:B:341:GLY:HA3	1:B:345:VAL:HG11	1.90	0.54
1:A:508:ILE:HD11	1:A:514:MET:HE2	1.90	0.54
1:C:508:ILE:HD11	1:C:514:MET:HE2	1.90	0.54
1:B:489:GLU:OE2	1:B:522:ARG:NE	2.31	0.54
1:C:259:VAL:HG23	1:C:262:GLN:HG3	1.90	0.54
1:B:323:LYS:NZ	1:B:329:GLY:O	2.40	0.54
1:A:981:TYR:HB2	3:A:1401:3PH:H3C2	1.89	0.54
1:D:138:THR:O	1:D:268:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1005:LYS:HD2	1:D:1121:VAL:HG13	1.88	0.53
1:B:317:LYS:O	1:B:320:SER:N	2.42	0.53
1:D:136:SER:O	2:H:8:UNK:N	2.42	0.53
1:C:993:ASN:HD22	1:C:995:TYR:H	1.58	0.52
1:C:239:ASP:O	1:C:243:LYS:NZ	2.41	0.52
1:A:346:ILE:HD11	1:A:370:ALA:HB1	1.89	0.52
1:B:188:VAL:O	1:B:312:ARG:NH2	2.40	0.52
1:C:317:LYS:C	1:C:319:ILE:H	2.16	0.52
1:C:524:GLU:O	1:C:528:ASN:ND2	2.38	0.52
1:A:194:ASN:HD22	1:A:231:ARG:HH21	1.58	0.52
1:B:947:ASP:OD1	1:B:981:TYR:OH	2.26	0.52
1:B:318:HIS:CG	1:B:318:HIS:O	2.63	0.52
1:B:317:LYS:C	1:B:319:ILE:H	2.18	0.52
1:A:990:PHE:HE1	5:A:1403:PIO:H6BA	1.75	0.51
1:B:165:LYS:HB2	1:B:168:LEU:HD23	1.93	0.51
1:C:947:ASP:OD2	1:C:985:ARG:NH2	2.42	0.51
1:D:402:THR:OG1	1:D:409:GLN:NE2	2.43	0.51
1:C:1218:GLU:OE2	1:C:1221:ARG:NH2	2.39	0.51
1:D:947:ASP:OD1	1:D:981:TYR:OH	2.25	0.51
1:B:186:ILE:HG22	1:B:186:ILE:O	2.09	0.51
1:C:318:HIS:CG	1:C:318:HIS:O	2.63	0.51
1:B:542:ARG:HG2	1:B:549:LEU:HD13	1.92	0.51
1:A:167:ASP:N	1:A:167:ASP:OD1	2.44	0.51
1:B:167:ASP:OD1	1:B:167:ASP:N	2.42	0.51
1:C:688:VAL:HG23	1:C:690:ASP:H	1.76	0.51
1:D:524:GLU:O	1:D:528:ASN:ND2	2.38	0.51
1:D:688:VAL:HG23	1:D:690:ASP:H	1.76	0.51
1:C:173:MET:HE1	1:C:315:LEU:HD21	1.93	0.50
1:D:167:ASP:N	1:D:167:ASP:OD1	2.45	0.50
1:A:993:ASN:HD22	1:A:995:TYR:H	1.59	0.50
4:B:1402:9Z9:C07	4:B:1402:9Z9:C02	2.89	0.50
1:C:976:CYS:O	1:C:979:ILE:HG12	2.12	0.50
1:D:524:GLU:OE2	1:D:585:TYR:OH	2.23	0.50
1:C:890:ASN:ND2	1:C:983:TYR:OH	2.37	0.50
1:C:167:ASP:OD1	1:C:167:ASP:N	2.43	0.50
1:C:317:LYS:C	1:C:319:ILE:N	2.69	0.50
1:A:208:GLY:HA3	1:A:440:ILE:HB	1.93	0.50
1:B:136:SER:O	2:F:8:UNK:N	2.45	0.50
1:C:136:SER:O	2:G:8:UNK:N	2.45	0.50
1:A:259:VAL:HG23	1:A:262:GLN:HG3	1.94	0.49
1:C:768:ARG:O	1:C:770:ARG:NE	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1218:GLU:OE2	1:D:1221:ARG:NH2	2.39	0.49
1:A:1006:MET:HG3	1:D:1109:LEU:HD13	1.94	0.49
1:D:175:LYS:O	1:D:178:GLN:NE2	2.43	0.49
1:C:644:TRP:NE1	1:C:648:MET:SD	2.86	0.49
1:A:644:TRP:NE1	1:A:648:MET:SD	2.86	0.49
1:A:768:ARG:O	1:A:770:ARG:NE	2.46	0.49
1:D:1081:LEU:HD12	1:D:1082:PRO:HD2	1.95	0.49
1:A:421:MET:HA	1:A:424:LYS:HB2	1.94	0.48
1:A:975:TYR:O	1:A:979:ILE:HG23	2.13	0.48
4:D:1402:9Z9:C06	4:D:1402:9Z9:C09	2.91	0.48
1:A:1053:MET:HE1	1:A:1095:MET:HG3	1.95	0.48
1:C:259:VAL:O	1:C:262:GLN:NE2	2.47	0.48
1:D:993:ASN:ND2	1:D:995:TYR:H	2.12	0.48
1:A:136:SER:O	2:E:8:UNK:N	2.47	0.48
1:A:993:ASN:ND2	1:A:995:TYR:H	2.12	0.48
1:C:1053:MET:HE1	1:C:1095:MET:HG3	1.95	0.48
4:A:1402:9Z9:C06	4:A:1402:9Z9:C09	2.91	0.48
1:C:1007:MET:HE1	3:C:1401:3PH:H251	1.93	0.48
4:D:1402:9Z9:C07	4:D:1402:9Z9:C02	2.89	0.48
4:C:1402:9Z9:C06	4:C:1402:9Z9:C09	2.91	0.48
4:A:1402:9Z9:C07	4:A:1402:9Z9:C02	2.89	0.48
1:B:314:GLN:O	1:B:315:LEU:C	2.51	0.48
1:C:314:GLN:O	1:C:315:LEU:C	2.51	0.48
1:B:258:ILE:HG22	1:B:285:THR:HG22	1.96	0.47
1:B:413:LEU:HD22	1:B:416:ILE:HD12	1.96	0.47
1:C:258:ILE:HG22	1:C:285:THR:HG22	1.97	0.47
1:C:993:ASN:ND2	1:C:995:TYR:H	2.11	0.47
1:B:644:TRP:NE1	1:B:648:MET:SD	2.87	0.47
4:B:1402:9Z9:C06	4:B:1402:9Z9:C09	2.91	0.47
1:D:993:ASN:HD22	1:D:995:TYR:H	1.62	0.47
1:B:187:SER:OG	1:B:316:GLU:OE2	2.28	0.47
4:C:1402:9Z9:C07	4:C:1402:9Z9:C02	2.89	0.47
1:D:353:LEU:HG	1:D:426:LEU:HD12	1.96	0.47
1:D:401:LYS:HB2	1:D:411:GLN:HE22	1.78	0.47
1:A:340:GLU:HG3	1:A:369:ARG:HG2	1.97	0.47
1:D:260:GLU:N	1:D:285:THR:O	2.48	0.47
1:A:1105:LEU:HD21	1:B:1003:ILE:HG23	1.97	0.47
1:A:1148:PRO:HA	1:A:1151:ILE:HB	1.97	0.47
1:C:165:LYS:HB2	1:C:168:LEU:HD23	1.97	0.47
1:C:186:ILE:O	1:C:186:ILE:HG22	2.14	0.47
1:C:194:ASN:HD22	1:C:231:ARG:HH21	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:GLY:HA3	1:D:440:ILE:HB	1.96	0.46
1:B:723:LYS:HZ2	1:B:1185:ILE:HD13	1.81	0.46
1:C:975:TYR:O	1:C:979:ILE:HG23	2.15	0.46
1:A:333:PRO:HB2	1:A:448:LEU:HD11	1.96	0.46
1:D:324:ILE:HG23	1:D:326:THR:H	1.81	0.46
1:A:345:VAL:HA	1:A:348:ILE:HG12	1.97	0.46
1:C:185:LEU:HD23	1:C:186:ILE:N	2.30	0.46
1:C:978:ASN:HD22	1:C:982:TRP:HE1	1.62	0.46
1:D:205:PHE:HA	1:D:440:ILE:HG13	1.98	0.46
1:A:205:PHE:HA	1:A:440:ILE:HG13	1.97	0.46
1:A:489:GLU:HG2	1:A:517:PHE:HD1	1.80	0.46
1:C:1148:PRO:HA	1:C:1151:ILE:HB	1.96	0.46
1:D:333:PRO:HB2	1:D:448:LEU:HD21	1.98	0.46
1:D:926:SER:HB3	1:D:934:LYS:HG2	1.97	0.46
1:C:315:LEU:O	1:C:316:GLU:C	2.57	0.46
1:B:544:VAL:HG21	1:B:563:VAL:HA	1.97	0.46
1:C:324:ILE:HG23	1:C:326:THR:H	1.80	0.46
1:A:324:ILE:HG23	1:A:326:THR:H	1.81	0.46
1:A:350:LEU:HD21	1:A:354:ARG:HH21	1.80	0.46
1:B:317:LYS:C	1:B:319:ILE:N	2.71	0.46
1:B:724:LEU:HD12	1:B:727:TYR:HE1	1.81	0.46
1:B:350:LEU:HD21	1:B:354:ARG:HH21	1.79	0.46
1:A:1063:ILE:HD12	1:A:1064:ASP:N	2.31	0.45
1:C:369:ARG:O	1:C:372:ASP:N	2.49	0.45
1:C:926:SER:HB3	1:C:934:LYS:HG2	1.97	0.45
1:B:401:LYS:HE2	1:B:412:HIS:HD2	1.82	0.45
1:D:345:VAL:HA	1:D:348:ILE:HG12	1.98	0.45
1:D:369:ARG:NH1	1:D:405:TYR:OH	2.50	0.45
1:D:379:LYS:HE3	1:D:379:LYS:HB3	1.84	0.45
1:A:1186:THR:OG1	1:A:1188:ASP:OD1	2.31	0.45
1:A:894:LEU:HD11	1:D:1046:ILE:HD11	1.98	0.45
1:B:279:ASN:OD1	1:B:279:ASN:N	2.40	0.45
1:A:549:LEU:HD12	1:A:550:PRO:HD2	1.99	0.45
1:B:163:ASP:OD1	1:B:163:ASP:N	2.50	0.45
1:B:1148:PRO:HA	1:B:1151:ILE:HB	1.97	0.45
1:A:897:MET:HE2	1:A:961:ARG:HE	1.82	0.45
1:C:724:LEU:HD12	1:C:727:TYR:HE1	1.82	0.45
1:A:333:PRO:HB2	1:A:448:LEU:HD21	1.99	0.45
1:D:210:ILE:HD13	1:D:210:ILE:HA	1.87	0.45
1:C:163:ASP:N	1:C:163:ASP:OD1	2.49	0.45
1:C:1105:LEU:HD21	1:D:1003:ILE:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:LEU:O	1:D:227:THR:OG1	2.32	0.45
1:B:317:LYS:HB2	1:B:317:LYS:HE2	1.45	0.45
1:B:478:ILE:HD12	1:B:478:ILE:HA	1.91	0.45
1:A:259:VAL:O	1:A:262:GLN:NE2	2.48	0.44
1:A:923:ILE:HD11	1:A:935:VAL:HA	1.98	0.44
1:B:369:ARG:O	1:B:372:ASP:N	2.49	0.44
1:D:1026:VAL:HG22	1:D:1046:ILE:HD13	1.98	0.44
1:D:269:ASP:OD1	1:D:269:ASP:N	2.49	0.44
1:B:239:ASP:O	1:B:243:LYS:NZ	2.50	0.44
1:D:421:MET:HE3	1:D:421:MET:HB3	1.73	0.44
1:A:1218:GLU:OE2	1:A:1221:ARG:NH2	2.39	0.44
1:C:649:LYS:NZ	1:C:694:GLU:OE1	2.49	0.44
1:B:432:MET:SD	1:B:432:MET:N	2.76	0.44
1:A:407:ARG:HB3	1:A:410:ALA:HB3	2.00	0.44
1:B:315:LEU:O	1:B:316:GLU:C	2.57	0.44
1:C:354:ARG:NH2	1:C:419:GLU:OE1	2.51	0.44
1:D:644:TRP:NE1	1:D:648:MET:SD	2.91	0.44
1:A:664:ALA:N	1:A:1197:GLU:OE2	2.30	0.43
3:D:1401:3PH:H3C1	3:D:1401:3PH:H3F1	1.75	0.43
1:C:317:LYS:O	1:C:319:ILE:N	2.51	0.43
1:D:165:LYS:HB2	1:D:168:LEU:HD23	1.99	0.43
1:D:664:ALA:N	1:D:1197:GLU:OE2	2.30	0.43
1:A:165:LYS:HB2	1:A:168:LEU:HD23	2.00	0.43
1:D:649:LYS:NZ	1:D:694:GLU:OE1	2.48	0.43
1:A:187:SER:O	1:A:337:LEU:N	2.50	0.43
1:A:724:LEU:HD12	1:A:727:TYR:HE1	1.83	0.43
1:B:697:HIS:CD2	1:B:700:ARG:HH21	2.36	0.43
1:A:978:ASN:ND2	1:A:982:TRP:HE1	2.16	0.43
1:C:697:HIS:CD2	1:C:700:ARG:HH21	2.37	0.43
1:B:1218:GLU:OE2	1:B:1221:ARG:NH2	2.39	0.43
1:C:448:LEU:HD23	1:C:448:LEU:HA	1.91	0.43
1:D:1024:PHE:HD1	1:D:1094:ILE:HG22	1.84	0.43
1:C:478:ILE:HG22	1:C:481:GLN:HE21	1.84	0.43
1:D:369:ARG:O	1:D:372:ASP:N	2.51	0.43
1:B:1186:THR:OG1	1:B:1187:ASP:N	2.52	0.43
1:C:172:LEU:HD12	1:C:176:GLU:HB3	1.99	0.43
1:C:188:VAL:O	1:C:312:ARG:NH2	2.51	0.43
1:D:478:ILE:HD12	1:D:478:ILE:HA	1.91	0.43
1:D:697:HIS:CD2	1:D:700:ARG:HH21	2.37	0.43
1:A:172:LEU:HD12	1:A:176:GLU:HB2	2.00	0.42
1:A:478:ILE:HD12	1:A:478:ILE:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:LYS:NZ	1:A:694:GLU:OE1	2.46	0.42
1:A:759:LEU:HD21	1:A:1134:TYR:HD1	1.84	0.42
1:C:179:LEU:HD21	1:C:249:CYS:SG	2.59	0.42
1:C:1238:ASN:HD22	1:D:1233:ARG:HD2	1.84	0.42
1:A:187:SER:OG	1:A:316:GLU:OE2	2.21	0.42
4:B:1402:9Z9:C05	4:B:1402:9Z9:C01	2.88	0.42
1:A:697:HIS:CD2	1:A:700:ARG:HH21	2.37	0.42
1:C:345:VAL:HA	1:C:348:ILE:HG12	2.00	0.42
1:C:356:THR:O	1:C:358:PRO:HD3	2.20	0.42
1:A:264:ASP:OD1	1:A:264:ASP:N	2.47	0.42
1:A:688:VAL:HG23	1:A:690:ASP:H	1.83	0.42
1:A:1188:ASP:OD1	1:A:1188:ASP:N	2.49	0.42
4:D:1402:9Z9:C05	4:D:1402:9Z9:C01	2.88	0.42
1:B:317:LYS:O	1:B:319:ILE:N	2.53	0.42
1:B:470:ASP:OD1	1:B:470:ASP:N	2.50	0.42
1:C:560:ILE:HA	1:C:563:VAL:HG12	2.00	0.42
1:A:157:TYR:OH	1:A:265:LEU:O	2.30	0.42
1:A:484:PRO:HG2	1:A:487:SER:HB3	2.02	0.42
1:C:885:TYR:HE1	1:C:908:VAL:HG13	1.85	0.42
1:B:192:LEU:O	1:B:227:THR:OG1	2.34	0.42
1:B:197:LEU:HB2	1:B:232:HIS:CE1	2.54	0.42
1:C:769:MET:HB3	1:C:773:SER:HB2	2.02	0.42
1:A:896:LYS:HE2	1:A:896:LYS:HB3	1.85	0.42
1:B:1012:TYR:HD1	1:B:1012:TYR:HA	1.78	0.42
1:B:1105:LEU:HD21	1:C:1003:ILE:HG23	2.02	0.42
1:B:1109:LEU:HD12	1:B:1109:LEU:HA	1.91	0.42
1:B:186:ILE:O	1:B:187:SER:C	2.61	0.41
1:D:336:ALA:HB3	1:D:361:VAL:HG12	2.02	0.41
1:D:497:VAL:HG22	1:D:529:THR:HG21	2.02	0.41
4:A:1402:9Z9:C05	4:A:1402:9Z9:C01	2.88	0.41
1:B:170:LEU:HD12	1:B:318:HIS:CE1	2.55	0.41
1:B:299:ASN:OD1	1:B:299:ASN:N	2.52	0.41
1:B:560:ILE:HA	1:B:563:VAL:HG12	2.01	0.41
1:B:723:LYS:NZ	1:B:1185:ILE:HD13	2.35	0.41
1:B:1046:ILE:HD11	1:C:894:LEU:HD11	2.01	0.41
1:C:224:GLY:HA3	1:C:254:ALA:HB2	2.02	0.41
1:D:239:ASP:O	1:D:243:LYS:NZ	2.47	0.41
1:A:540:LEU:HB3	1:A:563:VAL:HG21	2.02	0.41
1:B:1002:MET:HE2	1:B:1002:MET:HB2	1.87	0.41
1:C:892:ILE:HD12	1:C:892:ILE:HA	1.85	0.41
1:D:560:ILE:HA	1:D:563:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:432:MET:SD	1:C:432:MET:N	2.86	0.41
1:C:892:ILE:HG12	1:C:905:GLU:HB2	2.02	0.41
1:A:892:ILE:HG12	1:A:905:GLU:HB2	2.03	0.41
1:A:1012:TYR:HD1	1:A:1012:TYR:HA	1.79	0.41
1:B:920:MET:O	1:B:923:ILE:HG22	2.21	0.41
1:C:544:VAL:HG21	1:C:563:VAL:HA	2.01	0.41
1:D:185:LEU:HD12	1:D:219:TRP:HB2	2.03	0.41
1:A:560:ILE:HA	1:A:563:VAL:HG12	2.03	0.41
1:A:937:VAL:HA	1:A:940:GLN:HG2	2.03	0.41
1:B:310:LYS:O	1:B:314:GLN:HG2	2.21	0.41
1:C:316:GLU:O	1:C:317:LYS:C	2.62	0.41
1:A:1024:PHE:HD1	1:A:1094:ILE:HG22	1.85	0.41
1:B:540:LEU:HB3	1:B:563:VAL:HG21	2.03	0.41
1:B:896:LYS:HE2	1:B:896:LYS:HB3	1.86	0.41
1:C:299:ASN:OD1	1:C:299:ASN:N	2.54	0.41
1:C:897:MET:HE2	1:C:961:ARG:HE	1.85	0.41
1:D:565:GLU:OE2	1:D:577:THR:OG1	2.27	0.41
1:A:404:THR:HA	1:A:408:THR:HG22	2.02	0.41
1:B:319:ILE:HA	1:B:319:ILE:HD12	1.69	0.41
1:C:186:ILE:HD13	1:C:186:ILE:HG21	1.79	0.41
1:C:187:SER:OG	1:C:316:GLU:OE2	2.30	0.41
1:A:885:TYR:HE1	1:A:908:VAL:HG13	1.87	0.40
1:C:313:ARG:NH1	1:C:351:GLU:OE2	2.54	0.40
1:C:319:ILE:O	1:C:319:ILE:CG2	2.67	0.40
1:D:923:ILE:HD11	1:D:935:VAL:HA	2.03	0.40
1:B:316:GLU:O	1:B:317:LYS:C	2.64	0.40
1:A:545:LYS:NZ	1:A:559:ASP:OD1	2.45	0.40
1:A:1206:ARG:HE	1:D:245:ARG:HD3	1.87	0.40
1:B:497:VAL:HG22	1:B:529:THR:HG21	2.03	0.40
1:C:888:LEU:HD12	1:C:888:LEU:HA	1.96	0.40
1:D:454:ALA:HB1	1:D:458:ASP:HB2	2.04	0.40
1:A:298:ASP:OD2	2:E:9:UNK:N	2.55	0.40
1:B:778:ILE:HA	1:B:781:ILE:HG22	2.02	0.40
4:C:1402:9Z9:C05	4:C:1402:9Z9:C01	2.88	0.40
1:D:258:ILE:HG22	1:D:285:THR:HG22	2.02	0.40
1:D:549:LEU:HD12	1:D:549:LEU:HA	1.97	0.40
1:A:892:ILE:HD12	1:A:892:ILE:HA	1.85	0.40
1:B:175:LYS:HE2	1:B:175:LYS:HB3	1.96	0.40
1:C:920:MET:O	1:C:923:ILE:HG22	2.21	0.40
1:D:920:MET:O	1:D:923:ILE:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	956/1343 (71%)	900 (94%)	56 (6%)	0	100	100
1	B	956/1343 (71%)	894 (94%)	61 (6%)	1 (0%)	48	78
1	C	956/1343 (71%)	905 (95%)	51 (5%)	0	100	100
1	D	956/1343 (71%)	900 (94%)	56 (6%)	0	100	100
All	All	3824/5372 (71%)	3599 (94%)	224 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	184	LEU

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	858/1194 (72%)	834 (97%)	24 (3%)	38	60
1	B	859/1194 (72%)	828 (96%)	31 (4%)	31	56
1	C	859/1194 (72%)	836 (97%)	23 (3%)	39	60
1	D	859/1194 (72%)	837 (97%)	22 (3%)	40	61
All	All	3435/4776 (72%)	3335 (97%)	100 (3%)	38	60

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	HIS
1	A	167	ASP
1	A	173	MET
1	A	188	VAL
1	A	222	THR
1	A	309	VAL
1	A	335	VAL
1	A	356	THR
1	A	361	VAL
1	A	397	VAL
1	A	422	LYS
1	A	426	LEU
1	A	537	LEU
1	A	764	MET
1	A	767	LEU
1	A	877	PHE
1	A	888	LEU
1	A	889	PHE
1	A	1012	TYR
1	A	1013	PHE
1	A	1014	VAL
1	A	1058	VAL
1	A	1063	ILE
1	A	1209	ASP
1	B	151	HIS
1	B	167	ASP
1	B	168	LEU
1	B	170	LEU
1	B	184	LEU
1	B	185	LEU
1	B	197	LEU
1	B	200	LYS
1	B	264	ASP
1	B	279	ASN
1	B	309	VAL
1	B	317	LYS
1	B	334	VAL
1	B	339	VAL
1	B	345	VAL
1	B	356	THR
1	B	361	VAL
1	B	412	HIS
1	B	420	CYS

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Mol	Chain	Res	Type
1	B	448	LEU
1	B	501	VAL
1	B	537	LEU
1	B	549	LEU
1	B	764	MET
1	B	877	PHE
1	B	888	LEU
1	B	1002	MET
1	B	1012	TYR
1	B	1013	PHE
1	B	1014	VAL
1	B	1063	ILE
1	C	151	HIS
1	C	167	ASP
1	C	184	LEU
1	C	201	LEU
1	C	240	HIS
1	C	270	VAL
1	C	309	VAL
1	C	313	ARG
1	C	321	LEU
1	C	350	LEU
1	C	356	THR
1	C	361	VAL
1	C	417	LEU
1	C	420	CYS
1	C	501	VAL
1	C	764	MET
1	C	877	PHE
1	C	888	LEU
1	C	889	PHE
1	C	978	ASN
1	C	1012	TYR
1	C	1095	MET
1	C	1209	ASP
1	D	167	ASP
1	D	170	LEU
1	D	171	HIS
1	D	179	LEU
1	D	180	GLU
1	D	258	ILE
1	D	268	ARG

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Mol	Chain	Res	Type
1	D	269	ASP
1	D	275	GLN
1	D	309	VAL
1	D	356	THR
1	D	397	VAL
1	D	406	THR
1	D	408	THR
1	D	537	LEU
1	D	764	MET
1	D	877	PHE
1	D	888	LEU
1	D	1063	ILE
1	D	1090	ILE
1	D	1209	ASP
1	D	1241	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	ASN
1	A	194	ASN
1	A	240	HIS
1	A	411	GLN
1	A	659	GLN
1	A	697	HIS
1	A	734	ASN
1	A	940	GLN
1	A	944	ASN
1	A	965	GLN
1	A	978	ASN
1	A	1029	GLN
1	A	1115	ASN
1	A	1161	GLN
1	B	178	GLN
1	B	203	GLN
1	B	226	ASN
1	B	314	GLN
1	B	378	HIS
1	B	411	GLN
1	B	531	HIS
1	B	659	GLN
1	B	697	HIS

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Mol	Chain	Res	Type
1	B	719	GLN
1	B	940	GLN
1	B	965	GLN
1	B	978	ASN
1	B	1029	GLN
1	B	1115	ASN
1	B	1161	GLN
1	C	153	ASN
1	C	171	HIS
1	C	178	GLN
1	C	194	ASN
1	C	226	ASN
1	C	261	ASN
1	C	409	GLN
1	C	531	HIS
1	C	633	HIS
1	C	651	GLN
1	C	659	GLN
1	C	697	HIS
1	C	734	ASN
1	C	746	HIS
1	C	940	GLN
1	C	978	ASN
1	C	1029	GLN
1	C	1115	ASN
1	C	1161	GLN
1	C	1238	ASN
1	D	153	ASN
1	D	171	HIS
1	D	275	GLN
1	D	409	GLN
1	D	411	GLN
1	D	659	GLN
1	D	697	HIS
1	D	734	ASN
1	D	746	HIS
1	D	940	GLN
1	D	965	GLN
1	D	978	ASN
1	D	993	ASN
1	D	1115	ASN
1	D	1161	GLN

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Mol	Chain	Res	Type
1	D	1238	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	3PH	A	1401	-	44,44,47	1.15	3 (6%)	47,49,52	1.17	2 (4%)
3	3PH	B	1401	-	44,44,47	1.16	3 (6%)	47,49,52	1.16	2 (4%)
4	9Z9	B	1402	-	44,44,44	9.37	23 (52%)	64,68,68	5.01	24 (37%)
4	9Z9	C	1402	-	44,44,44	9.36	22 (50%)	64,68,68	5.01	24 (37%)
5	PIO	A	1403	-	47,47,47	1.20	6 (12%)	62,65,65	0.98	3 (4%)
4	9Z9	D	1402	-	44,44,44	9.37	22 (50%)	64,68,68	5.01	23 (35%)
5	PIO	C	1403	-	47,47,47	1.20	6 (12%)	62,65,65	1.03	2 (3%)
5	PIO	B	1403	-	47,47,47	1.24	6 (12%)	62,65,65	1.01	2 (3%)
3	3PH	D	1401	-	44,44,47	1.16	3 (6%)	47,49,52	1.17	2 (4%)
3	3PH	C	1401	-	44,44,47	1.16	3 (6%)	47,49,52	1.16	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PIO	D	1403	-	47,47,47	1.22	7 (14%)	62,65,65	1.02	2 (3%)
4	9Z9	A	1402	-	44,44,44	9.37	22 (50%)	64,68,68	5.01	23 (35%)

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	3PH	A	1401	-	-	26/46/46/49	-
3	3PH	B	1401	-	-	31/46/46/49	-
4	9Z9	B	1402	-	-	1/12/100/100	0/6/6/6
4	9Z9	C	1402	-	-	1/12/100/100	0/6/6/6
5	PIO	A	1403	-	-	9/44/68/68	0/1/1/1
4	9Z9	D	1402	-	-	1/12/100/100	0/6/6/6
5	PIO	C	1403	-	-	20/44/68/68	0/1/1/1
5	PIO	B	1403	-	-	17/44/68/68	0/1/1/1
3	3PH	D	1401	-	-	31/46/46/49	-
3	3PH	C	1401	-	-	25/46/46/49	-
5	PIO	D	1403	-	-	14/44/68/68	0/1/1/1
4	9Z9	A	1402	-	-	3/12/100/100	0/6/6/6

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1402	9Z9	C02-C03	-29.63	1.01	1.56
4	C	1402	9Z9	C02-C03	-29.61	1.01	1.56
4	D	1402	9Z9	C02-C03	-29.61	1.01	1.56
4	B	1402	9Z9	C02-C03	-29.58	1.01	1.56
4	D	1402	9Z9	C03-C74	-24.91	0.83	1.54
4	B	1402	9Z9	C03-C74	-24.90	0.83	1.54
4	A	1402	9Z9	C03-C74	-24.89	0.83	1.54
4	C	1402	9Z9	C03-C74	-24.86	0.84	1.54
4	A	1402	9Z9	C05-C06	-23.22	1.04	1.54
4	C	1402	9Z9	C05-C06	-23.21	1.04	1.54
4	D	1402	9Z9	C05-C06	-23.20	1.04	1.54
4	B	1402	9Z9	C05-C06	-23.18	1.04	1.54
4	A	1402	9Z9	O72-C73	-18.56	1.03	1.42
4	B	1402	9Z9	O72-C73	-18.52	1.03	1.42
4	D	1402	9Z9	O72-C73	-18.52	1.03	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1402	9Z9	O72-C73	-18.49	1.03	1.42
4	D	1402	9Z9	C75-C74	17.92	1.90	1.53
4	C	1402	9Z9	C75-C74	17.90	1.90	1.53
4	A	1402	9Z9	C75-C74	17.90	1.90	1.53
4	B	1402	9Z9	C75-C74	17.89	1.90	1.53
4	B	1402	9Z9	C07-C06	16.33	1.84	1.53
4	A	1402	9Z9	C07-C06	16.30	1.84	1.53
4	C	1402	9Z9	C07-C06	16.30	1.84	1.53
4	D	1402	9Z9	C07-C06	16.28	1.84	1.53
4	D	1402	9Z9	C73-C74	14.24	1.81	1.53
4	B	1402	9Z9	C73-C74	14.24	1.81	1.53
4	A	1402	9Z9	C73-C74	14.23	1.81	1.53
4	C	1402	9Z9	C73-C74	14.22	1.81	1.53
4	A	1402	9Z9	C02-C06	12.87	1.78	1.55
4	B	1402	9Z9	C02-C06	12.82	1.78	1.55
4	C	1402	9Z9	C02-C06	12.82	1.78	1.55
4	D	1402	9Z9	C02-C06	12.80	1.78	1.55
4	D	1402	9Z9	C10-C09	-12.12	1.29	1.53
4	C	1402	9Z9	C10-C09	-12.09	1.29	1.53
4	B	1402	9Z9	C10-C09	-12.08	1.29	1.53
4	A	1402	9Z9	C10-C09	-12.05	1.29	1.53
4	D	1402	9Z9	C15-C07	-10.12	1.36	1.53
4	C	1402	9Z9	C15-C07	-10.08	1.36	1.53
4	A	1402	9Z9	C15-C07	-10.07	1.36	1.53
4	B	1402	9Z9	C15-C07	-10.05	1.36	1.53
4	C	1402	9Z9	C10-C02	9.42	1.70	1.54
4	B	1402	9Z9	C10-C02	9.39	1.70	1.54
4	A	1402	9Z9	C10-C02	9.36	1.70	1.54
4	D	1402	9Z9	C10-C02	9.36	1.70	1.54
4	B	1402	9Z9	C03-C04	-5.86	1.43	1.54
4	C	1402	9Z9	C03-C04	-5.85	1.43	1.54
4	A	1402	9Z9	C03-C04	-5.84	1.43	1.54
4	D	1402	9Z9	C03-C04	-5.82	1.43	1.54
4	B	1402	9Z9	C14-C13	5.71	1.44	1.33
4	D	1402	9Z9	C14-C13	5.66	1.44	1.33
4	A	1402	9Z9	C14-C13	5.65	1.44	1.33
4	C	1402	9Z9	C14-C13	5.65	1.44	1.33
4	A	1402	9Z9	C09-C08	-4.74	1.46	1.53
4	B	1402	9Z9	C09-C08	-4.69	1.46	1.53
4	C	1402	9Z9	C09-C08	-4.67	1.46	1.53
4	D	1402	9Z9	C09-C08	-4.66	1.46	1.53
4	A	1402	9Z9	C15-C14	4.13	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1402	9Z9	C15-C14	4.08	1.58	1.50
4	B	1402	9Z9	C15-C14	4.08	1.58	1.50
4	C	1402	9Z9	C15-C14	4.08	1.58	1.50
4	B	1402	9Z9	C19-C18	3.82	1.61	1.53
4	C	1402	9Z9	C19-C18	3.78	1.60	1.53
4	D	1402	9Z9	C19-C18	3.76	1.60	1.53
4	A	1402	9Z9	C19-C18	3.76	1.60	1.53
5	B	1403	PIO	P4-O4	3.61	1.65	1.59
5	D	1403	PIO	P4-O4	3.56	1.65	1.59
5	B	1403	PIO	P5-O5	3.56	1.65	1.59
4	C	1402	9Z9	C11-C08	3.39	1.61	1.56
4	B	1402	9Z9	C11-C08	3.37	1.61	1.56
4	D	1402	9Z9	C11-C08	3.31	1.61	1.56
5	C	1403	PIO	P4-O4	3.30	1.65	1.59
5	D	1403	PIO	P5-O5	3.29	1.65	1.59
4	A	1402	9Z9	C11-C08	3.28	1.61	1.56
5	C	1403	PIO	P5-O5	3.27	1.65	1.59
5	A	1403	PIO	P4-O4	3.23	1.65	1.59
5	A	1403	PIO	P5-O5	3.23	1.65	1.59
4	A	1402	9Z9	C01-C02	3.21	1.59	1.54
4	B	1402	9Z9	C01-C02	3.21	1.59	1.54
4	C	1402	9Z9	C01-C02	3.20	1.59	1.54
4	D	1402	9Z9	C01-C02	3.20	1.59	1.54
4	B	1402	9Z9	C19-C11	-2.95	1.48	1.54
3	A	1401	3PH	O21-C21	2.95	1.42	1.34
4	D	1402	9Z9	C19-C11	-2.94	1.48	1.54
4	A	1402	9Z9	C19-C11	-2.92	1.48	1.54
3	A	1401	3PH	O31-C31	2.92	1.41	1.33
4	C	1402	9Z9	C19-C11	-2.92	1.48	1.54
3	D	1401	3PH	O21-C21	2.91	1.42	1.34
3	C	1401	3PH	O31-C31	2.91	1.41	1.33
3	B	1401	3PH	O31-C31	2.91	1.41	1.33
3	D	1401	3PH	O31-C31	2.89	1.41	1.33
3	B	1401	3PH	O21-C21	2.89	1.42	1.34
3	C	1401	3PH	O21-C21	2.83	1.42	1.34
4	A	1402	9Z9	C07-C08	-2.82	1.48	1.53
4	C	1402	9Z9	C07-C08	-2.82	1.48	1.53
4	B	1402	9Z9	C07-C08	-2.80	1.48	1.53
4	D	1402	9Z9	C07-C08	-2.77	1.48	1.53
4	C	1402	9Z9	C18-C17	2.75	1.58	1.51
4	D	1402	9Z9	C18-C17	2.75	1.58	1.51
4	B	1402	9Z9	C18-C17	2.73	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1403	PIO	O2C-C2C	-2.71	1.40	1.46
4	A	1402	9Z9	C18-C17	2.70	1.58	1.51
4	D	1402	9Z9	C76-C73	2.70	1.56	1.51
3	C	1401	3PH	O21-C2	-2.68	1.40	1.46
4	B	1402	9Z9	C76-C73	2.67	1.56	1.51
4	C	1402	9Z9	C76-C73	2.66	1.55	1.51
4	A	1402	9Z9	C76-C73	2.66	1.55	1.51
3	B	1401	3PH	O21-C2	-2.61	1.40	1.46
5	A	1403	PIO	O2C-C2C	-2.60	1.40	1.46
3	D	1401	3PH	O21-C2	-2.59	1.40	1.46
3	A	1401	3PH	O21-C2	-2.51	1.40	1.46
5	B	1403	PIO	O3C-C1B	2.41	1.40	1.33
5	A	1403	PIO	O3C-C1B	2.41	1.40	1.33
5	D	1403	PIO	O2C-C1A	2.36	1.40	1.34
5	C	1403	PIO	O2C-C1A	2.35	1.40	1.34
5	C	1403	PIO	O3C-C1B	2.35	1.40	1.33
5	D	1403	PIO	O2C-C2C	-2.34	1.41	1.46
5	D	1403	PIO	O3C-C1B	2.33	1.40	1.33
5	C	1403	PIO	O2C-C2C	-2.30	1.41	1.46
5	C	1403	PIO	O3C-C3C	-2.24	1.40	1.45
5	A	1403	PIO	O2C-C1A	2.23	1.40	1.34
5	D	1403	PIO	O3C-C3C	-2.20	1.40	1.45
5	B	1403	PIO	O3C-C3C	-2.16	1.40	1.45
5	D	1403	PIO	P1-O1	2.14	1.65	1.59
5	A	1403	PIO	O3C-C3C	-2.13	1.40	1.45
5	B	1403	PIO	O2C-C1A	2.12	1.40	1.34
4	B	1402	9Z9	O20-C17	-2.01	1.38	1.43

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1402	9Z9	C76-C73-C74	27.59	165.63	115.66
4	D	1402	9Z9	C76-C73-C74	27.59	165.63	115.66
4	C	1402	9Z9	C76-C73-C74	27.58	165.62	115.66
4	B	1402	9Z9	C76-C73-C74	27.57	165.60	115.66
4	C	1402	9Z9	O72-C73-C76	-18.85	70.26	108.54
4	A	1402	9Z9	O72-C73-C76	-18.85	70.27	108.54
4	D	1402	9Z9	O72-C73-C76	-18.84	70.29	108.54
4	B	1402	9Z9	O72-C73-C76	-18.82	70.32	108.54
4	B	1402	9Z9	O80-C73-O72	11.90	138.19	109.88
4	D	1402	9Z9	O80-C73-O72	11.90	138.19	109.88
4	C	1402	9Z9	O80-C73-O72	11.88	138.15	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1402	9Z9	O80-C73-O72	11.86	138.11	109.88
4	B	1402	9Z9	O80-C73-C74	-8.45	82.06	107.26
4	C	1402	9Z9	O80-C73-C74	-8.44	82.09	107.26
4	D	1402	9Z9	O80-C73-C74	-8.44	82.09	107.26
4	A	1402	9Z9	O80-C73-C74	-8.44	82.11	107.26
4	B	1402	9Z9	C02-C06-C07	-6.05	105.82	114.41
4	D	1402	9Z9	C02-C06-C07	-6.05	105.82	114.41
4	C	1402	9Z9	C02-C06-C07	-6.04	105.84	114.41
4	A	1402	9Z9	C02-C06-C07	-6.01	105.88	114.41
4	C	1402	9Z9	C10-C02-C06	-5.76	98.62	107.25
4	B	1402	9Z9	C10-C02-C06	-5.76	98.63	107.25
4	A	1402	9Z9	C10-C02-C06	-5.75	98.65	107.25
4	D	1402	9Z9	C10-C02-C06	-5.74	98.66	107.25
4	B	1402	9Z9	C07-C15-C14	-4.67	106.29	112.76
4	C	1402	9Z9	C07-C15-C14	-4.66	106.31	112.76
4	D	1402	9Z9	C07-C15-C14	-4.61	106.37	112.76
4	A	1402	9Z9	C07-C15-C14	-4.59	106.41	112.76
4	B	1402	9Z9	C06-C05-C04	-4.27	94.96	102.40
4	D	1402	9Z9	C06-C05-C04	-4.27	94.96	102.40
4	A	1402	9Z9	C06-C05-C04	-4.26	94.97	102.40
4	C	1402	9Z9	C06-C05-C04	-4.24	95.02	102.40
5	C	1403	PIO	O2C-C1A-C2A	4.08	120.30	111.48
3	B	1401	3PH	O21-C21-C22	4.07	120.29	111.48
3	D	1401	3PH	O21-C21-C22	4.07	120.29	111.48
4	A	1402	9Z9	C09-C08-C11	-4.03	108.12	113.08
3	C	1401	3PH	O21-C21-C22	4.02	120.19	111.48
4	B	1402	9Z9	C09-C08-C11	-4.00	108.15	113.08
4	D	1402	9Z9	C09-C08-C11	-3.99	108.16	113.08
3	A	1401	3PH	O21-C21-C22	3.98	120.08	111.48
4	C	1402	9Z9	C09-C08-C11	-3.97	108.19	113.08
5	A	1403	PIO	O2C-C1A-C2A	3.91	119.94	111.48
5	B	1403	PIO	O2C-C1A-C2A	3.89	119.89	111.48
5	D	1403	PIO	O2C-C1A-C2A	3.86	119.84	111.48
4	D	1402	9Z9	C73-C74-C03	3.79	108.95	103.37
4	C	1402	9Z9	C73-C74-C03	3.78	108.94	103.37
4	B	1402	9Z9	C73-C74-C03	3.77	108.92	103.37
4	A	1402	9Z9	C73-C74-C03	3.73	108.86	103.37
4	A	1402	9Z9	C09-C10-C02	-3.66	106.57	112.74
4	C	1402	9Z9	C09-C10-C02	-3.64	106.60	112.74
4	B	1402	9Z9	C09-C10-C02	-3.64	106.61	112.74
4	D	1402	9Z9	C09-C10-C02	-3.60	106.66	112.74
4	C	1402	9Z9	C01-C02-C03	3.44	119.07	111.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1402	9Z9	C01-C02-C03	3.44	119.07	111.58
4	B	1402	9Z9	C01-C02-C03	3.44	119.06	111.58
4	D	1402	9Z9	C01-C02-C03	3.42	119.02	111.58
4	A	1402	9Z9	O80-C79-C78	-3.28	107.96	112.17
4	B	1402	9Z9	O80-C79-C78	-3.23	108.02	112.17
4	D	1402	9Z9	O80-C79-C78	-3.22	108.03	112.17
4	C	1402	9Z9	O80-C79-C78	-3.18	108.08	112.17
4	A	1402	9Z9	C74-C03-C04	3.16	109.35	104.27
4	B	1402	9Z9	C74-C03-C04	3.15	109.34	104.27
4	D	1402	9Z9	C74-C03-C04	3.13	109.31	104.27
4	C	1402	9Z9	C74-C03-C04	3.10	109.26	104.27
4	D	1402	9Z9	C15-C14-C13	-2.95	120.03	125.02
4	C	1402	9Z9	C15-C14-C13	-2.95	120.03	125.02
4	B	1402	9Z9	C15-C14-C13	-2.95	120.04	125.02
4	A	1402	9Z9	C15-C14-C13	-2.93	120.07	125.02
5	B	1403	PIO	O3C-C1B-C2B	2.92	120.73	111.83
4	A	1402	9Z9	C10-C09-C08	2.88	118.03	113.14
4	C	1402	9Z9	C10-C09-C08	2.88	118.03	113.14
4	B	1402	9Z9	C10-C09-C08	2.87	118.02	113.14
4	D	1402	9Z9	C10-C09-C08	2.86	118.00	113.14
3	A	1401	3PH	O31-C31-C32	2.82	120.44	111.83
5	D	1403	PIO	O3C-C1B-C2B	2.78	120.33	111.83
4	C	1402	9Z9	O72-C04-C03	2.76	108.86	105.12
4	B	1402	9Z9	O72-C04-C03	2.74	108.84	105.12
4	D	1402	9Z9	O72-C04-C03	2.73	108.82	105.12
4	A	1402	9Z9	O72-C04-C03	2.71	108.80	105.12
5	C	1403	PIO	O3C-C1B-C2B	2.71	120.09	111.83
3	C	1401	3PH	O31-C31-C32	2.71	120.09	111.83
3	D	1401	3PH	O31-C31-C32	2.70	120.07	111.83
3	B	1401	3PH	O31-C31-C32	2.70	120.07	111.83
5	A	1403	PIO	O3C-C1B-C2B	2.69	120.04	111.83
4	B	1402	9Z9	C16-C13-C11	2.46	119.58	116.42
4	D	1402	9Z9	C16-C13-C11	2.46	119.57	116.42
4	A	1402	9Z9	C16-C13-C11	2.44	119.55	116.42
4	C	1402	9Z9	C16-C13-C11	2.44	119.55	116.42
4	D	1402	9Z9	C75-C74-C03	-2.19	110.13	114.50
4	D	1402	9Z9	C79-O80-C73	2.18	117.45	113.69
4	C	1402	9Z9	C75-C74-C03	-2.17	110.17	114.50
4	A	1402	9Z9	C79-O80-C73	2.16	117.41	113.69
4	B	1402	9Z9	C79-O80-C73	2.15	117.40	113.69
4	B	1402	9Z9	C75-C74-C03	-2.15	110.20	114.50
4	C	1402	9Z9	C79-O80-C73	2.15	117.39	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1402	9Z9	C75-C74-C03	-2.14	110.23	114.50
4	B	1402	9Z9	C01-C02-C06	-2.09	107.89	111.68
4	D	1402	9Z9	C01-C02-C06	-2.08	107.90	111.68
5	A	1403	PIO	P5-O5-C5	-2.08	117.89	123.43
4	A	1402	9Z9	C01-C02-C06	-2.07	107.92	111.68
4	C	1402	9Z9	C02-C03-C04	2.07	106.43	104.20
4	D	1402	9Z9	C10-C02-C03	2.06	118.30	115.36
4	C	1402	9Z9	C10-C02-C03	2.06	118.29	115.36
4	D	1402	9Z9	C02-C03-C04	2.05	106.42	104.20
4	B	1402	9Z9	C10-C02-C03	2.05	118.28	115.36
4	C	1402	9Z9	C01-C02-C06	-2.05	107.96	111.68
4	C	1402	9Z9	C15-C07-C06	-2.04	108.04	110.93
4	A	1402	9Z9	C15-C07-C06	-2.04	108.04	110.93
4	A	1402	9Z9	C10-C02-C03	2.02	118.24	115.36
4	B	1402	9Z9	C15-C07-C06	-2.02	108.08	110.93
4	B	1402	9Z9	C02-C03-C04	2.00	106.36	104.20

There are no chirality outliers.

All (179) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1401	3PH	C1-O11-P-O13
3	A	1401	3PH	C1-O11-P-O14
3	A	1401	3PH	C1-O11-P-O12
3	A	1401	3PH	O11-C1-C2-O21
3	A	1401	3PH	O22-C21-O21-C2
3	A	1401	3PH	C22-C21-O21-C2
3	B	1401	3PH	C1-O11-P-O13
3	B	1401	3PH	C1-O11-P-O14
3	B	1401	3PH	O22-C21-O21-C2
3	B	1401	3PH	C22-C21-O21-C2
3	C	1401	3PH	C22-C21-O21-C2
3	D	1401	3PH	C1-O11-P-O14
3	D	1401	3PH	O22-C21-O21-C2
5	B	1403	PIO	C1-O1-P1-O12
5	B	1403	PIO	C1-O1-P1-O13
5	B	1403	PIO	C5-C4-O4-P4
5	B	1403	PIO	C6-C5-O5-P5
5	B	1403	PIO	O1A-C1A-O2C-C2C
5	B	1403	PIO	C2A-C1A-O2C-C2C
5	B	1403	PIO	O2C-C2C-C3C-O3C
5	C	1403	PIO	C1-O1-P1-O13

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Mol	Chain	Res	Type	Atoms
5	C	1403	PIO	O1A-C1A-O2C-C2C
5	D	1403	PIO	C6-C1-O1-P1
5	D	1403	PIO	C1C-O13-P1-O1
5	D	1403	PIO	C1C-O13-P1-O11
5	D	1403	PIO	C3-C4-O4-P4
5	B	1403	PIO	O1B-C1B-O3C-C3C
5	B	1403	PIO	C2B-C1B-O3C-C3C
3	A	1401	3PH	O32-C31-O31-C3
3	C	1401	3PH	O22-C21-O21-C2
5	D	1403	PIO	O1A-C1A-O2C-C2C
3	D	1401	3PH	C22-C21-O21-C2
5	C	1403	PIO	C2A-C1A-O2C-C2C
3	A	1401	3PH	C32-C31-O31-C3
5	D	1403	PIO	C2A-C1A-O2C-C2C
5	C	1403	PIO	C2B-C1B-O3C-C3C
5	D	1403	PIO	C2B-C1B-O3C-C3C
3	A	1401	3PH	C21-C22-C23-C24
5	D	1403	PIO	O1B-C1B-O3C-C3C
5	C	1403	PIO	C1A-C2A-C3A-C4A
5	C	1403	PIO	C1B-C2B-C3B-C4B
5	C	1403	PIO	O1B-C1B-O3C-C3C
3	B	1401	3PH	C21-C22-C23-C24
3	A	1401	3PH	C31-C32-C33-C34
3	D	1401	3PH	C21-C22-C23-C24
3	A	1401	3PH	C35-C36-C37-C38
3	A	1401	3PH	C24-C25-C26-C27
3	B	1401	3PH	C23-C24-C25-C26
3	C	1401	3PH	C23-C24-C25-C26
3	D	1401	3PH	C23-C24-C25-C26
5	B	1403	PIO	C2B-C3B-C4B-C5B
3	B	1401	3PH	C35-C36-C37-C38
3	D	1401	3PH	C35-C36-C37-C38
3	C	1401	3PH	C38-C39-C3A-C3B
5	B	1403	PIO	C3B-C4B-C5B-C6B
3	B	1401	3PH	C32-C33-C34-C35
3	D	1401	3PH	C38-C39-C3A-C3B
3	B	1401	3PH	C38-C39-C3A-C3B
3	D	1401	3PH	C32-C33-C34-C35
3	C	1401	3PH	C32-C33-C34-C35
3	C	1401	3PH	C22-C23-C24-C25
3	A	1401	3PH	C38-C39-C3A-C3B
3	B	1401	3PH	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
3	A	1401	3PH	C29-C2A-C2B-C2C
5	D	1403	PIO	C1B-C2B-C3B-C4B
3	C	1401	3PH	C35-C36-C37-C38
3	A	1401	3PH	C23-C24-C25-C26
3	A	1401	3PH	C26-C27-C28-C29
3	D	1401	3PH	C39-C3A-C3B-C3C
3	A	1401	3PH	C28-C29-C2A-C2B
3	C	1401	3PH	C24-C25-C26-C27
3	D	1401	3PH	C24-C25-C26-C27
3	B	1401	3PH	C24-C25-C26-C27
3	B	1401	3PH	C34-C35-C36-C37
3	C	1401	3PH	C39-C3A-C3B-C3C
3	D	1401	3PH	C34-C35-C36-C37
3	C	1401	3PH	C34-C35-C36-C37
3	B	1401	3PH	C22-C23-C24-C25
3	A	1401	3PH	C39-C3A-C3B-C3C
3	B	1401	3PH	C33-C34-C35-C36
3	D	1401	3PH	C22-C23-C24-C25
3	B	1401	3PH	C1-C2-C3-O31
3	C	1401	3PH	C1-C2-C3-O31
3	D	1401	3PH	C1-C2-C3-O31
5	B	1403	PIO	C1C-C2C-C3C-O3C
3	D	1401	3PH	C33-C34-C35-C36
3	B	1401	3PH	C26-C27-C28-C29
3	B	1401	3PH	C2A-C2B-C2C-C2D
3	D	1401	3PH	C26-C27-C28-C29
3	B	1401	3PH	C1-O11-P-O12
3	A	1401	3PH	C33-C34-C35-C36
3	A	1401	3PH	C32-C33-C34-C35
5	D	1403	PIO	C1C-C2C-O2C-C1A
3	A	1401	3PH	C37-C38-C39-C3A
3	C	1401	3PH	C26-C27-C28-C29
3	C	1401	3PH	C33-C34-C35-C36
5	C	1403	PIO	O13-C1C-C2C-O2C
3	D	1401	3PH	C3C-C3D-C3E-C3F
5	A	1403	PIO	C4B-C5B-C6B-C7B
3	B	1401	3PH	C3C-C3D-C3E-C3F
3	D	1401	3PH	C2A-C2B-C2C-C2D
3	B	1401	3PH	C32-C31-O31-C3
4	A	1402	9Z9	C23-C24-O25-C26
4	A	1402	9Z9	C23-C48-O49-C50
3	C	1401	3PH	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
3	D	1401	3PH	C32-C31-O31-C3
3	A	1401	3PH	O11-C1-C2-C3
5	B	1403	PIO	C1B-C2B-C3B-C4B
5	A	1403	PIO	C3B-C4B-C5B-C6B
3	C	1401	3PH	C21-C22-C23-C24
5	A	1403	PIO	C4A-C5A-C6A-C7A
3	B	1401	3PH	O21-C2-C3-O31
3	C	1401	3PH	O21-C2-C3-O31
3	D	1401	3PH	O21-C2-C3-O31
3	C	1401	3PH	C3C-C3D-C3E-C3F
3	B	1401	3PH	O32-C31-O31-C3
3	A	1401	3PH	C2A-C2B-C2C-C2D
5	C	1403	PIO	O13-C1C-C2C-C3C
5	A	1403	PIO	C1A-C2A-C3A-C4A
3	D	1401	3PH	C1-O11-P-O13
3	A	1401	3PH	C36-C37-C38-C39
3	C	1401	3PH	O32-C31-O31-C3
3	D	1401	3PH	O32-C31-O31-C3
3	B	1401	3PH	C3D-C3E-C3F-C3G
5	C	1403	PIO	C3C-C2C-O2C-C1A
3	B	1401	3PH	C27-C28-C29-C2A
3	C	1401	3PH	O11-C1-C2-O21
3	D	1401	3PH	O11-C1-C2-O21
3	D	1401	3PH	C27-C28-C29-C2A
3	D	1401	3PH	C3D-C3E-C3F-C3G
5	C	1403	PIO	C2A-C3A-C4A-C5A
3	C	1401	3PH	C3A-C3B-C3C-C3D
4	B	1402	9Z9	C23-C24-O25-C26
5	C	1403	PIO	C1-O1-P1-O12
3	A	1401	3PH	C3C-C3D-C3E-C3F
3	C	1401	3PH	C2A-C2B-C2C-C2D
3	B	1401	3PH	O11-C1-C2-C3
3	C	1401	3PH	O11-C1-C2-C3
3	D	1401	3PH	O11-C1-C2-C3
5	C	1403	PIO	C2C-C1C-O13-P1
3	B	1401	3PH	O11-C1-C2-O21
3	C	1401	3PH	C2-C1-O11-P
3	A	1401	3PH	C3A-C3B-C3C-C3D
3	D	1401	3PH	C3F-C3G-C3H-C3I
3	D	1401	3PH	C1-O11-P-O12
3	B	1401	3PH	C3F-C3G-C3H-C3I
5	C	1403	PIO	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
4	C	1402	9Z9	C23-C24-O25-C26
4	D	1402	9Z9	C23-C24-O25-C26
5	A	1403	PIO	C5B-C6B-C7B-C8B
3	B	1401	3PH	C36-C37-C38-C39
3	D	1401	3PH	C36-C37-C38-C39
3	B	1401	3PH	C3A-C3B-C3C-C3D
5	C	1403	PIO	C3B-C4B-C5B-C6B
3	D	1401	3PH	C28-C29-C2A-C2B
5	A	1403	PIO	C2C-C1C-O13-P1
3	D	1401	3PH	C3A-C3B-C3C-C3D
3	B	1401	3PH	C28-C29-C2A-C2B
5	C	1403	PIO	C4-O4-P4-O42
5	C	1403	PIO	C5-O5-P5-O53
5	D	1403	PIO	C4-O4-P4-O42
3	D	1401	3PH	C37-C38-C39-C3A
4	A	1402	9Z9	O20-C21-C22-C23
5	A	1403	PIO	C2B-C3B-C4B-C5B
3	C	1401	3PH	C37-C38-C39-C3A
3	B	1401	3PH	C37-C38-C39-C3A
5	D	1403	PIO	O2C-C1A-C2A-C3A
5	B	1403	PIO	C1-O1-P1-O11
5	C	1403	PIO	C1-O1-P1-O11
5	C	1403	PIO	C3-C4-O4-P4
5	B	1403	PIO	C5-O5-P5-O51
5	C	1403	PIO	C5-O5-P5-O51
5	D	1403	PIO	C4A-C5A-C6A-C7A
3	C	1401	3PH	C28-C29-C2A-C2B
5	A	1403	PIO	O2C-C1A-C2A-C3A
5	B	1403	PIO	C4-O4-P4-O42
5	D	1403	PIO	O1A-C1A-C2A-C3A
5	B	1403	PIO	C4B-C5B-C6B-C7B
5	A	1403	PIO	O1A-C1A-C2A-C3A

There are no ring outliers.

9 monomers are involved in 66 short contacts:

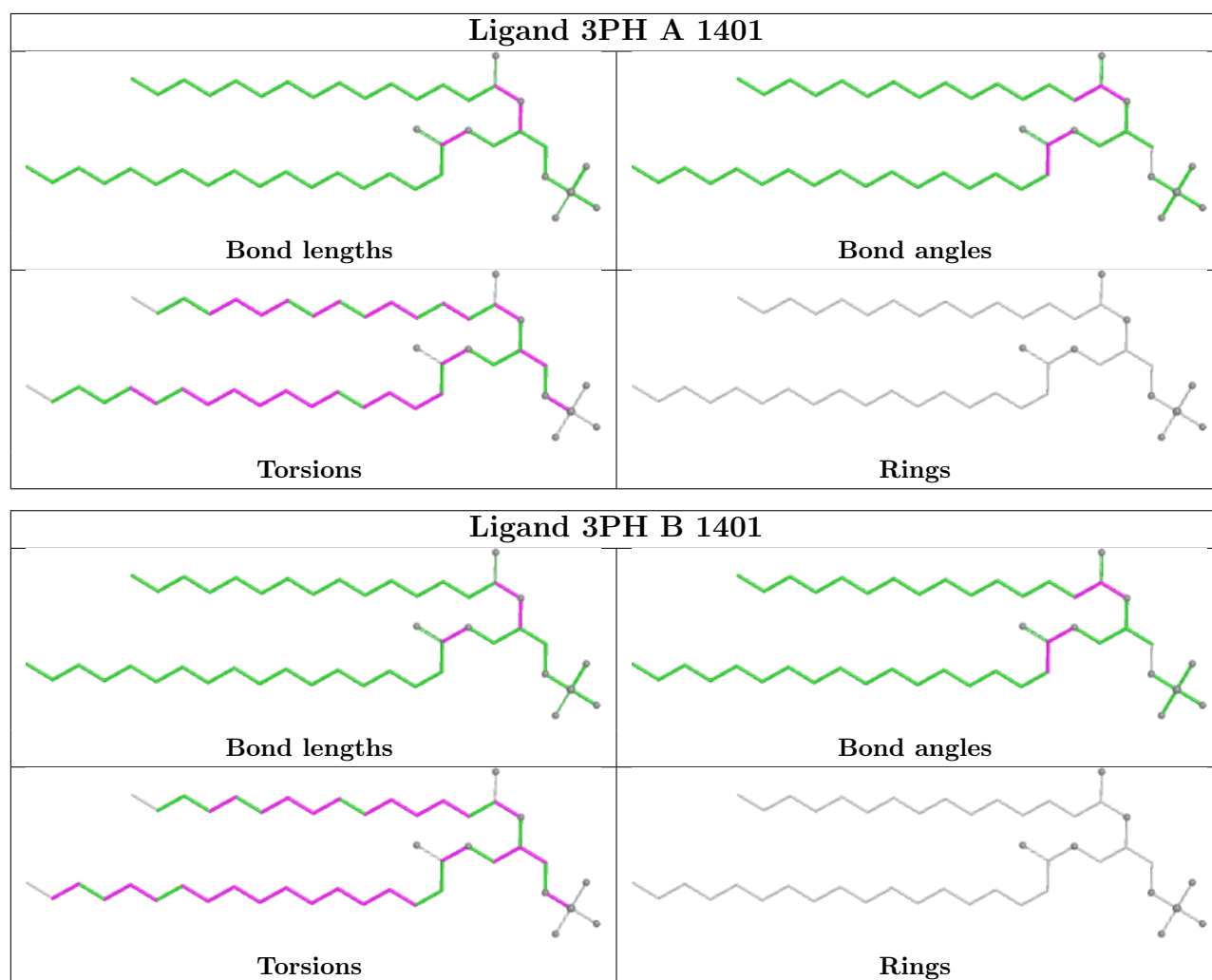
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1401	3PH	1	0
4	B	1402	9Z9	15	0
4	C	1402	9Z9	15	0
5	A	1403	PIO	1	0
4	D	1402	9Z9	15	0

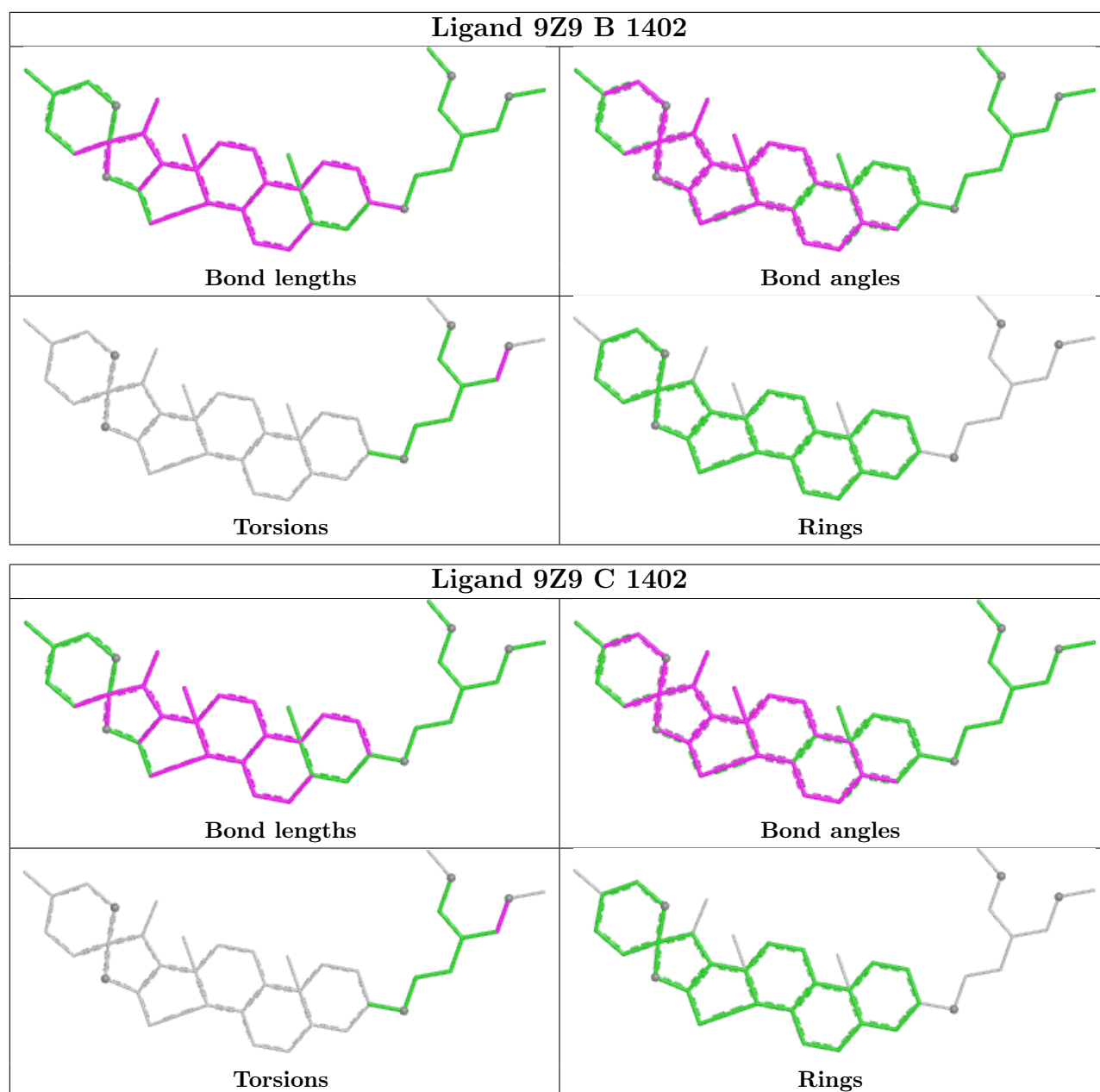
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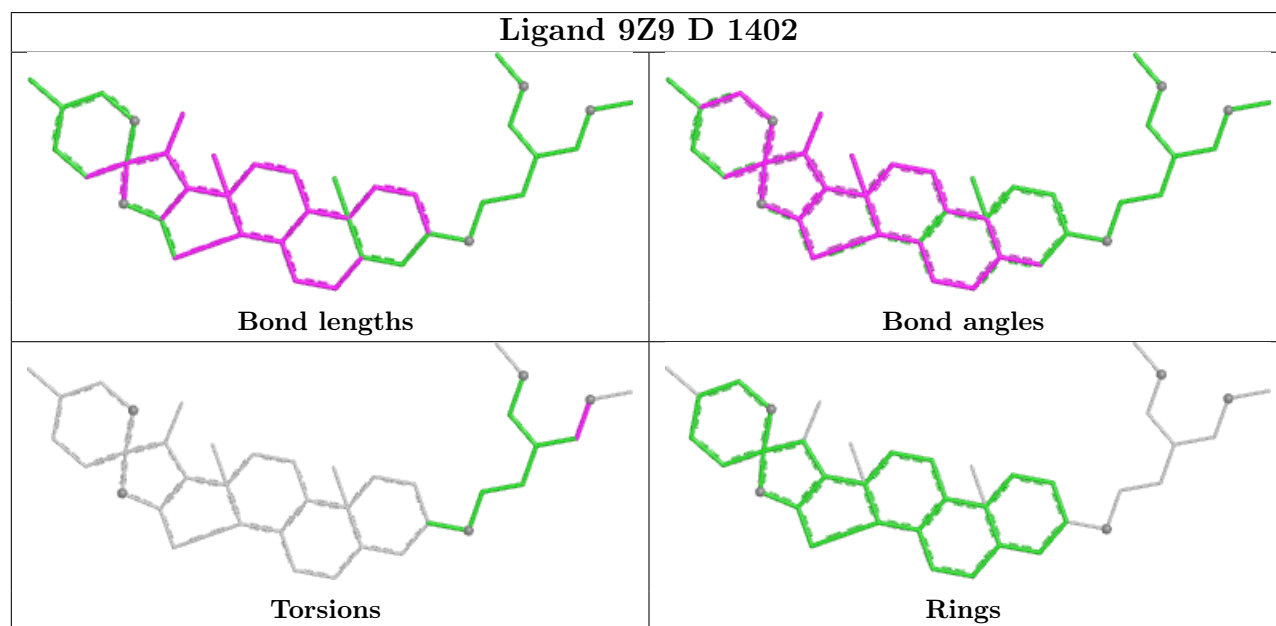
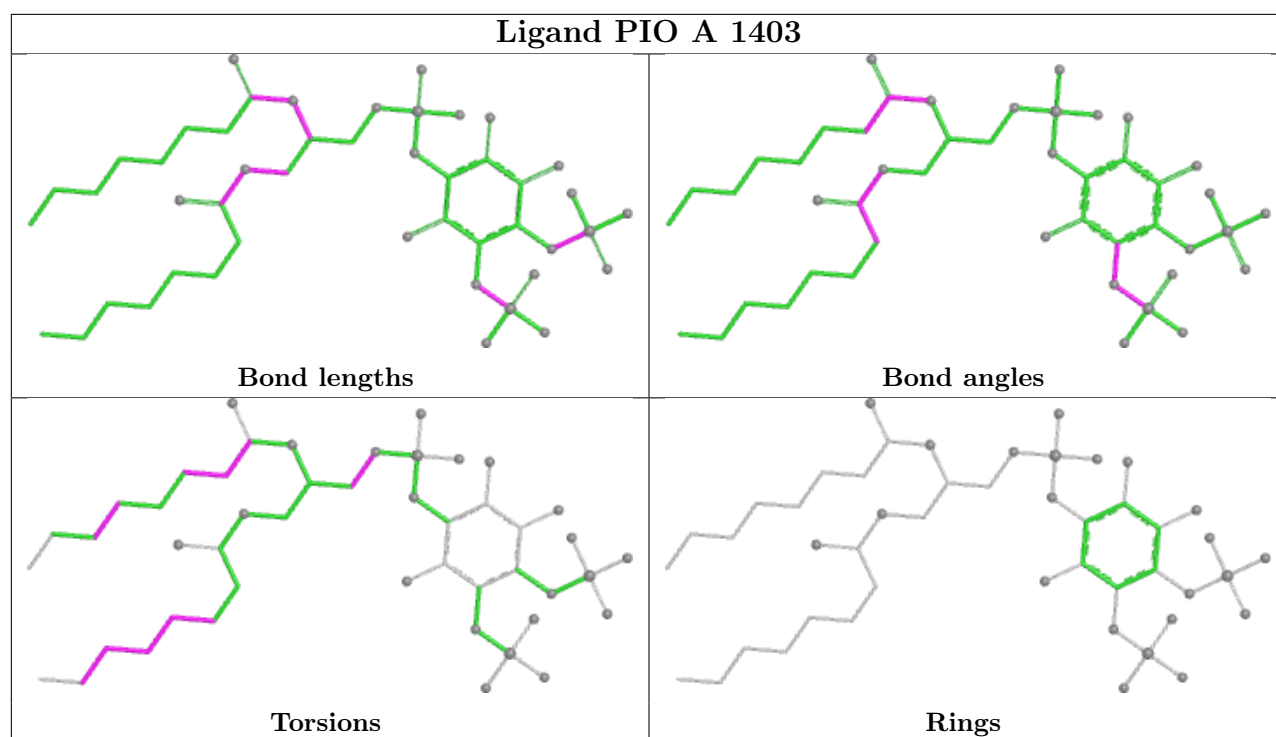
Continued from previous page...

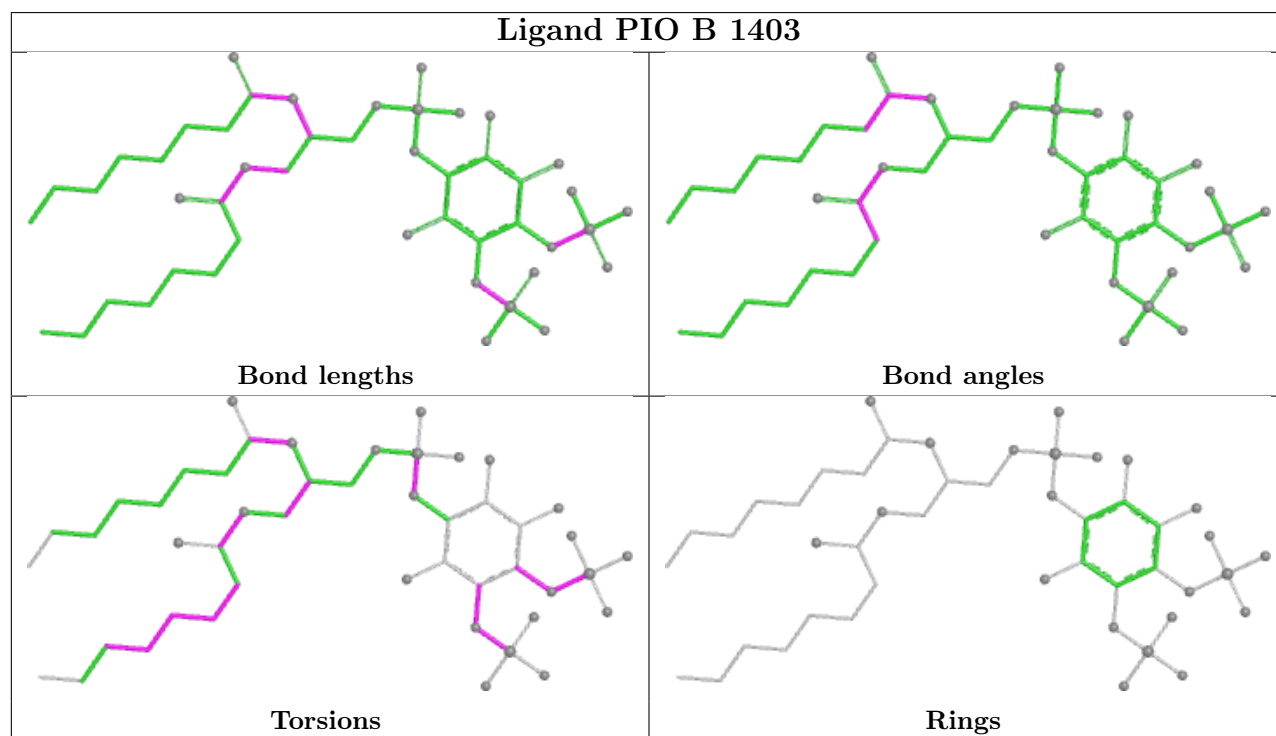
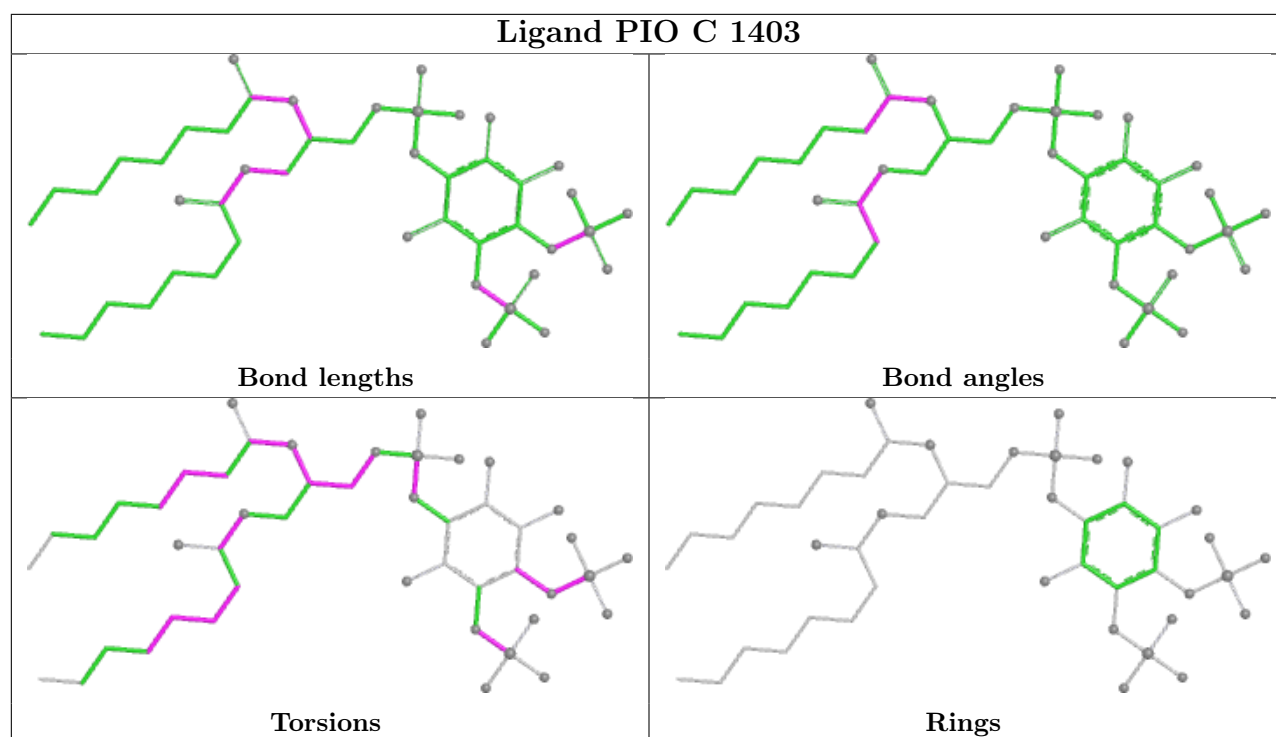
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1403	PIO	1	0
3	D	1401	3PH	1	0
3	C	1401	3PH	2	0
4	A	1402	9Z9	15	0

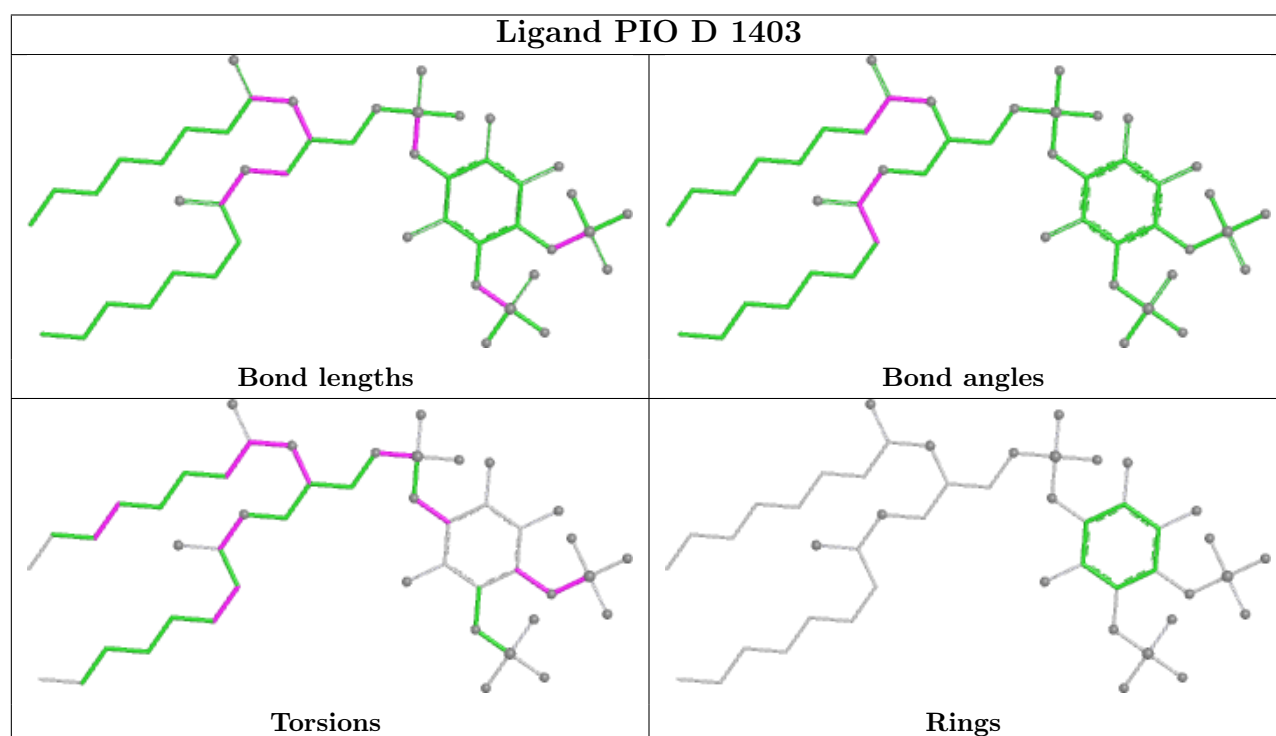
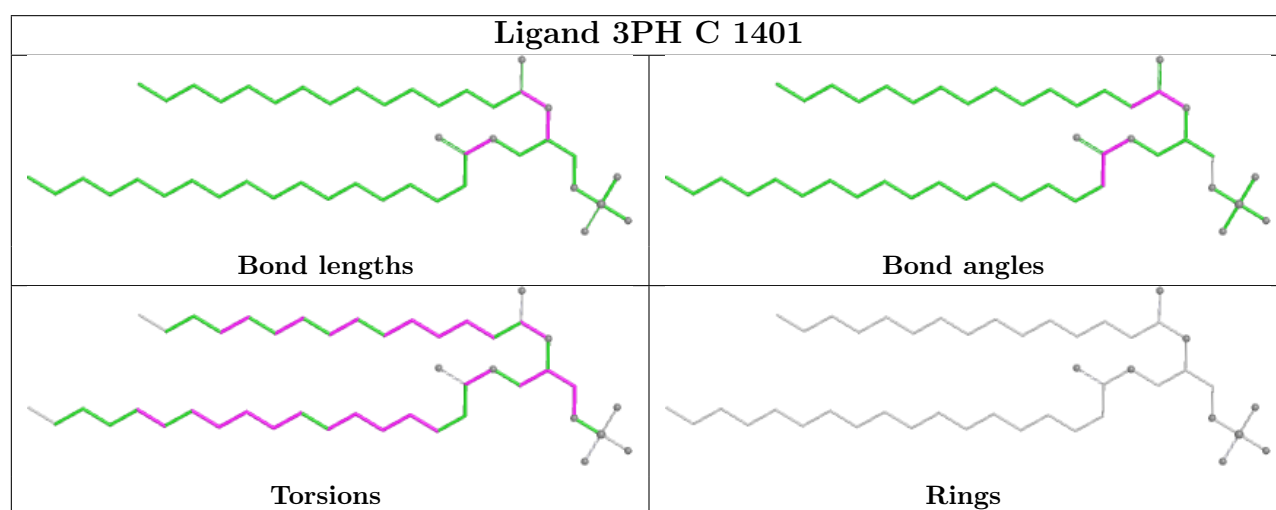
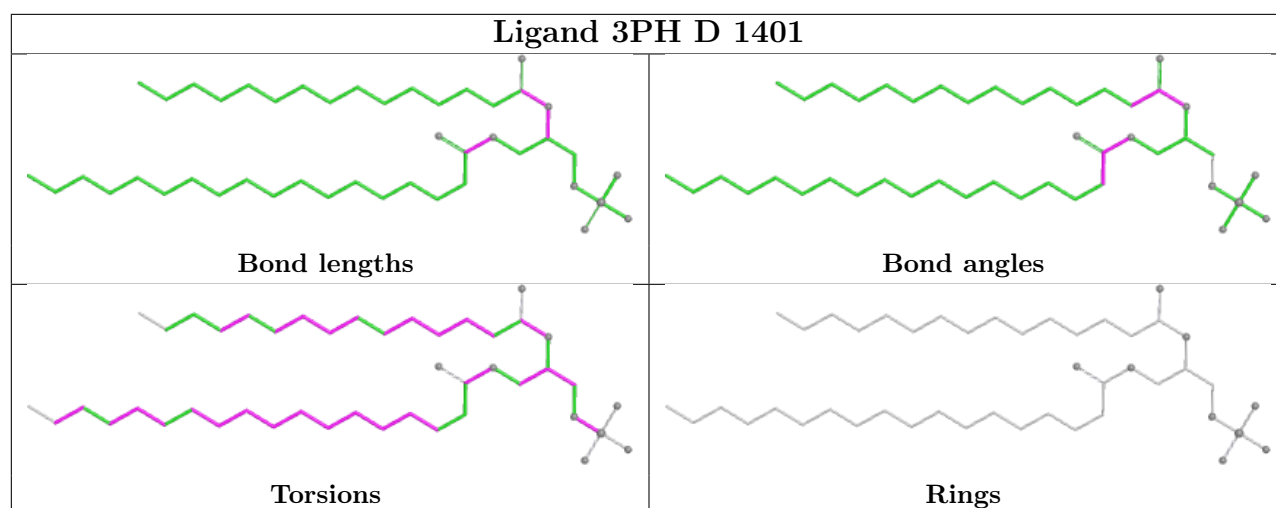
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

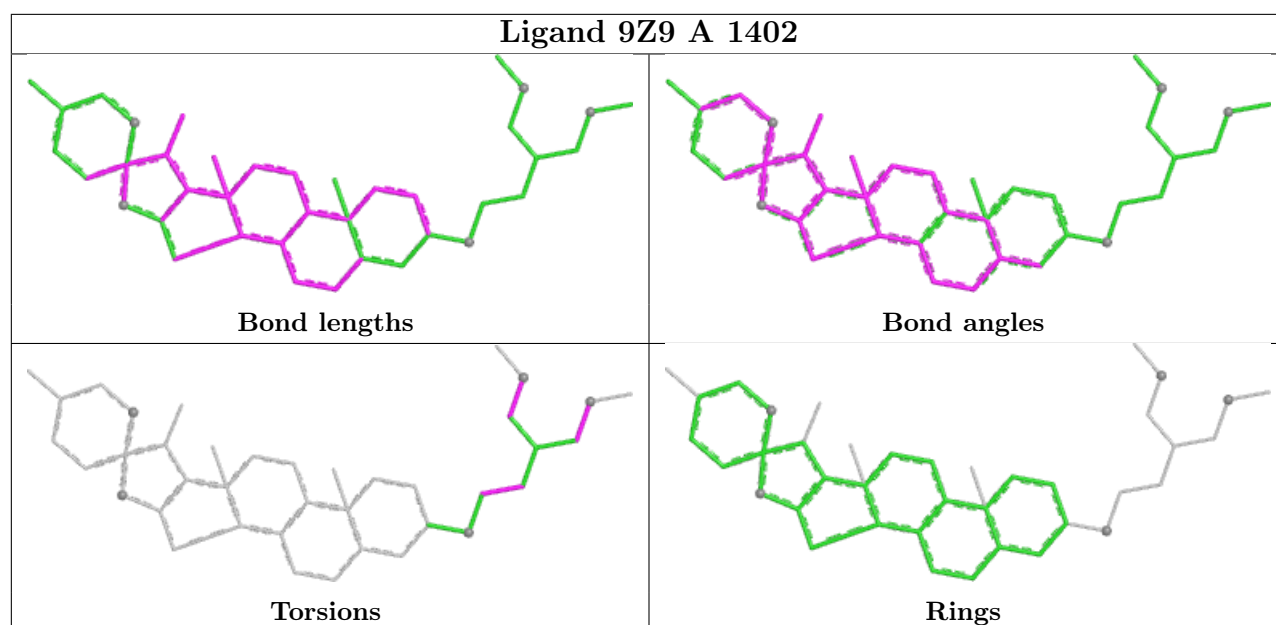












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

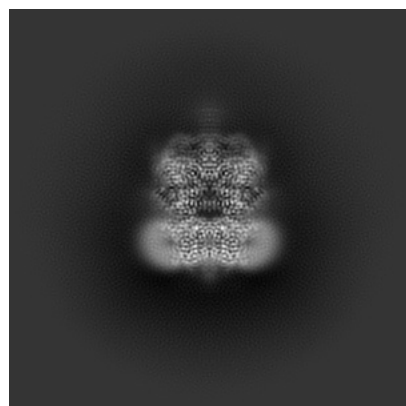
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28033. These allow visual inspection of the internal detail of the map and identification of artifacts.

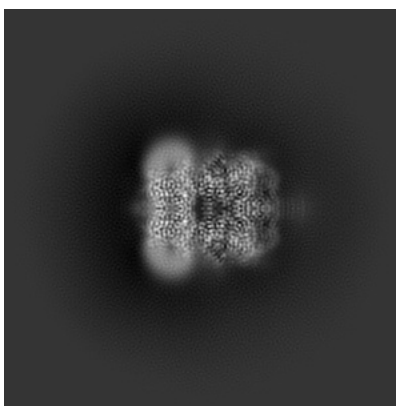
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

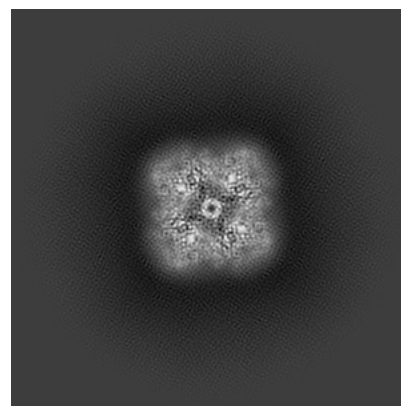
6.1.1 Primary map



X

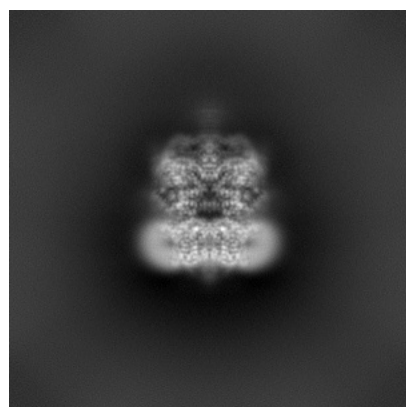


Y

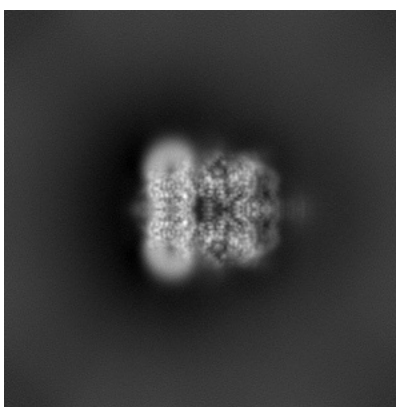


Z

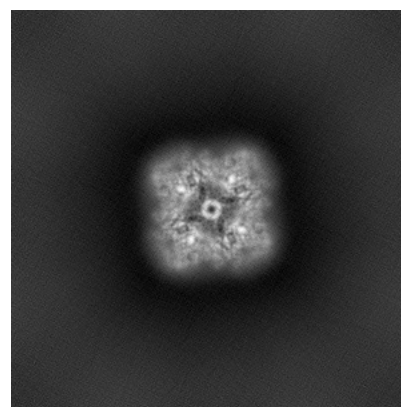
6.1.2 Raw map



X



Y

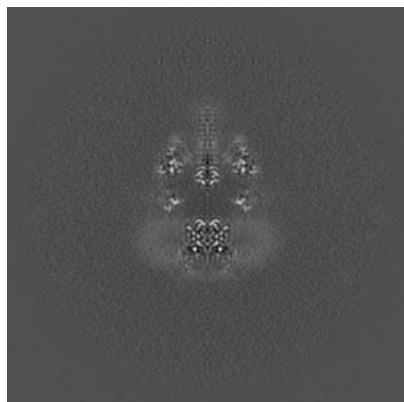


Z

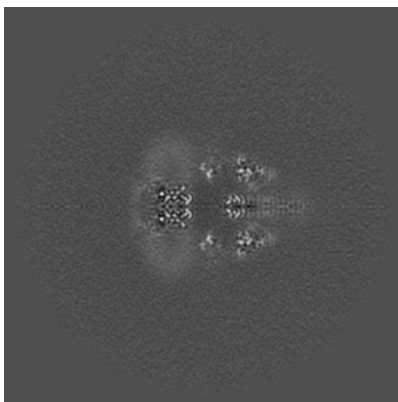
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

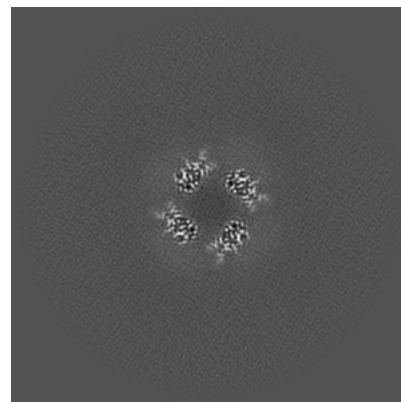
6.2.1 Primary map



X Index: 192

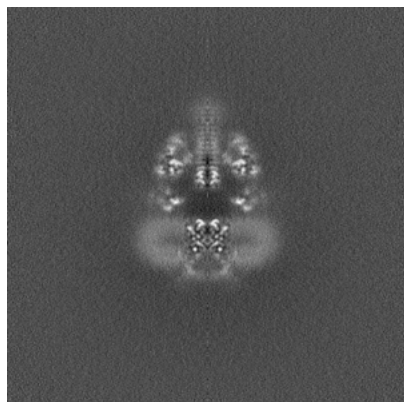


Y Index: 192

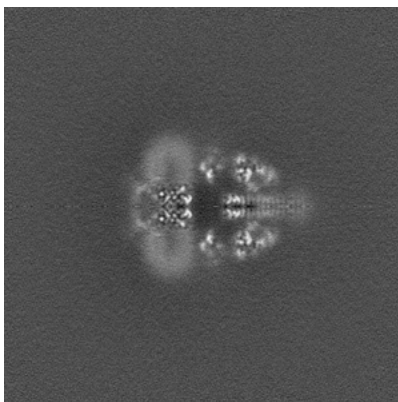


Z Index: 192

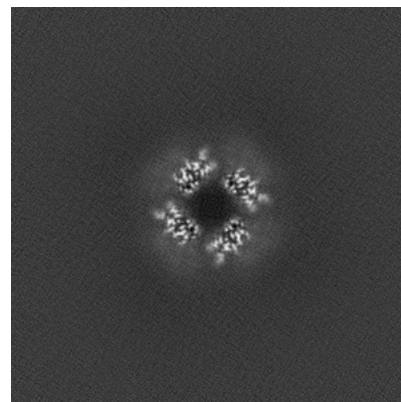
6.2.2 Raw map



X Index: 192



Y Index: 192

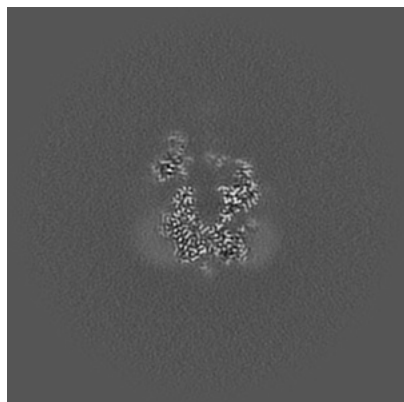


Z Index: 192

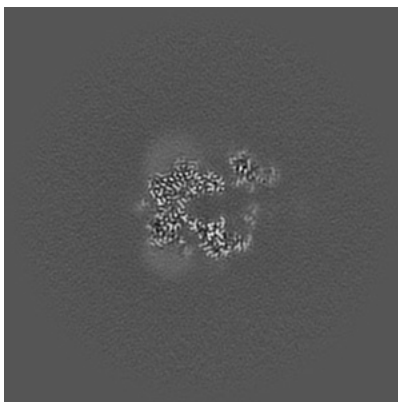
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

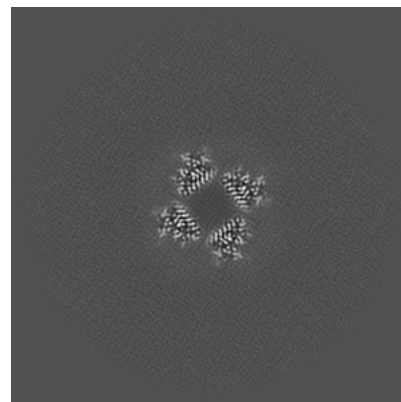
6.3.1 Primary map



X Index: 175

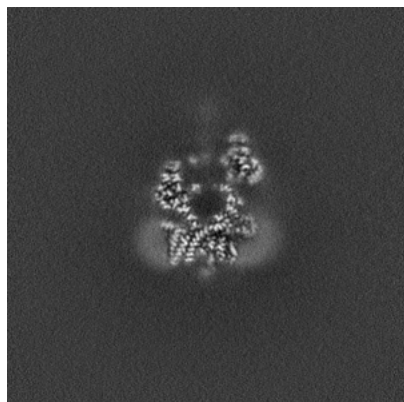


Y Index: 175

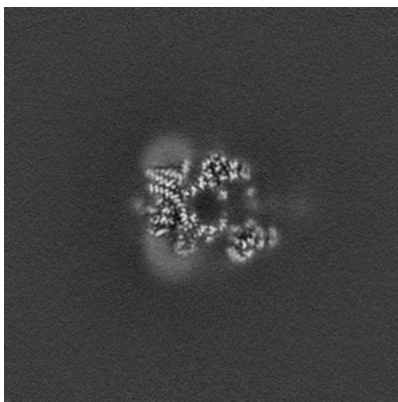


Z Index: 197

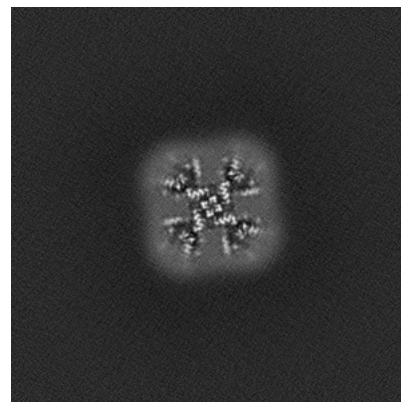
6.3.2 Raw map



X Index: 206



Y Index: 206

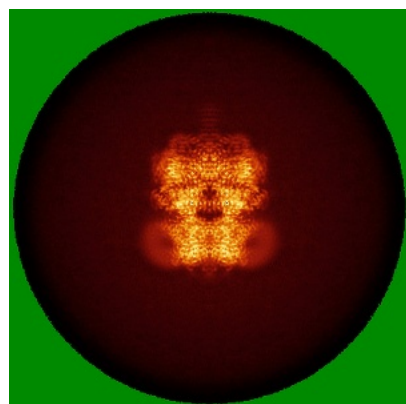


Z Index: 174

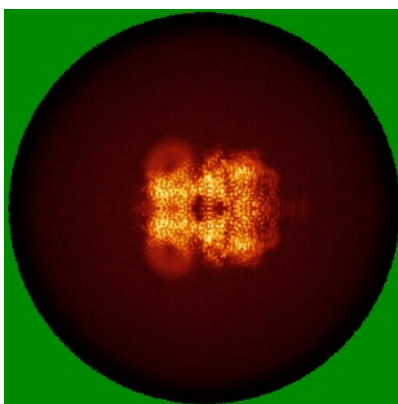
The images above show the largest variance slices of the map in three orthogonal directions.

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

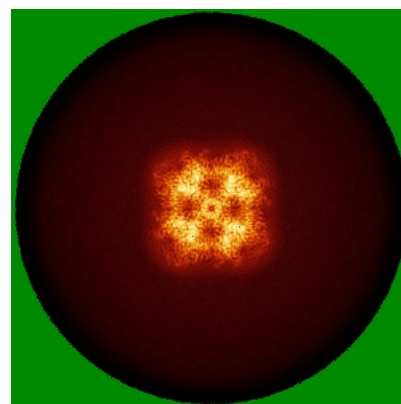
6.4.1 Primary map



X

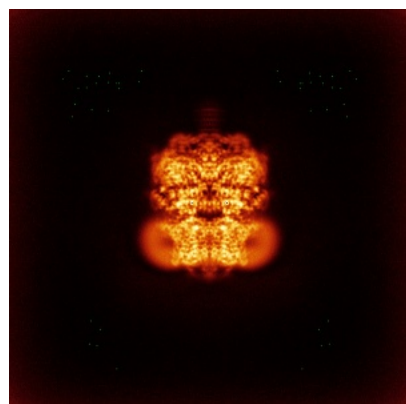


Y

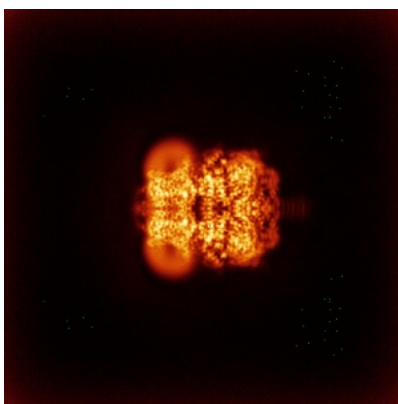


Z

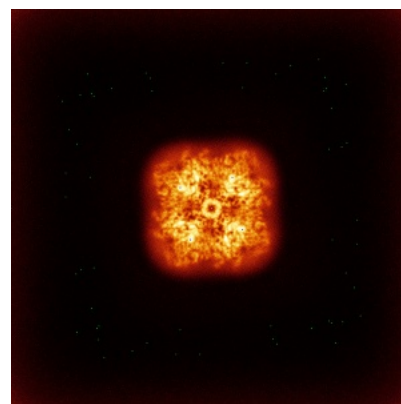
6.4.2 Raw map



X



Y

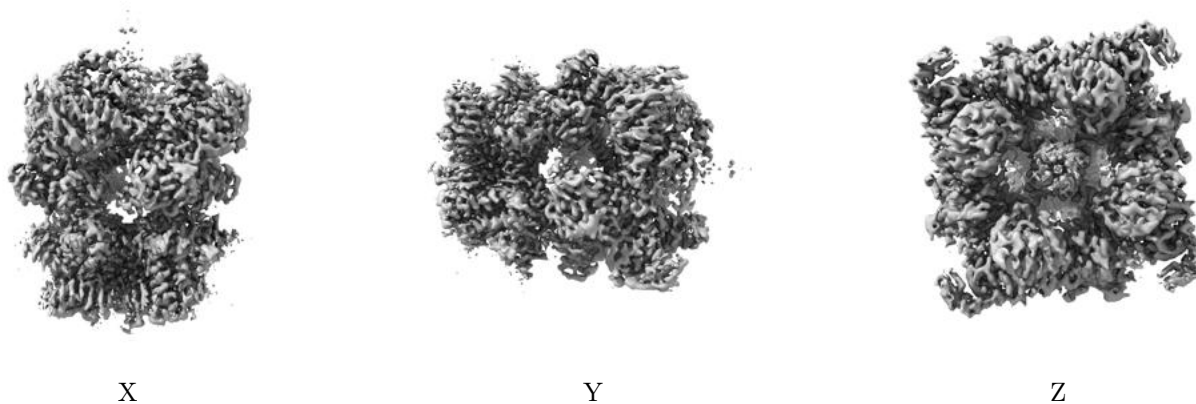


Z

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.

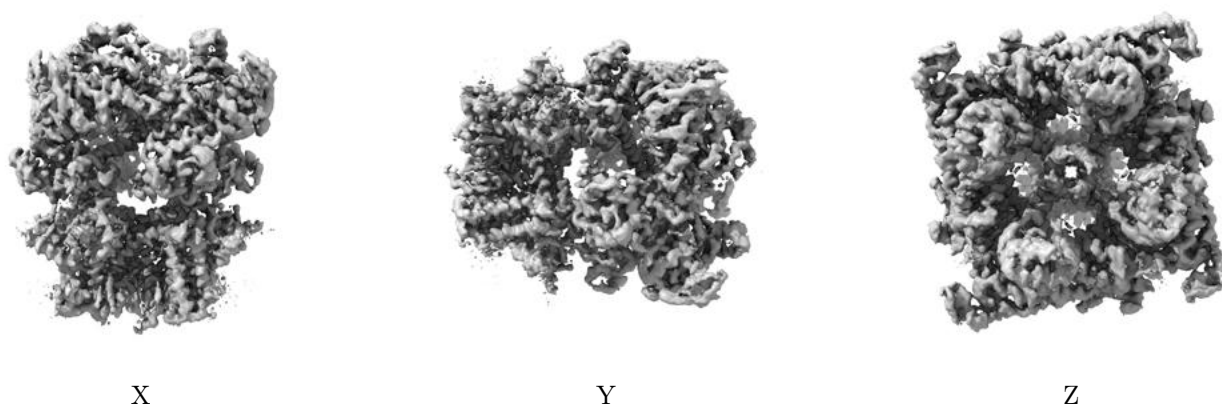
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

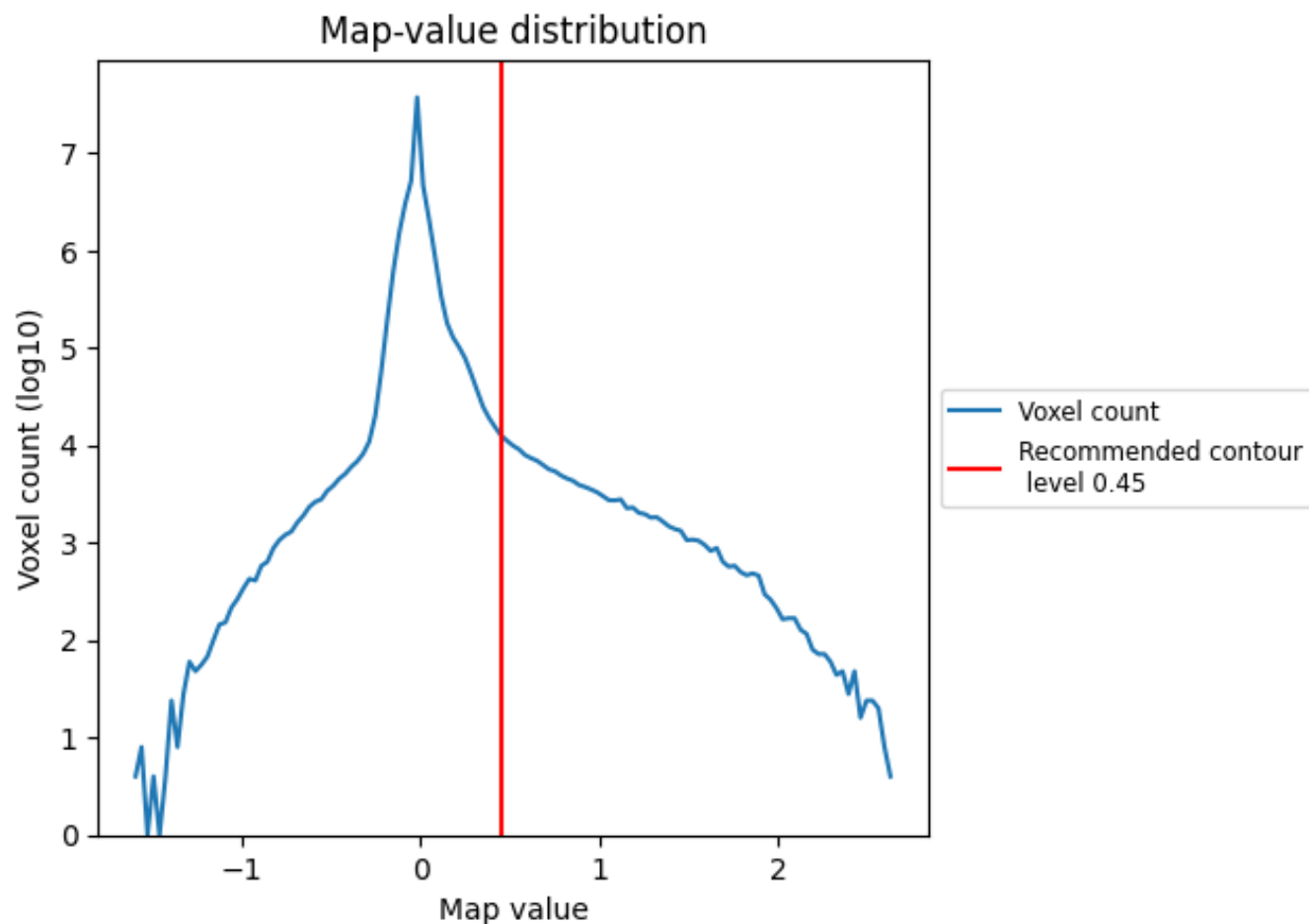
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

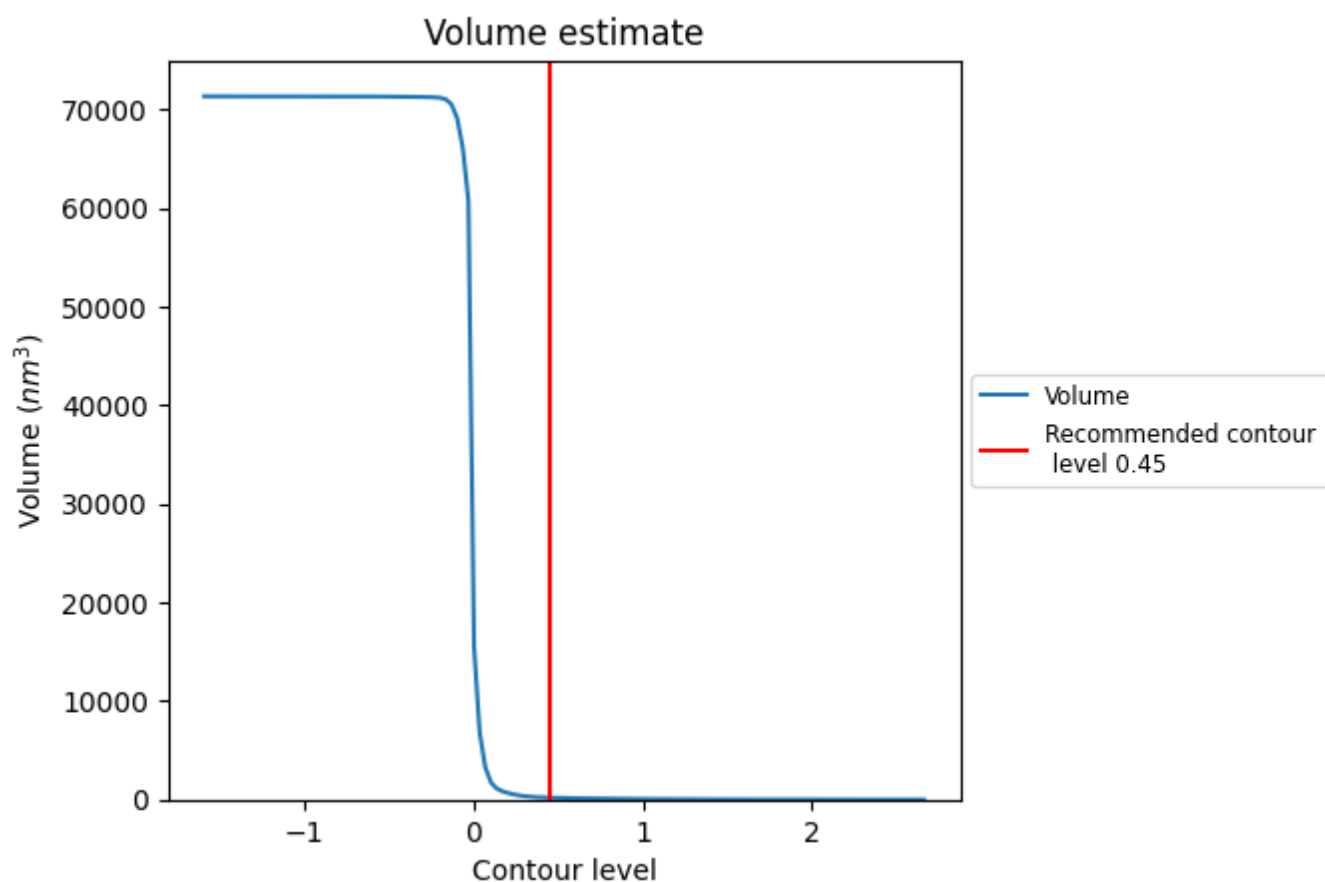
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

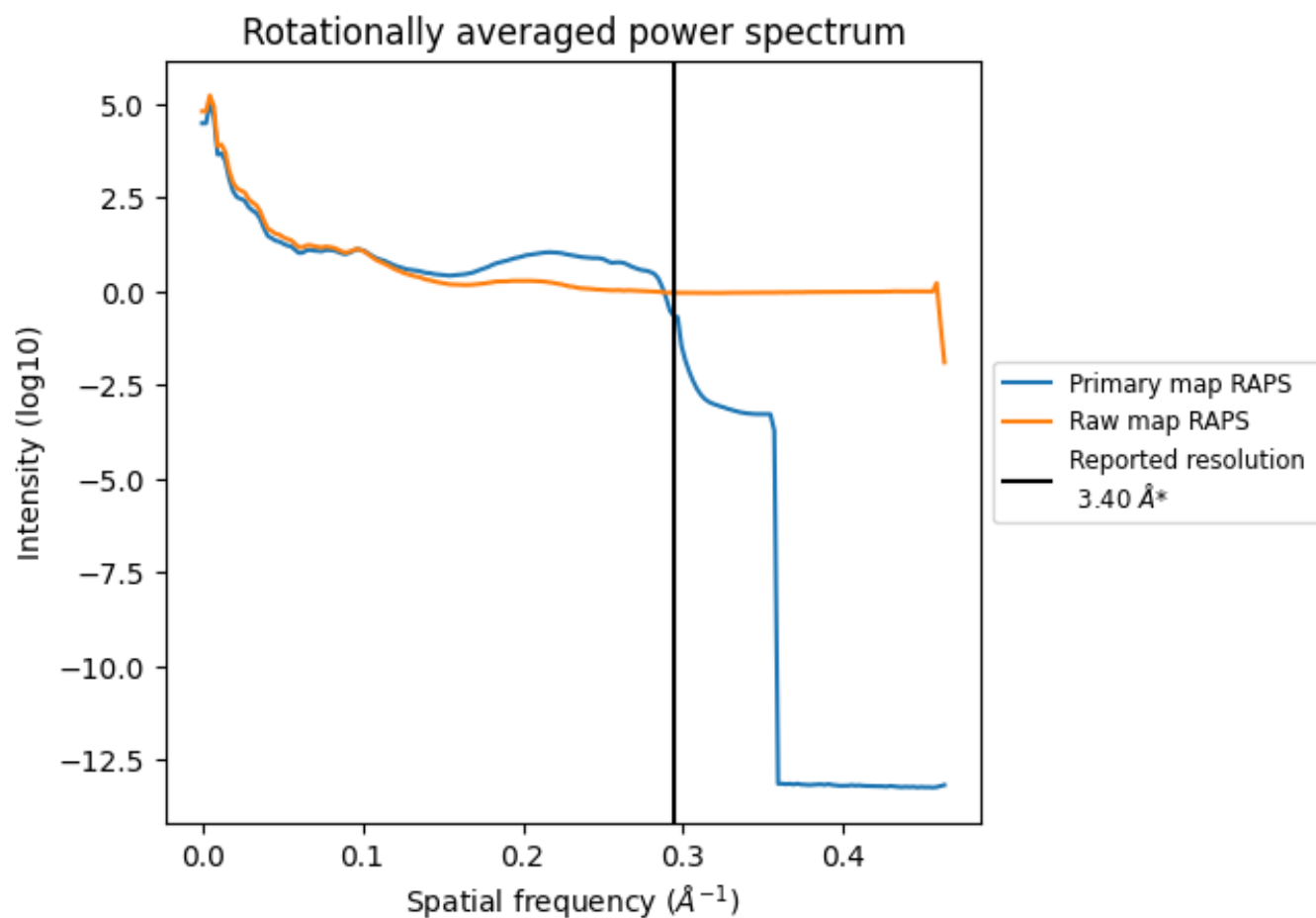
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 191 nm³; this corresponds to an approximate mass of 173 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 ⓘ

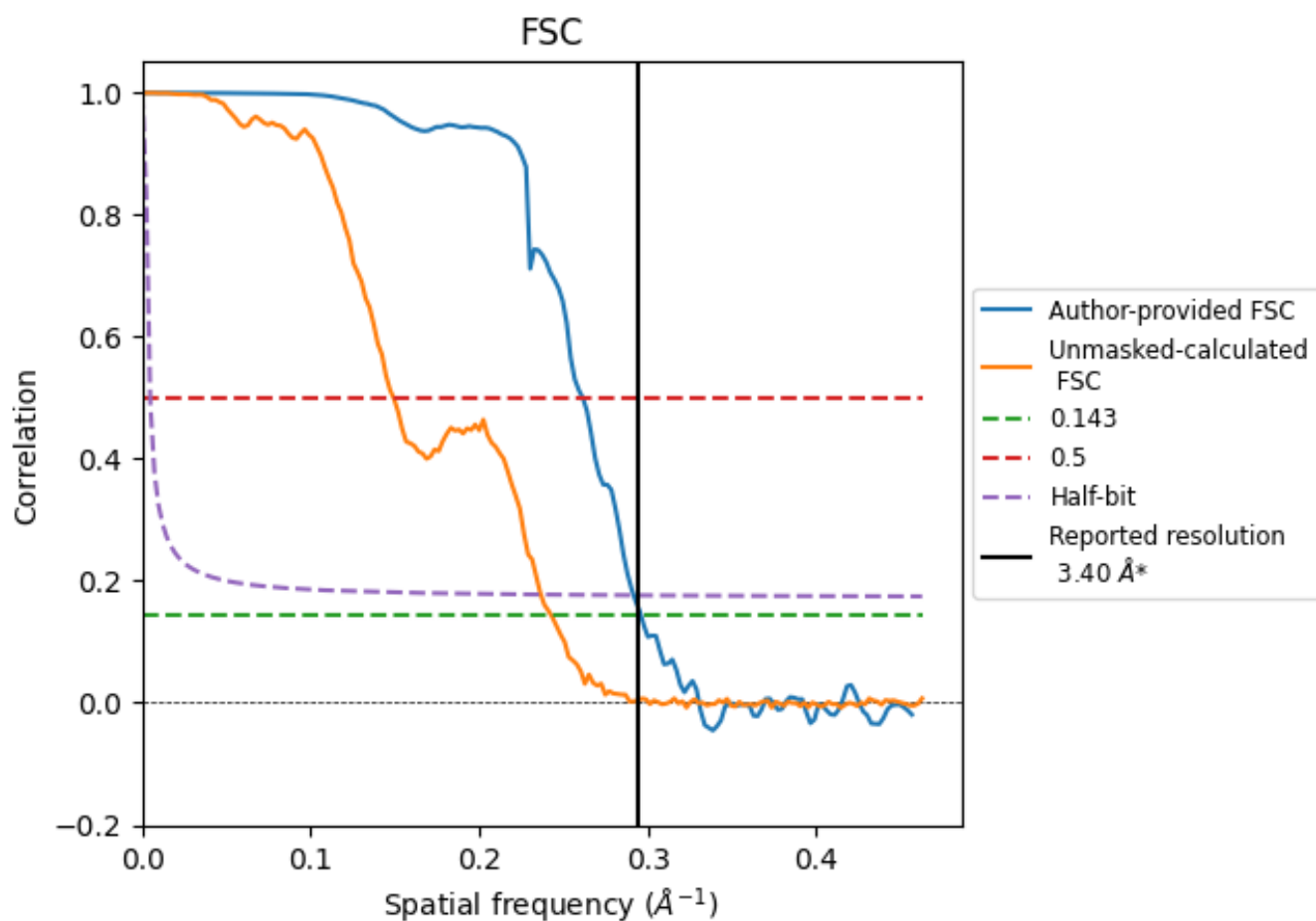


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

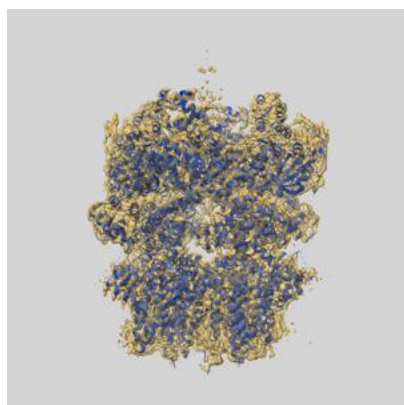
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.38	3.82	3.43
Unmasked-calculated*	4.12	6.70	4.23

*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 4.12 differs from the reported value 3.4 by more than 10 %

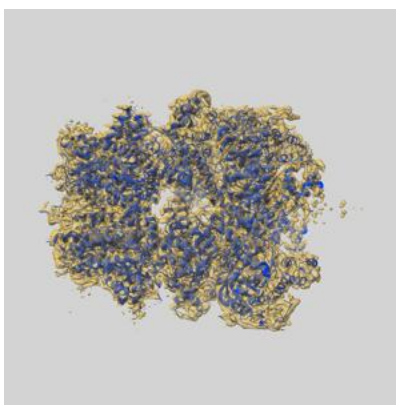
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-28033 and PDB model 8ED9. Per-residue inclusion information can be found in section [3](#) on page [7](#).

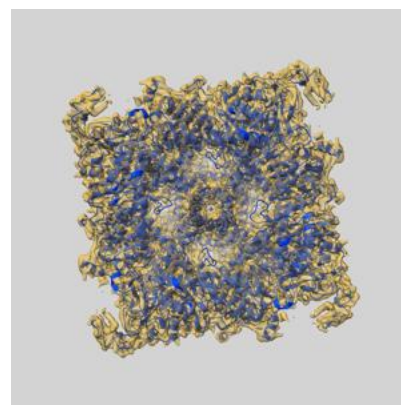
9.1 Map-model overlay [i](#)



X



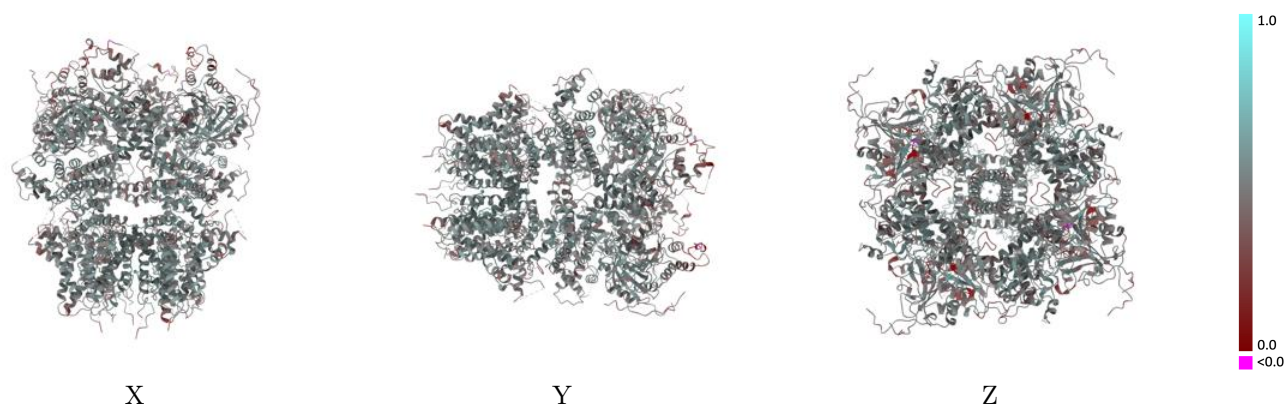
Y



Z

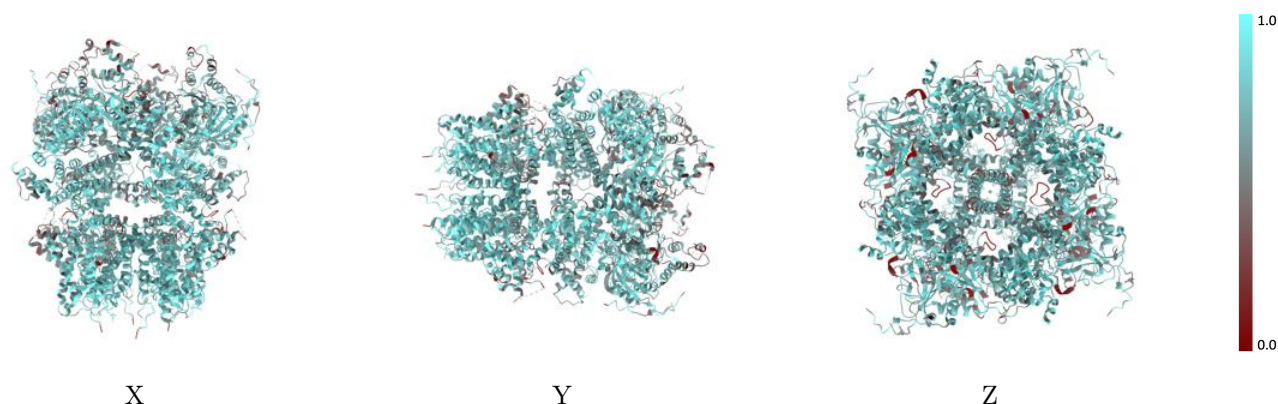
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



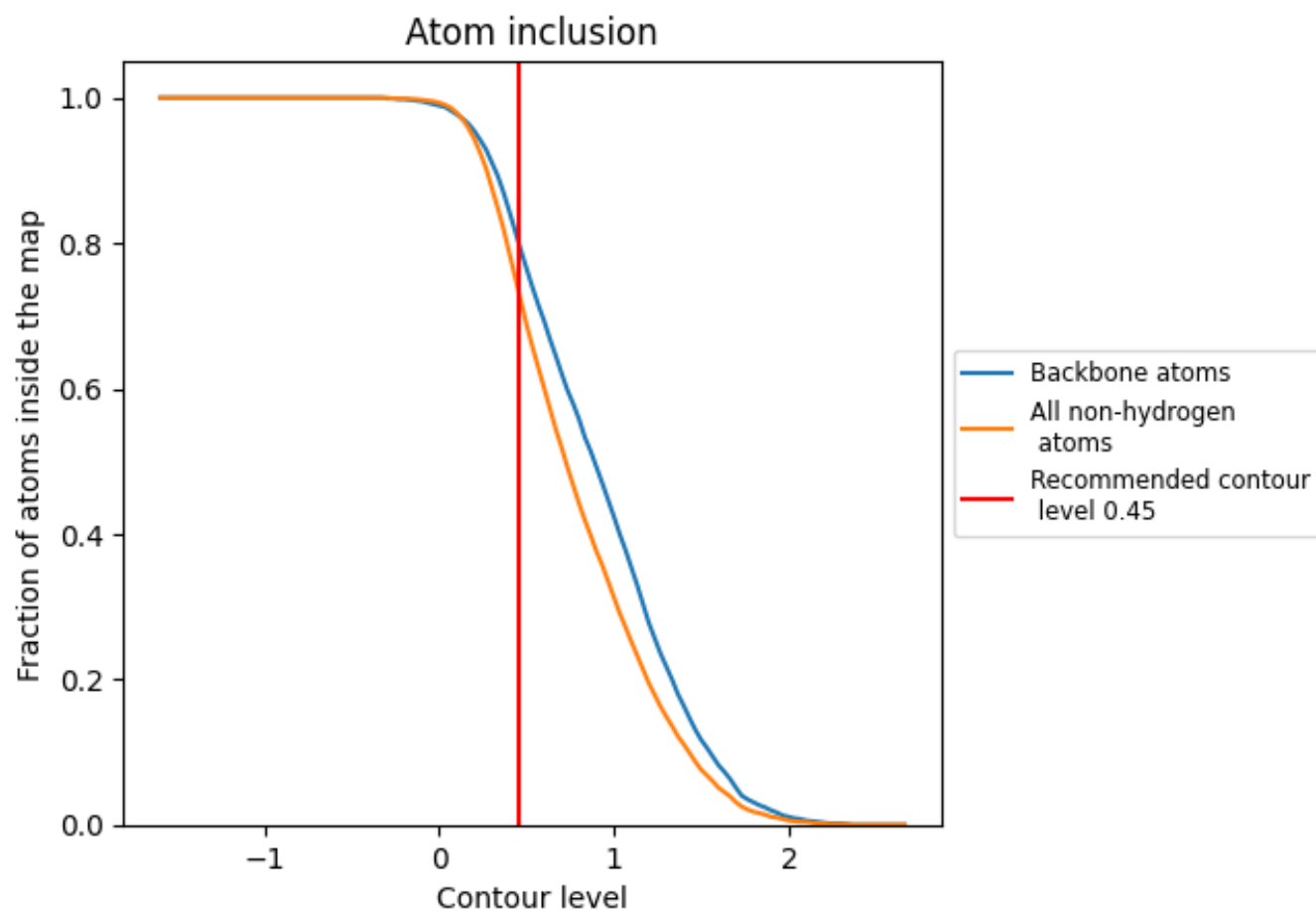
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 74% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7370	0.4880
A	0.7360	0.4870
B	0.7380	0.4900
C	0.7370	0.4880
D	0.7360	0.4900
E	0.7290	0.4360
F	0.7180	0.4420
G	0.7290	0.4270
H	0.7290	0.4290

