



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:19 PM UTC

PDB ID : 9B6H / pdb_00009b6h
EMDB ID : EMD-44259
Title : Cryo-EM structure of the mouse TRPM8 channel in complex with the antagonist TC-I 2014 and the cooling agonist C3
Authors : Yin, Y.; Park, C.-G.; Zhang, F.; Fedor, J.; Feng, S.; Suo, Y.; Im, W.; Lee, S.-Y.
Deposited on : 2024-03-25
Resolution : 2.76 Å(reported)
Based on initial model : .

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

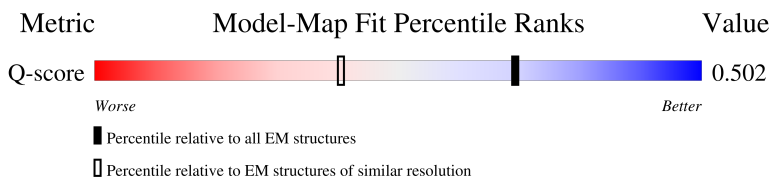
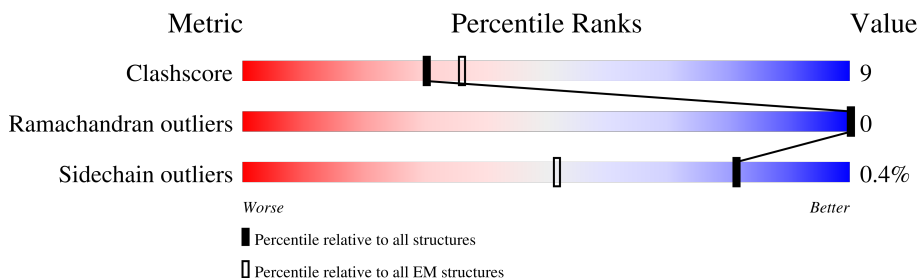
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.76 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	10642 (2.26 - 3.26)

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	1135	 70% 13% 18%
1	B	1135	 69% 13% 18%
1	C	1135	 69% 13% 18%

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Mol	Chain	Length	Quality of chain
1	D	1135	 69% 13% 18%

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
4	ULO	A	1301	-	X	-	-
4	ULO	B	1301	-	X	-	-
4	ULO	C	1301	-	X	-	-
4	ULO	D	1301	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 55880 atoms, of which 26884 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 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	934	Total	C	H	N	O	S	0	0
			13754	4637	6674	1166	1247	30		
1	B	934	Total	C	H	N	O	S	0	0
			13754	4637	6674	1166	1247	30		
1	C	934	Total	C	H	N	O	S	0	0
			13754	4637	6674	1166	1247	30		
1	D	934	Total	C	H	N	O	S	0	0
			13754	4637	6674	1166	1247	30		

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q8R4D5
A	1	ALA	-	expression tag	UNP Q8R4D5
A	1105	SER	-	expression tag	UNP Q8R4D5
A	1106	ASN	-	expression tag	UNP Q8R4D5
A	1107	SER	-	expression tag	UNP Q8R4D5
A	1108	LEU	-	expression tag	UNP Q8R4D5
A	1109	GLU	-	expression tag	UNP Q8R4D5
A	1110	VAL	-	expression tag	UNP Q8R4D5
A	1111	LEU	-	expression tag	UNP Q8R4D5
A	1112	PHE	-	expression tag	UNP Q8R4D5
A	1113	GLN	-	expression tag	UNP Q8R4D5
A	1114	GLY	-	expression tag	UNP Q8R4D5
A	1115	PRO	-	expression tag	UNP Q8R4D5
A	1116	ASP	-	expression tag	UNP Q8R4D5
A	1117	TYR	-	expression tag	UNP Q8R4D5
A	1118	LYS	-	expression tag	UNP Q8R4D5
A	1119	ASP	-	expression tag	UNP Q8R4D5
A	1120	ASP	-	expression tag	UNP Q8R4D5
A	1121	ASP	-	expression tag	UNP Q8R4D5
A	1122	ASP	-	expression tag	UNP Q8R4D5
A	1123	LYS	-	expression tag	UNP Q8R4D5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1124	ALA	-	expression tag	UNP Q8R4D5
A	1125	HIS	-	expression tag	UNP Q8R4D5
A	1126	HIS	-	expression tag	UNP Q8R4D5
A	1127	HIS	-	expression tag	UNP Q8R4D5
A	1128	HIS	-	expression tag	UNP Q8R4D5
A	1129	HIS	-	expression tag	UNP Q8R4D5
A	1130	HIS	-	expression tag	UNP Q8R4D5
A	1131	HIS	-	expression tag	UNP Q8R4D5
A	1132	HIS	-	expression tag	UNP Q8R4D5
A	1133	HIS	-	expression tag	UNP Q8R4D5
A	1134	HIS	-	expression tag	UNP Q8R4D5
B	0	MET	-	initiating methionine	UNP Q8R4D5
B	1	ALA	-	expression tag	UNP Q8R4D5
B	1105	SER	-	expression tag	UNP Q8R4D5
B	1106	ASN	-	expression tag	UNP Q8R4D5
B	1107	SER	-	expression tag	UNP Q8R4D5
B	1108	LEU	-	expression tag	UNP Q8R4D5
B	1109	GLU	-	expression tag	UNP Q8R4D5
B	1110	VAL	-	expression tag	UNP Q8R4D5
B	1111	LEU	-	expression tag	UNP Q8R4D5
B	1112	PHE	-	expression tag	UNP Q8R4D5
B	1113	GLN	-	expression tag	UNP Q8R4D5
B	1114	GLY	-	expression tag	UNP Q8R4D5
B	1115	PRO	-	expression tag	UNP Q8R4D5
B	1116	ASP	-	expression tag	UNP Q8R4D5
B	1117	TYR	-	expression tag	UNP Q8R4D5
B	1118	LYS	-	expression tag	UNP Q8R4D5
B	1119	ASP	-	expression tag	UNP Q8R4D5
B	1120	ASP	-	expression tag	UNP Q8R4D5
B	1121	ASP	-	expression tag	UNP Q8R4D5
B	1122	ASP	-	expression tag	UNP Q8R4D5
B	1123	LYS	-	expression tag	UNP Q8R4D5
B	1124	ALA	-	expression tag	UNP Q8R4D5
B	1125	HIS	-	expression tag	UNP Q8R4D5
B	1126	HIS	-	expression tag	UNP Q8R4D5
B	1127	HIS	-	expression tag	UNP Q8R4D5
B	1128	HIS	-	expression tag	UNP Q8R4D5
B	1129	HIS	-	expression tag	UNP Q8R4D5
B	1130	HIS	-	expression tag	UNP Q8R4D5
B	1131	HIS	-	expression tag	UNP Q8R4D5
B	1132	HIS	-	expression tag	UNP Q8R4D5
B	1133	HIS	-	expression tag	UNP Q8R4D5

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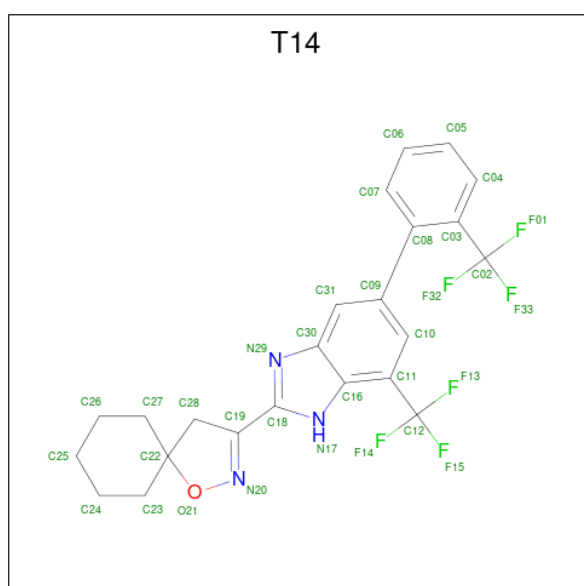
Chain	Residue	Modelled	Actual	Comment	Reference
B	1134	HIS	-	expression tag	UNP Q8R4D5
C	0	MET	-	initiating methionine	UNP Q8R4D5
C	1	ALA	-	expression tag	UNP Q8R4D5
C	1105	SER	-	expression tag	UNP Q8R4D5
C	1106	ASN	-	expression tag	UNP Q8R4D5
C	1107	SER	-	expression tag	UNP Q8R4D5
C	1108	LEU	-	expression tag	UNP Q8R4D5
C	1109	GLU	-	expression tag	UNP Q8R4D5
C	1110	VAL	-	expression tag	UNP Q8R4D5
C	1111	LEU	-	expression tag	UNP Q8R4D5
C	1112	PHE	-	expression tag	UNP Q8R4D5
C	1113	GLN	-	expression tag	UNP Q8R4D5
C	1114	GLY	-	expression tag	UNP Q8R4D5
C	1115	PRO	-	expression tag	UNP Q8R4D5
C	1116	ASP	-	expression tag	UNP Q8R4D5
C	1117	TYR	-	expression tag	UNP Q8R4D5
C	1118	LYS	-	expression tag	UNP Q8R4D5
C	1119	ASP	-	expression tag	UNP Q8R4D5
C	1120	ASP	-	expression tag	UNP Q8R4D5
C	1121	ASP	-	expression tag	UNP Q8R4D5
C	1122	ASP	-	expression tag	UNP Q8R4D5
C	1123	LYS	-	expression tag	UNP Q8R4D5
C	1124	ALA	-	expression tag	UNP Q8R4D5
C	1125	HIS	-	expression tag	UNP Q8R4D5
C	1126	HIS	-	expression tag	UNP Q8R4D5
C	1127	HIS	-	expression tag	UNP Q8R4D5
C	1128	HIS	-	expression tag	UNP Q8R4D5
C	1129	HIS	-	expression tag	UNP Q8R4D5
C	1130	HIS	-	expression tag	UNP Q8R4D5
C	1131	HIS	-	expression tag	UNP Q8R4D5
C	1132	HIS	-	expression tag	UNP Q8R4D5
C	1133	HIS	-	expression tag	UNP Q8R4D5
C	1134	HIS	-	expression tag	UNP Q8R4D5
D	0	MET	-	initiating methionine	UNP Q8R4D5
D	1	ALA	-	expression tag	UNP Q8R4D5
D	1105	SER	-	expression tag	UNP Q8R4D5
D	1106	ASN	-	expression tag	UNP Q8R4D5
D	1107	SER	-	expression tag	UNP Q8R4D5
D	1108	LEU	-	expression tag	UNP Q8R4D5
D	1109	GLU	-	expression tag	UNP Q8R4D5
D	1110	VAL	-	expression tag	UNP Q8R4D5
D	1111	LEU	-	expression tag	UNP Q8R4D5

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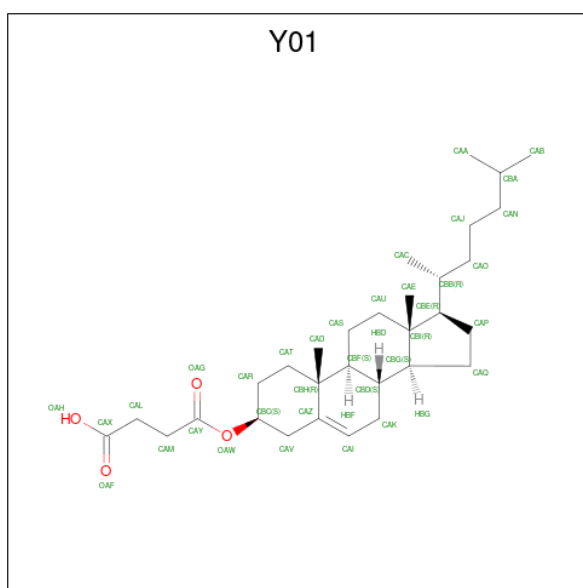
Chain	Residue	Modelled	Actual	Comment	Reference
D	1112	PHE	-	expression tag	UNP Q8R4D5
D	1113	GLN	-	expression tag	UNP Q8R4D5
D	1114	GLY	-	expression tag	UNP Q8R4D5
D	1115	PRO	-	expression tag	UNP Q8R4D5
D	1116	ASP	-	expression tag	UNP Q8R4D5
D	1117	TYR	-	expression tag	UNP Q8R4D5
D	1118	LYS	-	expression tag	UNP Q8R4D5
D	1119	ASP	-	expression tag	UNP Q8R4D5
D	1120	ASP	-	expression tag	UNP Q8R4D5
D	1121	ASP	-	expression tag	UNP Q8R4D5
D	1122	ASP	-	expression tag	UNP Q8R4D5
D	1123	LYS	-	expression tag	UNP Q8R4D5
D	1124	ALA	-	expression tag	UNP Q8R4D5
D	1125	HIS	-	expression tag	UNP Q8R4D5
D	1126	HIS	-	expression tag	UNP Q8R4D5
D	1127	HIS	-	expression tag	UNP Q8R4D5
D	1128	HIS	-	expression tag	UNP Q8R4D5
D	1129	HIS	-	expression tag	UNP Q8R4D5
D	1130	HIS	-	expression tag	UNP Q8R4D5
D	1131	HIS	-	expression tag	UNP Q8R4D5
D	1132	HIS	-	expression tag	UNP Q8R4D5
D	1133	HIS	-	expression tag	UNP Q8R4D5
D	1134	HIS	-	expression tag	UNP Q8R4D5

- Molecule 2 is 3-{7-(trifluoromethyl)-5-[2-(trifluoromethyl)phenyl]-1H-benzimidazol-2-yl}-1-oxa-2-azaspiro[4.5]dec-2-ene (CCD ID: T14) (formula: C₂₃H₁₉F₆N₃O).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 33	C 23	F 6	N 3	O 1	0
2	B	1	Total 33	C 23	F 6	N 3	O 1	0
2	C	1	Total 33	C 23	F 6	N 3	O 1	0
2	D	1	Total 33	C 23	F 6	N 3	O 1	0

- Molecule 3 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$).



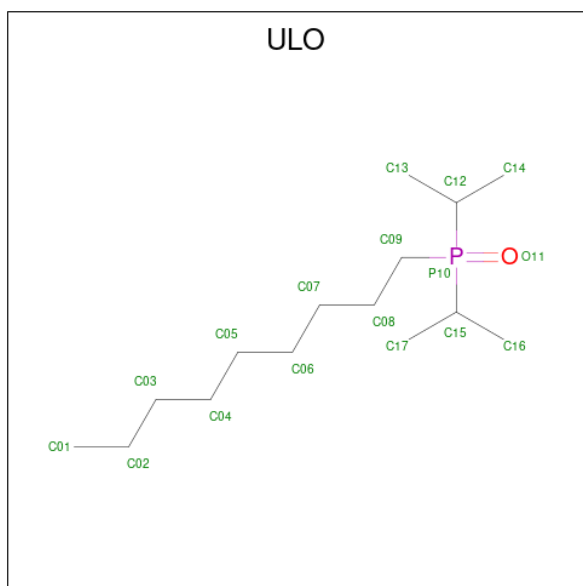
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total 35	C 31	O 4	0
3	A	1	Total 35	C 31	O 4	0
3	A	1	Total 35	C 31	O 4	0
3	B	1	Total 35	C 31	O 4	0
3	B	1	Total 35	C 31	O 4	0
3	B	1	Total 35	C 31	O 4	0
3	C	1	Total 35	C 31	O 4	0
3	C	1	Total 35	C 31	O 4	0

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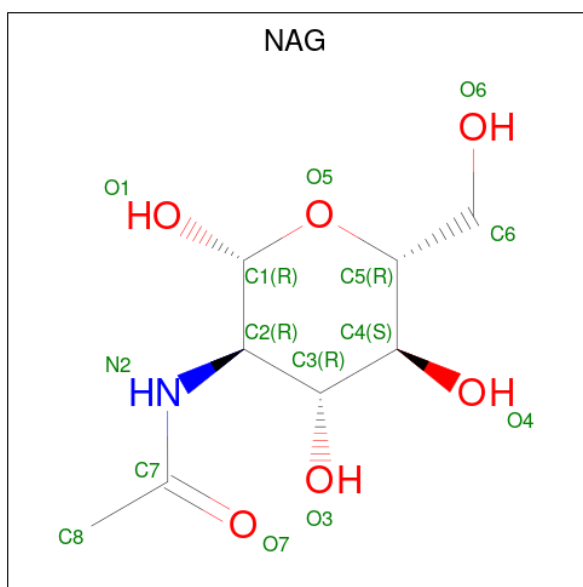
Mol	Chain	Residues	Atoms			AltConf
3	C	1	Total	C	O	0
			35	31	4	
3	D	1	Total	C	O	0
			35	31	4	
3	D	1	Total	C	O	0
			35	31	4	
3	D	1	Total	C	O	0
			35	31	4	

- Molecule 4 is nonyl(oxo)di(propan-2-yl)-lambda 5 -phosphane (CCD ID: ULO) (formula: C₁₅H₃₃OP).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	H	O	P	0
			50	15	33	1	1	
4	B	1	Total	C	H	O	P	0
			50	15	33	1	1	
4	C	1	Total	C	H	O	P	0
			50	15	33	1	1	
4	D	1	Total	C	H	O	P	0
			50	15	33	1	1	

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

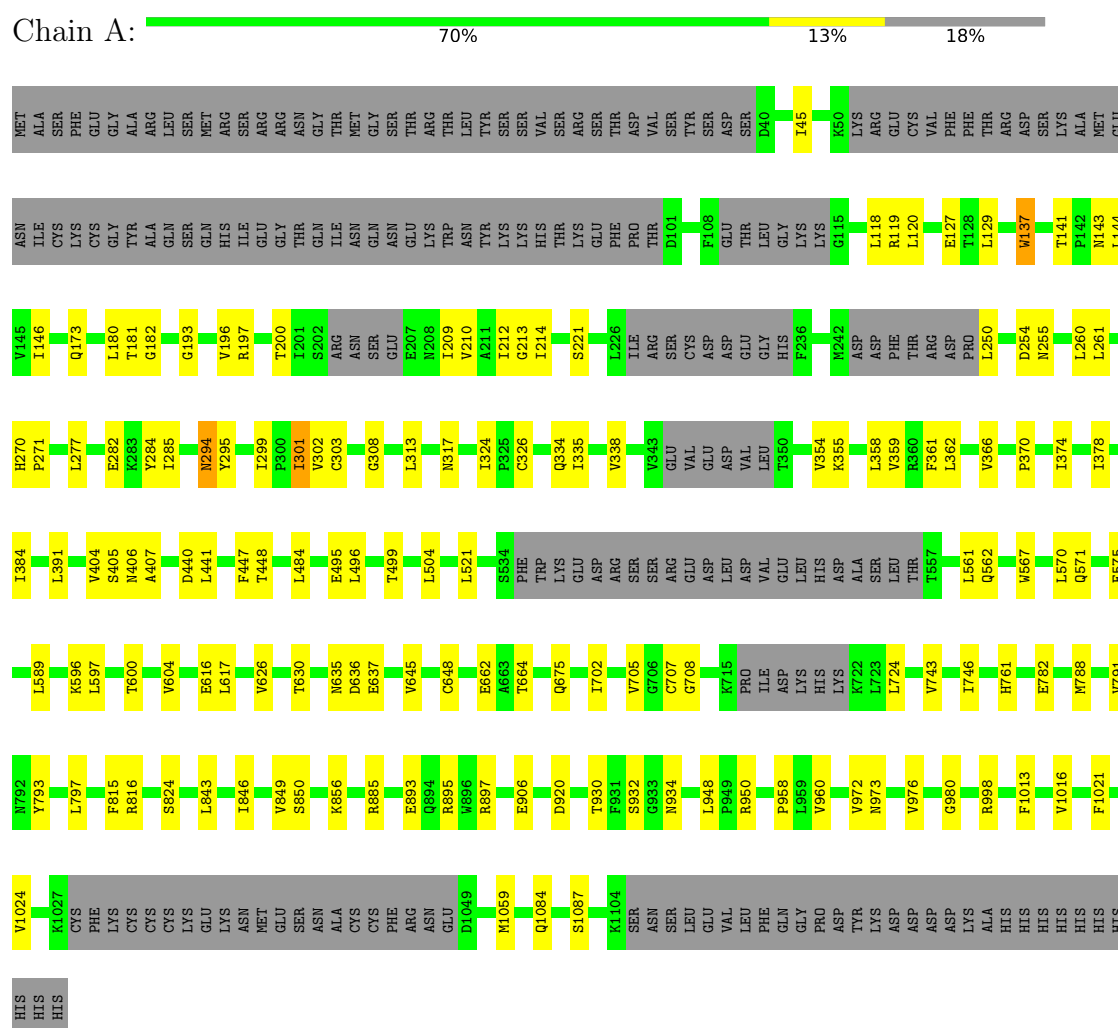


Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
5	A	1	28	8	14	1	5	0
5	B	1	28	8	14	1	5	0
5	C	1	28	8	14	1	5	0
5	D	1	28	8	14	1	5	0

3 Residue-property plots

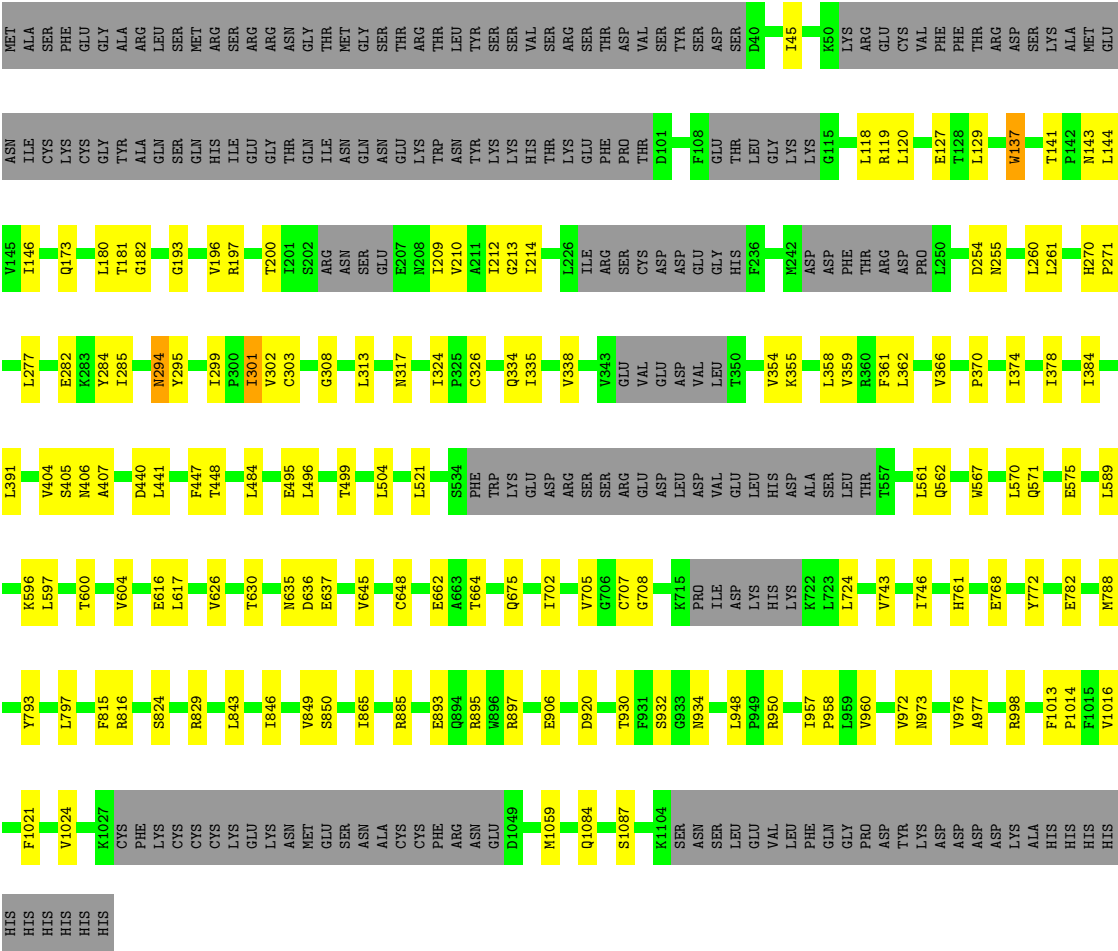
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Transient receptor potential cation channel subfamily M member 8

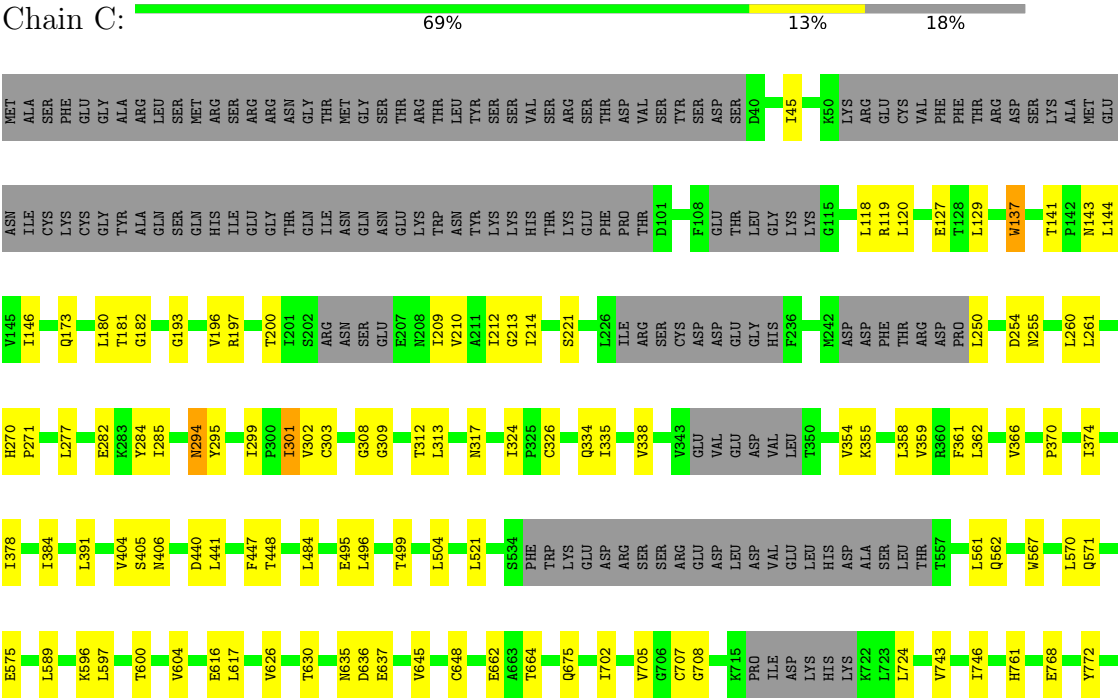


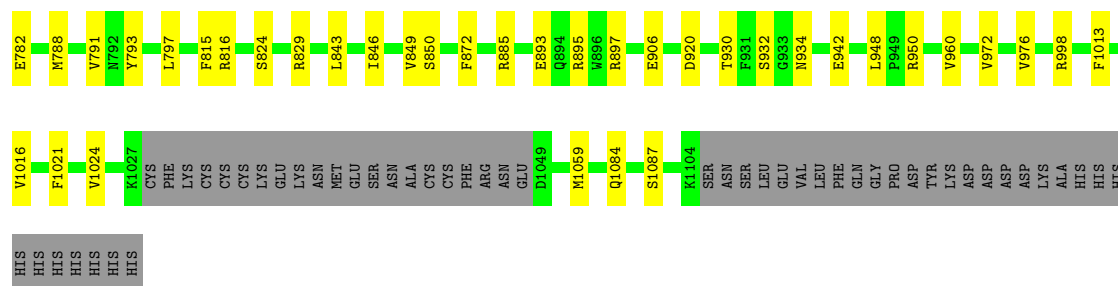
- Molecule 1: Transient receptor potential cation channel subfamily M member 8





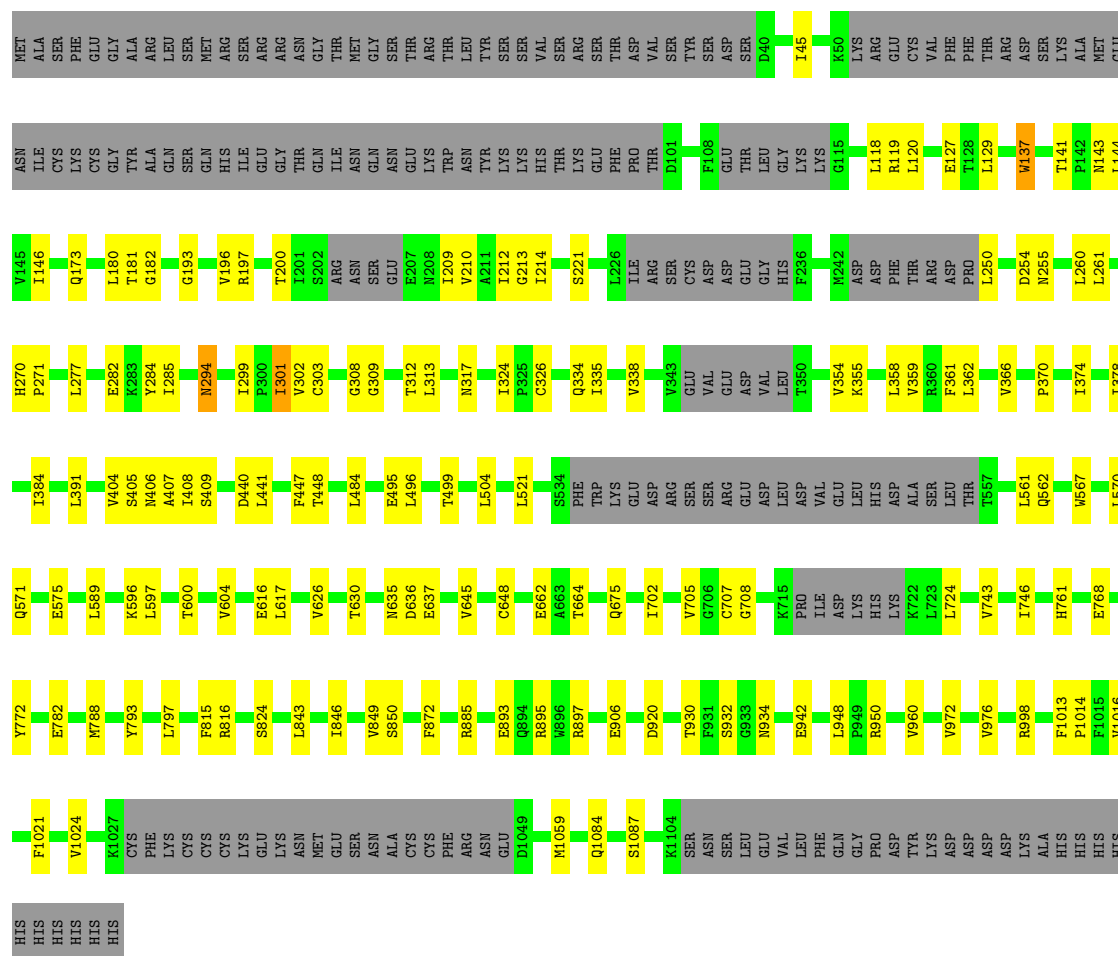
• Molecule 1: Transient receptor potential cation channel subfamily M member 8





- Molecule 1: Transient receptor potential cation channel subfamily M member 8

Chain D: 69% 13% 18%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	112062	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.827	Depositor
Minimum map value	-1.062	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	345.6, 345.6, 345.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ULO, Y01, NAG, T14

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	0.21	0/7243	0.34	4/9879 (0.0%)
1	B	0.22	0/7243	0.35	4/9879 (0.0%)
1	C	0.22	0/7243	0.35	4/9879 (0.0%)
1	D	0.22	0/7243	0.34	4/9879 (0.0%)
All	All	0.22	0/28972	0.35	16/39516 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	299	ILE	CA-C-N	-5.88	113.73	119.90
1	B	299	ILE	C-N-CA	-5.88	113.73	119.90
1	A	299	ILE	CA-C-N	-5.86	113.75	119.90
1	A	299	ILE	C-N-CA	-5.86	113.75	119.90
1	D	299	ILE	CA-C-N	-5.84	113.77	119.90
1	D	299	ILE	C-N-CA	-5.84	113.77	119.90
1	C	299	ILE	CA-C-N	-5.84	113.77	119.90
1	C	299	ILE	C-N-CA	-5.84	113.77	119.90
1	B	950	ARG	N-CA-C	5.80	120.51	113.38
1	D	950	ARG	N-CA-C	5.79	120.50	113.38
1	A	950	ARG	N-CA-C	5.78	120.49	113.38
1	C	950	ARG	N-CA-C	5.77	120.48	113.38
1	D	301	ILE	N-CA-C	-5.30	100.01	107.75
1	A	301	ILE	N-CA-C	-5.30	100.01	107.75
1	B	301	ILE	N-CA-C	-5.30	100.01	107.75
1	C	301	ILE	N-CA-C	-5.29	100.03	107.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7080	6674	6687	114	0
1	B	7080	6674	6687	113	0
1	C	7080	6674	6687	111	0
1	D	7080	6674	6687	113	0
2	A	33	0	0	0	0
2	B	33	0	0	0	0
2	C	33	0	0	0	0
2	D	33	0	0	0	0
3	A	105	0	147	26	0
3	B	105	0	147	23	0
3	C	105	0	147	25	0
3	D	105	0	147	21	0
4	A	17	33	0	0	0
4	B	17	33	0	0	0
4	C	17	33	0	0	0
4	D	17	33	0	0	0
5	A	14	14	13	1	0
5	B	14	14	13	1	0
5	C	14	14	13	1	0
5	D	14	14	13	1	0
All	All	28996	26884	27388	508	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 9.

All (508) 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:B:589:LEU:HD21	1:B:648:CYS:SG	1.69	1.32
1:C:589:LEU:HD21	1:C:648:CYS:SG	1.69	1.31
1:D:589:LEU:HD21	1:D:648:CYS:SG	1.69	1.30
1:A:589:LEU:HD21	1:A:648:CYS:SG	1.69	1.29
1:A:920:ASP:OD2	1:A:960:VAL:HG21	1.42	1.19
1:B:920:ASP:OD2	1:B:960:VAL:HG21	1.42	1.18
1:C:920:ASP:OD2	1:C:960:VAL:HG21	1.42	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:920:ASP:OD2	1:D:960:VAL:HG21	1.42	1.16
1:C:589:LEU:CD2	1:C:648:CYS:SG	2.55	0.95
1:B:589:LEU:CD2	1:B:648:CYS:SG	2.55	0.94
1:A:589:LEU:CD2	1:A:648:CYS:SG	2.55	0.94
1:D:589:LEU:CD2	1:D:648:CYS:SG	2.55	0.94
1:A:447:PHE:O	1:A:448:THR:OG1	1.97	0.83
1:A:920:ASP:OD2	1:A:960:VAL:CG2	2.26	0.83
1:B:920:ASP:OD2	1:B:960:VAL:CG2	2.26	0.81
1:C:447:PHE:O	1:C:448:THR:OG1	1.97	0.81
1:D:920:ASP:OD2	1:D:960:VAL:CG2	2.26	0.81
1:B:447:PHE:O	1:B:448:THR:OG1	1.97	0.81
1:D:447:PHE:O	1:D:448:THR:OG1	1.97	0.81
1:B:635:ASN:ND2	1:B:1059:MET:SD	2.55	0.80
1:D:635:ASN:ND2	1:D:1059:MET:SD	2.55	0.80
1:A:635:ASN:ND2	1:A:1059:MET:SD	2.55	0.80
1:C:635:ASN:ND2	1:C:1059:MET:SD	2.55	0.79
1:C:761:HIS:O	1:C:816:ARG:NH2	2.16	0.79
1:A:761:HIS:O	1:A:816:ARG:NH2	2.16	0.79
1:B:761:HIS:O	1:B:816:ARG:NH2	2.16	0.79
1:C:920:ASP:OD2	1:C:960:VAL:CG2	2.26	0.78
1:D:761:HIS:O	1:D:816:ARG:NH2	2.16	0.78
1:B:829:ARG:NH2	1:C:942:GLU:OE1	2.15	0.76
1:C:829:ARG:NH2	1:D:942:GLU:OE1	2.19	0.75
1:B:782:GLU:OE2	1:B:793:TYR:OH	2.05	0.75
1:A:141:THR:HG21	1:A:144:LEU:HD11	1.70	0.74
1:A:782:GLU:OE2	1:A:793:TYR:OH	2.05	0.74
1:D:141:THR:HG21	1:D:144:LEU:HD11	1.70	0.74
1:C:141:THR:HG21	1:C:144:LEU:HD11	1.70	0.74
1:C:782:GLU:OE2	1:C:793:TYR:OH	2.05	0.73
1:B:141:THR:HG21	1:B:144:LEU:HD11	1.70	0.73
1:D:782:GLU:OE2	1:D:793:TYR:OH	2.05	0.73
1:A:495:GLU:O	1:A:499:THR:HG22	1.89	0.73
3:C:1203:Y01:HAL2	3:C:1204:Y01:HAR1	1.71	0.72
1:D:495:GLU:O	1:D:499:THR:HG22	1.89	0.72
3:B:1203:Y01:HAL2	3:B:1204:Y01:HAR1	1.71	0.72
1:C:495:GLU:O	1:C:499:THR:HG22	1.89	0.72
1:A:850:SER:OG	3:A:1203:Y01:OAF	2.08	0.72
1:B:850:SER:OG	3:B:1203:Y01:OAF	2.08	0.72
3:A:1203:Y01:HAL2	3:A:1204:Y01:HAR1	1.71	0.71
1:B:495:GLU:O	1:B:499:THR:HG22	1.89	0.71
1:D:850:SER:OG	3:D:1203:Y01:OAF	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:850:SER:OG	3:C:1203:Y01:OAF	2.08	0.71
1:A:596:LYS:NZ	1:A:662:GLU:OE1	2.23	0.71
1:D:596:LYS:NZ	1:D:662:GLU:OE1	2.24	0.71
1:B:596:LYS:NZ	1:B:662:GLU:OE1	2.23	0.71
3:D:1203:Y01:HAL2	3:D:1204:Y01:HAR1	1.71	0.70
1:C:596:LYS:NZ	1:C:662:GLU:OE1	2.23	0.69
1:B:815:PHE:O	1:B:824:SER:OG	2.10	0.69
1:C:897:ARG:HD2	3:C:1202:Y01:HAM1	1.75	0.69
1:A:815:PHE:O	1:A:824:SER:OG	2.10	0.68
1:D:897:ARG:HD2	3:D:1202:Y01:HAM1	1.75	0.68
1:B:127:GLU:OE1	1:B:284:TYR:OH	2.07	0.68
1:B:355:LYS:NZ	1:B:374:ILE:HD12	2.09	0.68
1:B:897:ARG:HD2	3:B:1202:Y01:HAM1	1.75	0.67
1:A:897:ARG:HD2	3:A:1202:Y01:HAM1	1.75	0.67
1:C:355:LYS:NZ	1:C:374:ILE:HD12	2.09	0.67
1:D:815:PHE:O	1:D:824:SER:OG	2.10	0.67
1:A:370:PRO:O	1:A:374:ILE:HG12	1.95	0.67
1:D:355:LYS:NZ	1:D:374:ILE:HD12	2.09	0.67
1:A:355:LYS:NZ	1:A:374:ILE:HD12	2.09	0.66
1:B:370:PRO:O	1:B:374:ILE:HG12	1.95	0.66
1:C:815:PHE:O	1:C:824:SER:OG	2.10	0.66
1:C:308:GLY:HA2	1:C:335:ILE:HG22	1.78	0.66
1:D:308:GLY:HA2	1:D:335:ILE:HG22	1.78	0.66
1:C:370:PRO:O	1:C:374:ILE:HG12	1.95	0.65
1:D:370:PRO:O	1:D:374:ILE:HG12	1.95	0.65
1:A:308:GLY:HA2	1:A:335:ILE:HG22	1.78	0.65
1:B:1084:GLN:O	1:B:1087:SER:OG	2.14	0.64
1:D:743:VAL:HG22	3:D:1204:Y01:HAQ2	1.79	0.64
3:B:1203:Y01:HAR1	3:B:1204:Y01:HAS1	1.79	0.64
3:A:1203:Y01:HAR1	3:A:1204:Y01:HAS1	1.79	0.64
1:B:308:GLY:HA2	1:B:335:ILE:HG22	1.78	0.64
1:C:743:VAL:HG22	3:C:1204:Y01:HAQ2	1.79	0.64
1:B:743:VAL:HG22	3:B:1204:Y01:HAQ2	1.79	0.64
3:B:1203:Y01:HAE1	3:B:1203:Y01:HAD3	1.80	0.63
1:A:743:VAL:HG22	3:A:1204:Y01:HAQ2	1.79	0.63
3:A:1203:Y01:HAD3	3:A:1203:Y01:HAE1	1.80	0.63
3:D:1203:Y01:HAE1	3:D:1203:Y01:HAD3	1.80	0.63
1:C:127:GLU:OE1	1:C:284:TYR:OH	2.07	0.62
3:C:1203:Y01:HAR1	3:C:1204:Y01:HAS1	1.79	0.62
1:C:1021:PHE:O	1:C:1024:VAL:HG12	1.99	0.62
3:C:1202:Y01:HAE2	3:C:1202:Y01:HAC1	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1203:Y01:HAR1	3:D:1204:Y01:HAS1	1.79	0.62
1:A:973:ASN:HB3	1:D:976:VAL:HG22	1.81	0.62
1:B:1021:PHE:O	1:B:1024:VAL:HG12	1.99	0.62
3:B:1202:Y01:HAE2	3:B:1202:Y01:HAC1	1.82	0.62
1:D:1021:PHE:O	1:D:1024:VAL:HG12	1.99	0.61
1:A:1021:PHE:O	1:A:1024:VAL:HG12	1.99	0.61
3:B:1203:Y01:HAL2	3:B:1204:Y01:CAR	2.31	0.61
1:B:302:VAL:HG13	1:B:302:VAL:O	2.01	0.61
3:C:1203:Y01:HAD3	3:C:1203:Y01:HAE1	1.80	0.61
1:A:302:VAL:HG13	1:A:302:VAL:O	2.01	0.61
3:A:1203:Y01:HAL2	3:A:1204:Y01:CAR	2.31	0.61
1:C:302:VAL:O	1:C:302:VAL:HG13	2.01	0.61
3:C:1203:Y01:HAL2	3:C:1204:Y01:CAR	2.30	0.61
1:A:1084:GLN:O	1:A:1087:SER:OG	2.14	0.60
3:A:1202:Y01:HAC1	3:A:1202:Y01:HAE2	1.82	0.60
3:D:1202:Y01:HAE2	3:D:1202:Y01:HAC1	1.82	0.60
1:D:302:VAL:O	1:D:302:VAL:HG13	2.01	0.60
1:C:254:ASP:OD1	1:C:255:ASN:N	2.35	0.60
1:B:934:ASN:ND2	5:B:1302:NAG:O5	2.35	0.60
3:A:1202:Y01:HAS1	1:B:957:ILE:HG21	1.82	0.60
1:A:934:ASN:ND2	5:A:1302:NAG:O5	2.35	0.60
3:D:1203:Y01:HAL2	3:D:1204:Y01:CAR	2.31	0.60
1:B:254:ASP:OD1	1:B:255:ASN:N	2.35	0.59
1:D:843:LEU:HA	1:D:846:ILE:HG12	1.85	0.59
1:C:1084:GLN:O	1:C:1087:SER:OG	2.14	0.59
1:D:254:ASP:OD1	1:D:255:ASN:N	2.35	0.59
1:C:843:LEU:HA	1:C:846:ILE:HG12	1.85	0.59
1:D:355:LYS:HZ1	1:D:374:ILE:HD12	1.67	0.59
1:C:496:LEU:HD21	1:C:567:TRP:CE2	2.38	0.59
1:A:843:LEU:HA	1:A:846:ILE:HG12	1.85	0.59
1:D:496:LEU:HD21	1:D:567:TRP:CE2	2.38	0.59
1:B:496:LEU:HD21	1:B:567:TRP:CE2	2.38	0.58
1:C:934:ASN:ND2	5:C:1302:NAG:O5	2.35	0.58
1:A:496:LEU:HD21	1:A:567:TRP:CE2	2.38	0.58
1:D:934:ASN:ND2	5:D:1302:NAG:O5	2.35	0.58
1:A:254:ASP:OD1	1:A:255:ASN:N	2.35	0.58
1:D:1084:GLN:O	1:D:1087:SER:OG	2.14	0.58
1:B:843:LEU:HA	1:B:846:ILE:HG12	1.85	0.58
1:C:746:ILE:HG23	3:C:1203:Y01:HAC2	1.86	0.58
1:A:285:ILE:HG22	1:A:301:ILE:HD11	1.86	0.58
1:A:976:VAL:HG22	1:B:973:ASN:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:746:ILE:HG23	3:D:1203:Y01:HAC2	1.86	0.58
1:B:285:ILE:HG22	1:B:301:ILE:HD11	1.86	0.57
1:D:285:ILE:HG22	1:D:301:ILE:HD11	1.86	0.57
1:C:285:ILE:HG22	1:C:301:ILE:HD11	1.86	0.57
3:C:1203:Y01:HAE2	3:C:1203:Y01:HAC1	1.87	0.57
1:D:193:GLY:O	1:D:196:VAL:HG12	2.04	0.57
3:D:1203:Y01:HAE2	3:D:1203:Y01:HAC1	1.87	0.57
3:A:1203:Y01:HAE2	3:A:1203:Y01:HAC1	1.87	0.57
1:D:127:GLU:OE1	1:D:284:TYR:OH	2.07	0.57
1:C:355:LYS:HZ1	1:C:374:ILE:HD12	1.70	0.57
1:A:746:ILE:HG23	3:A:1203:Y01:HAC2	1.86	0.56
1:A:958:PRO:HG3	3:D:1202:Y01:HBG	1.87	0.56
1:B:193:GLY:O	1:B:196:VAL:HG12	2.04	0.56
1:C:193:GLY:O	1:C:196:VAL:HG12	2.04	0.56
1:A:1013:PHE:O	1:A:1016:VAL:HG12	2.06	0.56
1:A:976:VAL:HG22	1:B:973:ASN:CB	2.36	0.56
1:C:370:PRO:O	1:C:374:ILE:HG23	2.06	0.56
1:D:370:PRO:O	1:D:374:ILE:HG23	2.06	0.56
1:D:1013:PHE:O	1:D:1016:VAL:HG12	2.06	0.56
1:B:746:ILE:HG23	3:B:1203:Y01:HAC2	1.86	0.56
1:A:193:GLY:O	1:A:196:VAL:HG12	2.04	0.56
1:A:370:PRO:O	1:A:374:ILE:HG23	2.06	0.56
1:B:1013:PHE:O	1:B:1016:VAL:HG12	2.06	0.56
1:C:1013:PHE:O	1:C:1016:VAL:HG12	2.06	0.56
1:B:575:GLU:N	1:B:575:GLU:OE1	2.39	0.55
3:B:1203:Y01:HAE2	3:B:1203:Y01:HAC1	1.87	0.55
1:B:604:VAL:HG12	1:B:604:VAL:O	2.07	0.55
1:A:355:LYS:HZ1	1:A:374:ILE:HD12	1.71	0.55
1:A:575:GLU:OE1	1:A:575:GLU:N	2.39	0.55
1:B:370:PRO:O	1:B:374:ILE:HG23	2.06	0.55
1:C:930:THR:OG1	1:C:932:SER:O	2.25	0.55
1:A:604:VAL:HG12	1:A:604:VAL:O	2.07	0.55
1:B:301:ILE:HB	1:B:324:ILE:HD12	1.88	0.55
1:D:301:ILE:HB	1:D:324:ILE:HD12	1.88	0.55
1:A:301:ILE:HB	1:A:324:ILE:HD12	1.88	0.55
1:D:604:VAL:HG12	1:D:604:VAL:O	2.07	0.55
1:C:301:ILE:HB	1:C:324:ILE:HD12	1.88	0.55
1:C:604:VAL:HG12	1:C:604:VAL:O	2.07	0.55
1:C:575:GLU:OE1	1:C:575:GLU:N	2.39	0.54
1:D:575:GLU:N	1:D:575:GLU:OE1	2.40	0.54
1:A:932:SER:OG	1:A:934:ASN:ND2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:932:SER:OG	1:B:934:ASN:ND2	2.41	0.54
1:C:932:SER:OG	1:C:934:ASN:ND2	2.41	0.54
1:A:45:ILE:HG23	1:A:118:LEU:HD11	1.90	0.54
3:C:1203:Y01:HAV1	1:D:872:PHE:CD1	2.42	0.54
1:D:45:ILE:HG23	1:D:118:LEU:HD11	1.90	0.53
1:D:930:THR:OG1	1:D:932:SER:O	2.25	0.53
1:D:932:SER:OG	1:D:934:ASN:ND2	2.41	0.53
1:D:570:LEU:HD21	1:D:597:LEU:HD21	1.90	0.53
1:C:570:LEU:HD21	1:C:597:LEU:HD21	1.90	0.53
1:A:973:ASN:CB	1:D:976:VAL:HG22	2.38	0.53
1:D:221:SER:HG	1:D:250:LEU:N	2.07	0.53
1:D:210:VAL:HG12	1:D:212:ILE:HG13	1.91	0.53
1:B:570:LEU:HD21	1:B:597:LEU:HD21	1.90	0.52
1:A:221:SER:HG	1:A:250:LEU:N	2.08	0.52
1:B:45:ILE:HG23	1:B:118:LEU:HD11	1.90	0.52
1:B:355:LYS:HZ1	1:B:374:ILE:HD12	1.73	0.52
1:B:768:GLU:OE2	1:B:772:TYR:OH	2.19	0.52
1:D:440:ASP:OD1	1:D:441:LEU:N	2.43	0.52
1:A:570:LEU:HD21	1:A:597:LEU:HD21	1.90	0.52
1:A:146:ILE:HG22	1:A:180:LEU:HD12	1.92	0.52
1:C:440:ASP:OD1	1:C:441:LEU:N	2.43	0.52
1:A:743:VAL:CG2	3:A:1204:Y01:HAQ2	2.40	0.52
1:D:146:ILE:HG22	1:D:180:LEU:HD12	1.92	0.52
1:A:210:VAL:HG12	1:A:212:ILE:HG13	1.91	0.52
1:C:45:ILE:HG23	1:C:118:LEU:HD11	1.90	0.52
1:D:768:GLU:OE2	1:D:772:TYR:OH	2.19	0.52
1:A:440:ASP:OD1	1:A:441:LEU:N	2.43	0.52
1:C:743:VAL:CG2	3:C:1204:Y01:HAQ2	2.40	0.52
1:C:210:VAL:HG12	1:C:212:ILE:HG13	1.91	0.51
1:A:930:THR:OG1	1:A:932:SER:O	2.25	0.51
1:B:146:ILE:HG22	1:B:180:LEU:HD12	1.92	0.51
1:B:743:VAL:CG2	3:B:1204:Y01:HAQ2	2.40	0.51
1:C:496:LEU:C	1:C:496:LEU:HD23	2.35	0.51
1:B:496:LEU:C	1:B:496:LEU:HD23	2.35	0.51
1:A:317:ASN:HB2	1:A:384:ILE:HD11	1.92	0.51
1:A:980:GLY:HA2	1:B:977:ALA:HB1	1.91	0.51
3:A:1202:Y01:HBG	1:B:958:PRO:HG3	1.93	0.51
1:D:743:VAL:CG2	3:D:1204:Y01:HAQ2	2.40	0.51
3:D:1204:Y01:HAC1	3:D:1204:Y01:HAE2	1.93	0.51
1:C:146:ILE:HG22	1:C:180:LEU:HD12	1.92	0.51
1:C:562:GLN:N	1:C:562:GLN:OE1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:LEU:HD23	1:A:496:LEU:C	2.35	0.50
1:B:210:VAL:HG12	1:B:212:ILE:HG13	1.91	0.50
1:B:562:GLN:N	1:B:562:GLN:OE1	2.44	0.50
3:B:1204:Y01:HAE2	3:B:1204:Y01:HAC1	1.93	0.50
1:D:496:LEU:HD23	1:D:496:LEU:C	2.35	0.50
1:D:562:GLN:OE1	1:D:562:GLN:N	2.45	0.50
1:C:707:CYS:SG	1:C:708:GLY:N	2.85	0.50
1:B:930:THR:OG1	1:B:932:SER:O	2.25	0.50
1:C:317:ASN:HB2	1:C:384:ILE:HD11	1.92	0.50
1:A:562:GLN:N	1:A:562:GLN:OE1	2.44	0.50
1:B:143:ASN:C	1:B:144:LEU:HD12	2.37	0.50
1:A:301:ILE:HB	1:A:324:ILE:CD1	2.42	0.50
1:B:317:ASN:HB2	1:B:384:ILE:HD11	1.92	0.50
1:B:707:CYS:SG	1:B:708:GLY:N	2.85	0.50
1:C:301:ILE:HB	1:C:324:ILE:CD1	2.42	0.50
1:D:317:ASN:HB2	1:D:384:ILE:HD11	1.92	0.50
1:A:143:ASN:C	1:A:144:LEU:HD12	2.37	0.50
3:A:1204:Y01:HAE2	3:A:1204:Y01:HAC1	1.93	0.50
1:B:440:ASP:OD1	1:B:441:LEU:N	2.43	0.50
3:C:1202:Y01:HAC1	3:C:1202:Y01:HAU2	1.94	0.50
1:A:702:ILE:O	1:A:705:VAL:HG12	2.12	0.50
1:C:143:ASN:C	1:C:144:LEU:HD12	2.37	0.50
3:A:1204:Y01:HAJ2	3:A:1204:Y01:HAP1	1.94	0.49
3:D:1202:Y01:HAC1	3:D:1202:Y01:HAU2	1.94	0.49
1:B:301:ILE:HB	1:B:324:ILE:CD1	2.42	0.49
3:A:1202:Y01:HAC1	3:A:1202:Y01:HAU2	1.94	0.49
3:B:1202:Y01:HAC1	3:B:1202:Y01:HAU2	1.94	0.49
1:D:143:ASN:C	1:D:144:LEU:HD12	2.37	0.49
1:D:702:ILE:O	1:D:705:VAL:HG12	2.12	0.49
1:D:301:ILE:HB	1:D:324:ILE:CD1	2.42	0.49
3:D:1204:Y01:HAP1	3:D:1204:Y01:HAJ2	1.95	0.49
3:C:1204:Y01:HAE2	3:C:1204:Y01:HAC1	1.93	0.49
1:D:707:CYS:SG	1:D:708:GLY:N	2.85	0.49
1:C:797:LEU:HD13	1:C:797:LEU:C	2.38	0.49
1:C:181:THR:HG22	1:C:182:GLY:N	2.28	0.49
1:C:702:ILE:O	1:C:705:VAL:HG12	2.12	0.49
1:D:484:LEU:HD23	1:D:561:LEU:HD21	1.95	0.49
1:D:797:LEU:C	1:D:797:LEU:HD13	2.38	0.49
1:A:181:THR:HG22	1:A:182:GLY:N	2.28	0.48
1:A:636:ASP:OD1	1:A:637:GLU:N	2.46	0.48
1:B:702:ILE:O	1:B:705:VAL:HG12	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1204:Y01:HAJ2	3:B:1204:Y01:HAP1	1.94	0.48
1:A:504:LEU:C	1:A:504:LEU:HD23	2.39	0.48
1:C:636:ASP:OD1	1:C:637:GLU:N	2.46	0.48
1:C:484:LEU:HD23	1:C:561:LEU:HD21	1.95	0.48
3:C:1204:Y01:HAJ2	3:C:1204:Y01:HAP1	1.94	0.48
1:B:797:LEU:C	1:B:797:LEU:HD13	2.38	0.48
3:C:1203:Y01:HAV1	1:D:872:PHE:HD1	1.78	0.48
1:D:636:ASP:OD1	1:D:637:GLU:N	2.46	0.48
1:B:181:THR:HG22	1:B:182:GLY:N	2.28	0.48
1:B:636:ASP:OD1	1:B:637:GLU:N	2.46	0.48
1:C:118:LEU:HD23	1:C:119:ARG:N	2.29	0.48
1:D:571:GLN:N	1:D:571:GLN:OE1	2.47	0.48
1:A:118:LEU:HD23	1:A:119:ARG:N	2.29	0.48
1:A:797:LEU:HD13	1:A:797:LEU:C	2.38	0.48
1:C:504:LEU:C	1:C:504:LEU:HD23	2.39	0.48
1:D:118:LEU:HD23	1:D:119:ARG:N	2.29	0.48
1:D:181:THR:HG22	1:D:182:GLY:N	2.28	0.48
1:D:521:LEU:HD21	1:D:600:THR:HG21	1.96	0.48
1:A:334:GLN:HG3	1:A:362:LEU:HD21	1.96	0.48
1:B:743:VAL:HG22	3:B:1204:Y01:CAQ	2.44	0.48
1:C:849:VAL:HG22	1:C:849:VAL:O	2.14	0.48
1:D:849:VAL:O	1:D:849:VAL:HG22	2.14	0.48
1:D:675:GLN:OE1	1:D:998:ARG:NH1	2.47	0.48
1:A:303:CYS:O	1:A:326:CYS:HB2	2.14	0.47
1:A:484:LEU:HD23	1:A:561:LEU:HD21	1.95	0.47
3:A:1204:Y01:HAP1	3:A:1204:Y01:CAJ	2.44	0.47
1:B:118:LEU:HD23	1:B:119:ARG:N	2.29	0.47
1:C:571:GLN:OE1	1:C:571:GLN:N	2.47	0.47
1:B:303:CYS:O	1:B:326:CYS:HB2	2.14	0.47
3:B:1204:Y01:HAP1	3:B:1204:Y01:CAJ	2.44	0.47
1:C:521:LEU:HD21	1:C:600:THR:HG21	1.96	0.47
1:D:504:LEU:HD23	1:D:504:LEU:C	2.39	0.47
1:A:707:CYS:SG	1:A:708:GLY:N	2.85	0.47
1:B:484:LEU:HD23	1:B:561:LEU:HD21	1.95	0.47
1:B:521:LEU:HD21	1:B:600:THR:HG21	1.96	0.47
1:B:675:GLN:OE1	1:B:998:ARG:NH1	2.47	0.47
3:C:1204:Y01:HAP1	3:C:1204:Y01:CAJ	2.44	0.47
1:A:743:VAL:HG22	3:A:1204:Y01:CAQ	2.44	0.47
3:B:1203:Y01:HAT2	3:B:1203:Y01:HAS2	1.37	0.47
1:A:571:GLN:OE1	1:A:571:GLN:N	2.47	0.47
1:B:849:VAL:O	1:B:849:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:675:GLN:OE1	1:C:998:ARG:NH1	2.47	0.47
3:D:1204:Y01:HAP1	3:D:1204:Y01:CAJ	2.44	0.47
1:A:675:GLN:OE1	1:A:998:ARG:NH1	2.47	0.47
1:B:334:GLN:HG3	1:B:362:LEU:HD21	1.96	0.47
1:A:521:LEU:HD21	1:A:600:THR:HG21	1.96	0.47
1:A:849:VAL:HG22	1:A:849:VAL:O	2.14	0.47
1:B:504:LEU:HD23	1:B:504:LEU:C	2.39	0.47
1:B:571:GLN:N	1:B:571:GLN:OE1	2.47	0.47
1:C:743:VAL:HG22	3:C:1204:Y01:CAQ	2.44	0.47
1:A:173:GLN:CD	1:A:209:ILE:HD11	2.40	0.47
1:D:334:GLN:HG3	1:D:362:LEU:HD21	1.96	0.47
1:D:788:MET:HE2	1:D:788:MET:HA	1.97	0.47
1:C:146:ILE:HG12	1:C:303:CYS:HA	1.97	0.47
1:B:173:GLN:CD	1:B:209:ILE:HD11	2.40	0.46
1:D:303:CYS:O	1:D:326:CYS:HB2	2.14	0.46
1:B:146:ILE:HG12	1:B:303:CYS:HA	1.97	0.46
1:C:303:CYS:O	1:C:326:CYS:HB2	2.15	0.46
1:C:334:GLN:HG3	1:C:362:LEU:HD21	1.96	0.46
3:B:1202:Y01:HAJ2	3:B:1202:Y01:HAP1	1.97	0.46
1:C:213:GLY:O	1:C:214:ILE:HD12	2.15	0.46
1:D:173:GLN:CD	1:D:209:ILE:HD11	2.40	0.46
1:B:885:ARG:NH2	1:B:906:GLU:OE1	2.44	0.46
1:D:146:ILE:HG12	1:D:303:CYS:HA	1.97	0.46
1:B:213:GLY:O	1:B:214:ILE:HD12	2.15	0.46
3:C:1204:Y01:HAS2	3:C:1204:Y01:HAT2	1.65	0.46
1:D:743:VAL:HG22	3:D:1204:Y01:CAQ	2.44	0.46
1:A:788:MET:HA	1:A:788:MET:HE2	1.97	0.46
3:C:1202:Y01:HAJ2	3:C:1202:Y01:HAP1	1.98	0.46
1:A:213:GLY:O	1:A:214:ILE:HD12	2.15	0.46
1:A:338:VAL:HG22	1:A:361:PHE:CD2	2.51	0.46
1:B:724:LEU:HD13	1:B:724:LEU:C	2.41	0.46
1:C:788:MET:HA	1:C:788:MET:HE2	1.97	0.46
1:D:213:GLY:O	1:D:214:ILE:HD12	2.15	0.46
1:A:146:ILE:HG12	1:A:303:CYS:HA	1.97	0.46
1:C:391:LEU:C	1:C:391:LEU:HD23	2.41	0.46
1:D:309:GLY:O	1:D:312:THR:OG1	2.32	0.46
1:A:270:HIS:N	1:A:271:PRO:HD3	2.31	0.46
1:A:724:LEU:C	1:A:724:LEU:HD13	2.41	0.46
1:C:173:GLN:CD	1:C:209:ILE:HD11	2.40	0.46
1:D:338:VAL:HG22	1:D:361:PHE:CD2	2.51	0.46
3:A:1204:Y01:HAD2	3:A:1204:Y01:HAS2	1.85	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:LEU:HD23	1:D:119:ARG:C	2.41	0.46
1:A:626:VAL:O	1:A:630:THR:HG23	2.16	0.45
1:C:118:LEU:HD23	1:C:119:ARG:C	2.41	0.45
1:C:129:LEU:C	1:C:129:LEU:HD23	2.41	0.45
1:D:270:HIS:N	1:D:271:PRO:HD3	2.31	0.45
1:A:129:LEU:C	1:A:129:LEU:HD23	2.41	0.45
3:A:1204:Y01:HAC1	3:A:1204:Y01:HAU2	1.99	0.45
1:B:118:LEU:HD23	1:B:119:ARG:C	2.41	0.45
1:B:129:LEU:HD23	1:B:129:LEU:C	2.41	0.45
1:D:724:LEU:C	1:D:724:LEU:HD13	2.41	0.45
1:A:118:LEU:HD23	1:A:119:ARG:C	2.41	0.45
1:C:338:VAL:HG22	1:C:361:PHE:CD2	2.51	0.45
1:C:626:VAL:O	1:C:630:THR:HG23	2.16	0.45
3:C:1203:Y01:HAT2	3:C:1203:Y01:HAS2	1.37	0.45
1:D:129:LEU:C	1:D:129:LEU:HD23	2.41	0.45
1:D:626:VAL:O	1:D:630:THR:HG23	2.16	0.45
1:B:338:VAL:HG22	1:B:361:PHE:CD2	2.51	0.45
1:B:391:LEU:C	1:B:391:LEU:HD23	2.41	0.45
1:C:221:SER:HG	1:C:250:LEU:N	2.13	0.45
1:D:197:ARG:O	1:D:200:THR:HG22	2.17	0.45
1:D:391:LEU:HD23	1:D:391:LEU:C	2.41	0.45
1:D:645:VAL:HG12	1:D:645:VAL:O	2.17	0.45
1:B:626:VAL:O	1:B:630:THR:HG23	2.16	0.45
1:A:197:ARG:O	1:A:200:THR:HG22	2.17	0.45
3:A:1202:Y01:HAP1	3:A:1202:Y01:HAJ2	1.97	0.45
1:C:724:LEU:HD13	1:C:724:LEU:C	2.41	0.45
3:D:1202:Y01:HAJ2	3:D:1202:Y01:HAP1	1.97	0.45
1:A:391:LEU:C	1:A:391:LEU:HD23	2.41	0.45
1:A:447:PHE:O	1:A:448:THR:CB	2.65	0.45
1:B:788:MET:HE2	1:B:788:MET:HA	1.97	0.45
3:B:1204:Y01:HAC1	3:B:1204:Y01:HAU2	1.99	0.45
1:C:137:TRP:CD1	1:C:137:TRP:N	2.85	0.45
1:C:143:ASN:OD1	1:C:144:LEU:N	2.50	0.45
1:D:137:TRP:CD1	1:D:137:TRP:N	2.85	0.45
1:A:137:TRP:N	1:A:137:TRP:CD1	2.85	0.45
1:B:197:ARG:O	1:B:200:THR:HG22	2.17	0.45
1:B:270:HIS:N	1:B:271:PRO:HD3	2.31	0.45
1:C:197:ARG:O	1:C:200:THR:HG22	2.17	0.45
1:C:270:HIS:N	1:C:271:PRO:HD3	2.31	0.45
1:C:645:VAL:HG12	1:C:645:VAL:O	2.17	0.44
1:B:137:TRP:CD1	1:B:137:TRP:N	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:447:PHE:O	1:D:448:THR:CB	2.65	0.44
1:D:702:ILE:HD12	1:D:702:ILE:N	2.32	0.44
1:A:127:GLU:OE1	1:A:284:TYR:OH	2.07	0.44
1:B:143:ASN:OD1	1:B:144:LEU:N	2.50	0.44
1:A:702:ILE:N	1:A:702:ILE:HD12	2.32	0.44
1:C:309:GLY:O	1:C:312:THR:OG1	2.32	0.44
3:D:1204:Y01:HAC1	3:D:1204:Y01:HAU2	1.99	0.44
1:D:143:ASN:OD1	1:D:144:LEU:N	2.50	0.44
1:B:702:ILE:HD12	1:B:702:ILE:N	2.32	0.44
1:C:141:THR:CG2	1:C:144:LEU:HD11	2.45	0.44
1:A:645:VAL:O	1:A:645:VAL:HG12	2.17	0.44
1:B:129:LEU:HD23	1:B:129:LEU:O	2.18	0.44
1:A:143:ASN:OD1	1:A:144:LEU:N	2.50	0.44
1:C:354:VAL:HG13	1:C:378:ILE:HD12	2.00	0.44
1:B:447:PHE:O	1:B:448:THR:CB	2.65	0.43
1:A:885:ARG:NH2	1:A:906:GLU:OE1	2.44	0.43
1:C:129:LEU:HD23	1:C:129:LEU:O	2.18	0.43
3:B:1204:Y01:HAD2	3:B:1204:Y01:HAS2	1.85	0.43
1:C:702:ILE:N	1:C:702:ILE:HD12	2.32	0.43
3:C:1204:Y01:HAC1	3:C:1204:Y01:HAU2	1.99	0.43
1:D:354:VAL:HG13	1:D:378:ILE:HD12	2.00	0.43
1:A:354:VAL:HG13	1:A:378:ILE:HD12	2.00	0.43
1:D:129:LEU:HD23	1:D:129:LEU:O	2.18	0.43
1:A:129:LEU:HD23	1:A:129:LEU:O	2.18	0.43
1:B:354:VAL:HG13	1:B:378:ILE:HD12	2.00	0.43
1:B:645:VAL:HG12	1:B:645:VAL:O	2.17	0.43
1:C:447:PHE:O	1:C:448:THR:CB	2.65	0.43
3:B:1203:Y01:HAV1	1:C:872:PHE:CD1	2.54	0.43
1:C:146:ILE:CG2	1:C:180:LEU:HD12	2.49	0.43
1:C:213:GLY:C	1:C:214:ILE:HD12	2.44	0.43
1:A:118:LEU:HD22	1:A:120:LEU:HG	2.01	0.43
1:C:294:ASN:OD1	1:C:294:ASN:C	2.62	0.43
1:D:146:ILE:CG2	1:D:180:LEU:HD12	2.49	0.43
3:A:1203:Y01:HAS2	3:A:1203:Y01:HAT2	1.37	0.42
1:B:118:LEU:HD22	1:B:120:LEU:HG	2.01	0.42
1:C:885:ARG:NH2	1:C:906:GLU:OE1	2.44	0.42
3:D:1204:Y01:HAS2	3:D:1204:Y01:HAT2	1.65	0.42
1:B:213:GLY:C	1:B:214:ILE:HD12	2.44	0.42
1:A:294:ASN:OD1	1:A:294:ASN:C	2.62	0.42
1:A:146:ILE:CG2	1:A:180:LEU:HD12	2.49	0.42
1:B:616:GLU:OE1	1:B:617:LEU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ILE:HD13	1:A:282:GLU:OE2	2.20	0.42
1:A:664:THR:HG22	1:A:664:THR:O	2.20	0.42
1:B:338:VAL:HG22	1:B:361:PHE:HD2	1.85	0.42
3:C:1202:Y01:HAD2	3:C:1202:Y01:HAS2	1.84	0.42
1:D:213:GLY:C	1:D:214:ILE:HD12	2.44	0.42
1:D:616:GLU:OE1	1:D:617:LEU:N	2.53	0.42
1:B:294:ASN:OD1	1:B:294:ASN:C	2.62	0.42
1:C:146:ILE:HD13	1:C:282:GLU:OE2	2.20	0.42
1:C:405:SER:O	1:C:406:ASN:C	2.63	0.42
1:D:146:ILE:HD13	1:D:282:GLU:OE2	2.20	0.42
1:B:146:ILE:CG2	1:B:180:LEU:HD12	2.49	0.42
1:D:294:ASN:OD1	1:D:294:ASN:C	2.62	0.42
1:A:277:LEU:HD13	1:A:277:LEU:C	2.45	0.42
3:A:1203:Y01:HAE1	3:A:1203:Y01:HBD	1.86	0.42
1:B:405:SER:O	1:B:406:ASN:C	2.63	0.42
1:D:277:LEU:HD13	1:D:277:LEU:C	2.45	0.42
1:A:213:GLY:C	1:A:214:ILE:HD12	2.44	0.41
1:A:358:LEU:HD23	1:A:358:LEU:C	2.45	0.41
1:A:616:GLU:OE1	1:A:617:LEU:N	2.53	0.41
1:C:118:LEU:HD22	1:C:120:LEU:HG	2.01	0.41
1:C:358:LEU:C	1:C:358:LEU:HD23	2.45	0.41
1:C:616:GLU:OE1	1:C:617:LEU:N	2.53	0.41
3:C:1203:Y01:OAG	3:C:1204:Y01:HAT2	2.20	0.41
1:D:118:LEU:HD22	1:D:120:LEU:HG	2.01	0.41
1:A:972:VAL:O	1:A:976:VAL:HG23	2.20	0.41
3:C:1202:Y01:HAS2	3:C:1202:Y01:HAT2	1.76	0.41
1:D:885:ARG:NH2	1:D:906:GLU:OE1	2.44	0.41
1:D:893:GLU:OE2	1:D:895:ARG:NH2	2.47	0.41
1:D:972:VAL:O	1:D:976:VAL:HG23	2.20	0.41
1:B:972:VAL:O	1:B:976:VAL:HG23	2.20	0.41
1:C:664:THR:HG22	1:C:664:THR:O	2.20	0.41
1:C:893:GLU:OE2	1:C:895:ARG:NH2	2.47	0.41
1:A:338:VAL:HG22	1:A:361:PHE:HD2	1.85	0.41
1:B:146:ILE:HD13	1:B:282:GLU:OE2	2.20	0.41
1:B:359:VAL:HG22	1:B:366:VAL:HG21	2.03	0.41
1:B:295:TYR:O	1:B:295:TYR:CG	2.74	0.41
1:D:359:VAL:HG22	1:D:366:VAL:HG21	2.03	0.41
1:A:856:LYS:HE3	1:B:865:ILE:HG22	2.03	0.41
1:B:358:LEU:C	1:B:358:LEU:HD23	2.45	0.41
1:B:404:VAL:O	1:B:405:SER:C	2.63	0.41
1:B:664:THR:O	1:B:664:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:VAL:HG22	1:C:361:PHE:HD2	1.85	0.41
1:C:359:VAL:HG22	1:C:366:VAL:HG21	2.03	0.41
1:C:972:VAL:O	1:C:976:VAL:HG23	2.20	0.41
1:D:404:VAL:O	1:D:405:SER:C	2.63	0.41
1:D:788:MET:HE2	1:D:788:MET:CA	2.51	0.41
1:A:260:LEU:O	1:A:261:LEU:HD12	2.21	0.41
1:A:405:SER:O	1:A:406:ASN:C	2.63	0.41
1:C:295:TYR:O	1:C:295:TYR:CG	2.74	0.41
1:D:358:LEU:HD23	1:D:358:LEU:C	2.45	0.41
3:D:1203:Y01:OAG	3:D:1204:Y01:HAT2	2.20	0.41
1:A:404:VAL:O	1:A:405:SER:C	2.63	0.41
1:B:277:LEU:HD13	1:B:277:LEU:C	2.45	0.41
1:B:313:LEU:HB2	1:B:335:ILE:CD1	2.51	0.41
1:B:788:MET:HE2	1:B:788:MET:CA	2.51	0.41
1:C:277:LEU:C	1:C:277:LEU:HD13	2.45	0.41
1:C:768:GLU:OE2	1:C:772:TYR:OH	2.19	0.41
1:C:791:VAL:O	1:C:791:VAL:HG12	2.21	0.41
1:D:260:LEU:O	1:D:261:LEU:HD12	2.21	0.41
1:D:406:ASN:O	1:D:407:ALA:C	2.64	0.41
1:D:664:THR:O	1:D:664:THR:HG22	2.20	0.41
1:A:295:TYR:O	1:A:295:TYR:CG	2.74	0.41
1:A:359:VAL:HG22	1:A:366:VAL:HG21	2.03	0.41
1:A:791:VAL:HG12	1:A:791:VAL:O	2.21	0.41
1:A:893:GLU:OE2	1:A:895:ARG:NH2	2.47	0.41
3:B:1204:Y01:HAD3	3:B:1204:Y01:HBD	1.92	0.41
1:C:788:MET:HE2	1:C:788:MET:CA	2.51	0.41
1:A:141:THR:CG2	1:A:144:LEU:HD11	2.45	0.40
1:A:146:ILE:HD13	1:A:282:GLU:CD	2.46	0.40
1:A:313:LEU:HB2	1:A:335:ILE:CD1	2.51	0.40
3:A:1202:Y01:HAS2	3:A:1202:Y01:HAD2	1.84	0.40
3:A:1204:Y01:HAS2	3:A:1204:Y01:HAT2	1.65	0.40
1:B:141:THR:CG2	1:B:144:LEU:HD11	2.45	0.40
1:B:260:LEU:O	1:B:261:LEU:HD12	2.21	0.40
1:D:313:LEU:HB2	1:D:335:ILE:CD1	2.51	0.40
1:D:405:SER:O	1:D:406:ASN:C	2.63	0.40
3:B:1203:Y01:OAG	3:B:1204:Y01:HAT2	2.20	0.40
1:C:260:LEU:O	1:C:261:LEU:HD12	2.21	0.40
1:B:893:GLU:OE2	1:B:895:ARG:NH2	2.47	0.40
1:B:1013:PHE:N	1:B:1014:PRO:HD2	2.36	0.40
1:C:146:ILE:HD13	1:C:282:GLU:CD	2.46	0.40
1:D:408:ILE:O	1:D:409:SER:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:788:MET:HE2	1:A:788:MET:CA	2.51	0.40
1:C:313:LEU:HB2	1:C:335:ILE:CD1	2.51	0.40
1:D:338:VAL:HG22	1:D:361:PHE:HD2	1.85	0.40
1:D:1013:PHE:N	1:D:1014:PRO:HD2	2.37	0.40
1:A:406:ASN:O	1:A:407:ALA:C	2.64	0.40
3:A:1203:Y01:OAG	3:A:1204:Y01:HAT2	2.20	0.40
1:B:406:ASN:O	1:B:407:ALA:C	2.64	0.40
1:C:404:VAL:O	1:C:405:SER:C	2.63	0.40
1:D:146:ILE:HD13	1:D:282:GLU:CD	2.46	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	914/1135 (80%)	885 (97%)	29 (3%)	0	100	100
1	B	914/1135 (80%)	885 (97%)	29 (3%)	0	100	100
1	C	914/1135 (80%)	885 (97%)	29 (3%)	0	100	100
1	D	914/1135 (80%)	885 (97%)	29 (3%)	0	100	100
All	All	3656/4540 (80%)	3540 (97%)	116 (3%)	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	689/1022 (67%)	686 (100%)	3 (0%)	84	91
1	B	689/1022 (67%)	686 (100%)	3 (0%)	84	91
1	C	689/1022 (67%)	686 (100%)	3 (0%)	84	91
1	D	689/1022 (67%)	686 (100%)	3 (0%)	84	91
All	All	2756/4088 (67%)	2744 (100%)	12 (0%)	81	91

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	TRP
1	A	294	ASN
1	A	948	LEU
1	B	137	TRP
1	B	294	ASN
1	B	948	LEU
1	C	137	TRP
1	C	294	ASN
1	C	948	LEU
1	D	137	TRP
1	D	294	ASN
1	D	948	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	ASN
1	A	438	GLN
1	A	459	GLN
1	A	671	GLN
1	A	928	HIS
1	A	934	ASN
1	A	973	ASN
1	A	1003	GLN
1	B	256	ASN
1	B	438	GLN
1	B	459	GLN
1	B	671	GLN
1	B	914	GLN
1	B	928	HIS
1	B	934	ASN

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Mol	Chain	Res	Type
1	B	987	GLN
1	B	1003	GLN
1	C	438	GLN
1	C	459	GLN
1	C	671	GLN
1	C	892	ASN
1	C	914	GLN
1	C	928	HIS
1	C	934	ASN
1	C	987	GLN
1	C	992	GLN
1	C	1003	GLN
1	D	256	ASN
1	D	438	GLN
1	D	459	GLN
1	D	671	GLN
1	D	914	GLN
1	D	928	HIS
1	D	934	ASN
1	D	1003	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 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
5	NAG	C	1302	-	14,14,15	2.65	7 (50%)	17,19,21	1.26	2 (11%)
3	Y01	D	1202	-	38,38,38	1.07	3 (7%)	57,57,57	3.11	17 (29%)
3	Y01	B	1203	-	38,38,38	1.10	3 (7%)	57,57,57	3.38	21 (36%)
3	Y01	D	1204	-	38,38,38	1.08	3 (7%)	57,57,57	3.22	20 (35%)
4	ULO	D	1301	-	15,16,16	2.00	3 (20%)	17,20,20	1.61	3 (17%)
3	Y01	C	1203	-	38,38,38	1.10	3 (7%)	57,57,57	3.38	21 (36%)
3	Y01	A	1202	-	38,38,38	1.07	3 (7%)	57,57,57	3.11	17 (29%)
2	T14	A	1201	-	36,37,37	3.26	9 (25%)	47,58,58	1.54	6 (12%)
4	ULO	B	1301	-	15,16,16	2.01	3 (20%)	17,20,20	1.61	3 (17%)
2	T14	C	1201	-	36,37,37	3.26	8 (22%)	47,58,58	1.53	6 (12%)
5	NAG	B	1302	-	14,14,15	2.66	7 (50%)	17,19,21	1.26	2 (11%)
3	Y01	C	1204	-	38,38,38	1.08	3 (7%)	57,57,57	3.21	19 (33%)
4	ULO	A	1301	-	15,16,16	1.99	3 (20%)	17,20,20	1.61	3 (17%)
3	Y01	A	1203	-	38,38,38	1.10	3 (7%)	57,57,57	3.38	20 (35%)
3	Y01	B	1202	-	38,38,38	1.07	3 (7%)	57,57,57	3.11	17 (29%)
3	Y01	D	1203	-	38,38,38	1.10	3 (7%)	57,57,57	3.38	20 (35%)
2	T14	B	1201	-	36,37,37	3.26	8 (22%)	47,58,58	1.54	6 (12%)
3	Y01	C	1202	-	38,38,38	1.07	3 (7%)	57,57,57	3.11	17 (29%)
3	Y01	B	1204	-	38,38,38	1.08	3 (7%)	57,57,57	3.21	19 (33%)
5	NAG	D	1302	-	14,14,15	2.65	7 (50%)	17,19,21	1.26	2 (11%)
4	ULO	C	1301	-	15,16,16	1.98	3 (20%)	17,20,20	1.62	3 (17%)
3	Y01	A	1204	-	38,38,38	1.08	3 (7%)	57,57,57	3.22	20 (35%)
5	NAG	A	1302	-	14,14,15	2.66	7 (50%)	17,19,21	1.26	2 (11%)
2	T14	D	1201	-	36,37,37	3.27	9 (25%)	47,58,58	1.54	6 (12%)

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
5	NAG	C	1302	-	-	0/6/23/26	0/1/1/1
3	Y01	D	1202	-	-	9/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	Y01	B	1203	-	-	4/19/77/77	0/4/4/4
3	Y01	D	1204	-	-	6/19/77/77	0/4/4/4
4	ULO	D	1301	-	-	19/22/22/22	-
3	Y01	C	1203	-	-	4/19/77/77	0/4/4/4
3	Y01	A	1202	-	-	9/19/77/77	0/4/4/4
2	T14	A	1201	-	-	6/17/41/41	0/5/5/5
4	ULO	B	1301	-	-	19/22/22/22	-
2	T14	C	1201	-	-	6/17/41/41	0/5/5/5
5	NAG	B	1302	-	-	0/6/23/26	0/1/1/1
3	Y01	C	1204	-	-	6/19/77/77	0/4/4/4
4	ULO	A	1301	-	-	19/22/22/22	-
3	Y01	A	1203	-	-	4/19/77/77	0/4/4/4
3	Y01	B	1202	-	-	9/19/77/77	0/4/4/4
3	Y01	D	1203	-	-	4/19/77/77	0/4/4/4
2	T14	B	1201	-	-	6/17/41/41	0/5/5/5
3	Y01	C	1202	-	-	9/19/77/77	0/4/4/4
3	Y01	B	1204	-	-	6/19/77/77	0/4/4/4
5	NAG	D	1302	-	-	0/6/23/26	0/1/1/1
4	ULO	C	1301	-	-	19/22/22/22	-
3	Y01	A	1204	-	-	6/19/77/77	0/4/4/4
5	NAG	A	1302	-	-	0/6/23/26	0/1/1/1
2	T14	D	1201	-	-	6/17/41/41	0/5/5/5

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1201	T14	O21-N20	-13.72	1.20	1.42
2	A	1201	T14	O21-N20	-13.67	1.20	1.42
2	C	1201	T14	O21-N20	-13.65	1.20	1.42
2	B	1201	T14	O21-N20	-13.63	1.21	1.42
2	B	1201	T14	C18-C19	-9.38	1.34	1.47
2	C	1201	T14	C18-C19	-9.34	1.34	1.47
2	A	1201	T14	C18-C19	-9.33	1.34	1.47
2	D	1201	T14	C18-C19	-9.29	1.34	1.47
4	D	1301	ULO	P10-C15	5.26	1.86	1.82
4	B	1301	ULO	P10-C15	5.26	1.86	1.82
4	A	1301	ULO	P10-C15	5.23	1.86	1.82
4	B	1301	ULO	P10-C12	5.23	1.86	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1302	NAG	O5-C5	5.22	1.53	1.43
2	B	1201	T14	C16-C30	-5.21	1.35	1.40
2	A	1201	T14	C16-C30	-5.20	1.35	1.40
5	A	1302	NAG	O5-C5	5.19	1.53	1.43
4	C	1301	ULO	P10-C15	5.19	1.86	1.82
5	D	1302	NAG	O5-C5	5.19	1.53	1.43
2	D	1201	T14	C16-C30	-5.19	1.35	1.40
4	D	1301	ULO	P10-C12	5.18	1.86	1.82
4	A	1301	ULO	P10-C12	5.16	1.86	1.82
2	C	1201	T14	C16-C30	-5.15	1.35	1.40
5	C	1302	NAG	O5-C5	5.15	1.53	1.43
4	C	1301	ULO	P10-C12	5.13	1.86	1.82
2	B	1201	T14	C18-N17	-4.92	1.28	1.36
2	A	1201	T14	C18-N17	-4.92	1.28	1.36
2	D	1201	T14	C18-N17	-4.92	1.28	1.36
2	C	1201	T14	C18-N17	-4.90	1.28	1.36
5	A	1302	NAG	C2-N2	4.20	1.53	1.46
5	C	1302	NAG	C2-N2	4.20	1.53	1.46
5	B	1302	NAG	C2-N2	4.18	1.53	1.46
5	D	1302	NAG	C2-N2	4.18	1.53	1.46
2	D	1201	T14	C30-N29	3.74	1.47	1.39
2	A	1201	T14	C30-N29	3.71	1.47	1.39
2	C	1201	T14	C30-N29	3.70	1.47	1.39
2	B	1201	T14	C30-N29	3.67	1.47	1.39
5	A	1302	NAG	C7-N2	3.49	1.45	1.34
5	B	1302	NAG	C7-N2	3.49	1.45	1.34
5	D	1302	NAG	C7-N2	3.47	1.45	1.34
5	C	1302	NAG	C7-N2	3.47	1.45	1.34
2	B	1201	T14	C16-N17	3.44	1.45	1.38
2	C	1201	T14	C16-N17	3.43	1.45	1.38
2	A	1201	T14	C16-N17	3.43	1.45	1.38
2	D	1201	T14	C16-N17	3.42	1.45	1.38
5	C	1302	NAG	C3-C2	-3.32	1.45	1.52
5	D	1302	NAG	C3-C2	-3.30	1.45	1.52
5	A	1302	NAG	C3-C2	-3.29	1.45	1.52
5	B	1302	NAG	C3-C2	-3.27	1.45	1.52
3	C	1204	Y01	OAW-CAY	3.22	1.43	1.34
3	B	1203	Y01	OAW-CAY	3.21	1.43	1.34
3	D	1204	Y01	OAW-CAY	3.21	1.43	1.34
3	C	1203	Y01	OAW-CAY	3.21	1.43	1.34
3	B	1204	Y01	OAW-CAY	3.21	1.43	1.34
3	D	1203	Y01	OAW-CAY	3.21	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1204	Y01	OAW-CAY	3.21	1.43	1.34
3	A	1203	Y01	OAW-CAY	3.20	1.43	1.34
3	C	1202	Y01	OAW-CAY	3.19	1.43	1.34
3	A	1202	Y01	OAW-CAY	3.19	1.43	1.34
3	D	1202	Y01	OAW-CAY	3.18	1.43	1.34
3	B	1202	Y01	OAW-CAY	3.17	1.43	1.34
5	A	1302	NAG	C6-C5	-3.08	1.41	1.51
5	C	1302	NAG	C6-C5	-3.08	1.41	1.51
5	D	1302	NAG	C6-C5	-3.07	1.41	1.51
5	B	1302	NAG	C6-C5	-3.06	1.41	1.51
3	B	1203	Y01	OAH-CAX	-2.88	1.21	1.30
3	A	1204	Y01	OAH-CAX	-2.87	1.21	1.30
3	A	1203	Y01	OAH-CAX	-2.86	1.21	1.30
3	D	1202	Y01	OAH-CAX	-2.86	1.21	1.30
3	B	1204	Y01	OAH-CAX	-2.86	1.21	1.30
3	C	1204	Y01	OAH-CAX	-2.86	1.21	1.30
3	D	1203	Y01	OAH-CAX	-2.85	1.21	1.30
3	C	1202	Y01	OAH-CAX	-2.85	1.21	1.30
3	C	1203	Y01	OAH-CAX	-2.84	1.21	1.30
3	A	1202	Y01	OAH-CAX	-2.84	1.21	1.30
3	D	1204	Y01	OAH-CAX	-2.83	1.21	1.30
3	B	1202	Y01	OAH-CAX	-2.83	1.21	1.30
2	D	1201	T14	C08-C09	2.81	1.54	1.49
2	A	1201	T14	C08-C09	2.78	1.54	1.49
2	C	1201	T14	C08-C09	2.76	1.54	1.49
2	B	1201	T14	C08-C09	2.74	1.54	1.49
3	D	1203	Y01	CAK-CAI	2.38	1.55	1.50
3	B	1203	Y01	CAK-CAI	2.36	1.55	1.50
3	C	1203	Y01	CAK-CAI	2.35	1.55	1.50
3	A	1203	Y01	CAK-CAI	2.34	1.55	1.50
5	D	1302	NAG	O3-C3	2.28	1.48	1.43
4	D	1301	ULO	P10-O11	-2.28	1.46	1.49
4	A	1301	ULO	P10-O11	-2.26	1.46	1.49
5	C	1302	NAG	O3-C3	2.26	1.48	1.43
5	B	1302	NAG	O5-C1	2.26	1.47	1.43
5	A	1302	NAG	O3-C3	2.25	1.48	1.43
3	B	1204	Y01	CAK-CAI	2.24	1.54	1.50
5	B	1302	NAG	O3-C3	2.24	1.48	1.43
3	C	1202	Y01	CAK-CAI	2.22	1.54	1.50
4	B	1301	ULO	P10-O11	-2.21	1.46	1.49
3	A	1202	Y01	CAK-CAI	2.21	1.54	1.50
5	A	1302	NAG	O5-C1	2.21	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1202	Y01	CAK-CAI	2.21	1.54	1.50
3	A	1204	Y01	CAK-CAI	2.20	1.54	1.50
5	C	1302	NAG	O5-C1	2.20	1.47	1.43
3	C	1204	Y01	CAK-CAI	2.20	1.54	1.50
3	B	1202	Y01	CAK-CAI	2.19	1.54	1.50
5	D	1302	NAG	O5-C1	2.18	1.47	1.43
3	D	1204	Y01	CAK-CAI	2.18	1.54	1.50
4	C	1301	ULO	P10-O11	-2.17	1.46	1.49
2	D	1201	T14	C18-N29	-2.08	1.29	1.32
2	B	1201	T14	C18-N29	-2.05	1.29	1.32
2	C	1201	T14	C16-C11	-2.04	1.38	1.42
2	A	1201	T14	C18-N29	-2.03	1.29	1.32
2	D	1201	T14	C16-C11	-2.02	1.38	1.42
2	A	1201	T14	C16-C11	-2.00	1.38	1.42

All (272) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1204	Y01	CAT-CBH-CBF	-14.49	89.56	108.74
3	B	1204	Y01	CAT-CBH-CBF	-14.48	89.57	108.74
3	D	1204	Y01	CAT-CBH-CBF	-14.47	89.59	108.74
3	C	1204	Y01	CAT-CBH-CBF	-14.47	89.59	108.74
3	C	1202	Y01	CAT-CBH-CBF	-14.30	89.81	108.74
3	D	1202	Y01	CAT-CBH-CBF	-14.30	89.82	108.74
3	B	1202	Y01	CAT-CBH-CBF	-14.29	89.83	108.74
3	A	1202	Y01	CAT-CBH-CBF	-14.29	89.83	108.74
3	C	1203	Y01	CAT-CBH-CBF	-13.87	90.39	108.74
3	A	1203	Y01	CAT-CBH-CBF	-13.86	90.40	108.74
3	D	1203	Y01	CAT-CBH-CBF	-13.86	90.40	108.74
3	B	1203	Y01	CAT-CBH-CBF	-13.85	90.41	108.74
3	C	1203	Y01	CAV-CAZ-CAI	9.22	133.06	120.57
3	A	1203	Y01	CAV-CAZ-CAI	9.21	133.06	120.57
3	B	1203	Y01	CAV-CAZ-CAI	9.21	133.06	120.57
3	D	1203	Y01	CAV-CAZ-CAI	9.20	133.04	120.57
3	D	1204	Y01	CAV-CAZ-CAI	8.87	132.60	120.57
3	A	1204	Y01	CAV-CAZ-CAI	8.86	132.58	120.57
3	C	1204	Y01	CAV-CAZ-CAI	8.83	132.54	120.57
3	B	1204	Y01	CAV-CAZ-CAI	8.82	132.52	120.57
3	B	1202	Y01	CAV-CAZ-CAI	8.76	132.44	120.57
3	A	1202	Y01	CAV-CAZ-CAI	8.72	132.39	120.57
3	C	1202	Y01	CAV-CAZ-CAI	8.70	132.36	120.57
3	D	1202	Y01	CAV-CAZ-CAI	8.70	132.36	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1203	Y01	CBH-CBF-CBD	-6.91	102.61	112.71
3	B	1203	Y01	CBH-CBF-CBD	-6.90	102.63	112.71
3	D	1203	Y01	CBH-CBF-CBD	-6.90	102.64	112.71
3	A	1203	Y01	CBH-CBF-CBD	-6.89	102.64	112.71
3	A	1204	Y01	CBH-CBF-CBD	-6.32	103.48	112.71
3	C	1204	Y01	CBH-CBF-CBD	-6.31	103.48	112.71
3	D	1204	Y01	CBH-CBF-CBD	-6.31	103.50	112.71
3	B	1204	Y01	CBH-CBF-CBD	-6.30	103.50	112.71
3	C	1202	Y01	CAS-CBF-CBH	-5.99	105.70	113.08
3	A	1202	Y01	CAS-CBF-CBH	-5.97	105.72	113.08
3	D	1202	Y01	CAS-CBF-CBH	-5.94	105.75	113.08
3	B	1202	Y01	CAS-CBF-CBH	-5.94	105.76	113.08
3	D	1202	Y01	CBH-CBF-CBD	-5.90	104.09	112.71
3	C	1202	Y01	CBH-CBF-CBD	-5.88	104.12	112.71
3	B	1202	Y01	CBH-CBF-CBD	-5.88	104.12	112.71
3	A	1202	Y01	CBH-CBF-CBD	-5.88	104.13	112.71
3	D	1203	Y01	CAK-CBD-CBG	5.81	119.16	110.93
3	A	1203	Y01	CAK-CBD-CBG	5.80	119.14	110.93
3	C	1203	Y01	CAK-CBD-CBG	5.78	119.11	110.93
3	B	1203	Y01	CAK-CBD-CBG	5.77	119.10	110.93
3	D	1204	Y01	CAS-CBF-CBH	-5.66	106.11	113.08
3	C	1204	Y01	CAS-CBF-CBH	-5.65	106.12	113.08
3	A	1204	Y01	CAS-CBF-CBH	-5.63	106.14	113.08
3	B	1204	Y01	CAS-CBF-CBH	-5.62	106.16	113.08
3	A	1204	Y01	CBH-CAZ-CAI	-5.35	115.11	122.93
3	D	1204	Y01	CBH-CAZ-CAI	-5.35	115.11	122.93
3	C	1204	Y01	CBH-CAZ-CAI	-5.34	115.14	122.93
3	B	1202	Y01	CBH-CAZ-CAI	-5.32	115.16	122.93
3	B	1204	Y01	CBH-CAZ-CAI	-5.32	115.16	122.93
3	A	1202	Y01	CBH-CAZ-CAI	-5.32	115.17	122.93
3	D	1202	Y01	CBH-CAZ-CAI	-5.31	115.18	122.93
3	C	1202	Y01	CBH-CAZ-CAI	-5.30	115.19	122.93
3	A	1203	Y01	CAD-CBH-CAZ	5.14	116.23	108.38
3	C	1203	Y01	CAD-CBH-CAZ	5.14	116.23	108.38
3	B	1203	Y01	CAD-CBH-CAZ	5.13	116.23	108.38
3	D	1203	Y01	CAD-CBH-CAZ	5.13	116.22	108.38
3	D	1204	Y01	CAD-CBH-CAZ	5.12	116.20	108.38
3	A	1204	Y01	CAD-CBH-CAZ	5.11	116.19	108.38
3	B	1204	Y01	CAD-CBH-CAZ	5.10	116.18	108.38
3	C	1204	Y01	CAD-CBH-CAZ	5.10	116.17	108.38
3	A	1202	Y01	CAD-CBH-CAZ	5.06	116.11	108.38
3	D	1202	Y01	CAD-CBH-CAZ	5.04	116.09	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1202	Y01	CAD-CBH-CAZ	5.04	116.08	108.38
3	C	1202	Y01	CAD-CBH-CAZ	5.03	116.07	108.38
3	B	1203	Y01	CAK-CBD-CBF	-5.01	103.93	109.72
3	C	1203	Y01	CAK-CBD-CBF	-5.01	103.93	109.72
3	A	1203	Y01	CAK-CBD-CBF	-5.00	103.95	109.72
3	D	1203	Y01	CAK-CBD-CBF	-5.00	103.95	109.72
3	C	1203	Y01	CBI-CBG-CBD	-4.87	107.50	114.41
3	B	1203	Y01	CBI-CBG-CBD	-4.86	107.52	114.41
3	A	1203	Y01	CBI-CBG-CBD	-4.85	107.53	114.41
3	D	1203	Y01	CBI-CBG-CBD	-4.83	107.56	114.41
3	D	1203	Y01	CBI-CBE-CBB	-4.76	112.14	119.50
3	B	1203	Y01	CBI-CBE-CBB	-4.76	112.14	119.50
3	C	1203	Y01	CBI-CBE-CBB	-4.75	112.16	119.50
3	A	1203	Y01	CBI-CBE-CBB	-4.75	112.16	119.50
3	C	1203	Y01	CBH-CAZ-CAI	-4.74	116.01	122.93
3	B	1203	Y01	CBH-CAZ-CAI	-4.73	116.02	122.93
3	A	1203	Y01	CBH-CAZ-CAI	-4.72	116.04	122.93
3	D	1203	Y01	CBH-CAZ-CAI	-4.71	116.05	122.93
3	C	1204	Y01	CBI-CBE-CBB	-4.56	112.46	119.50
3	D	1204	Y01	CBI-CBE-CBB	-4.56	112.46	119.50
3	A	1204	Y01	CBI-CBE-CBB	-4.54	112.48	119.50
3	B	1204	Y01	CBI-CBE-CBB	-4.54	112.49	119.50
3	D	1204	Y01	CAU-CBI-CBE	-4.49	109.99	116.60
3	C	1204	Y01	CAU-CBI-CBE	-4.46	110.03	116.60
3	A	1204	Y01	CAU-CBI-CBE	-4.45	110.05	116.60
3	B	1204	Y01	CAU-CBI-CBE	-4.43	110.07	116.60
3	B	1202	Y01	CAU-CBI-CBE	-4.31	110.25	116.60
3	C	1203	Y01	CAU-CBI-CBE	-4.31	110.25	116.60
3	A	1203	Y01	CAV-CAZ-CBH	-4.31	110.90	116.42
3	D	1203	Y01	CAV-CAZ-CBH	-4.31	110.91	116.42
3	B	1203	Y01	CAV-CAZ-CBH	-4.30	110.92	116.42
3	D	1203	Y01	CAU-CBI-CBE	-4.30	110.27	116.60
3	A	1203	Y01	CAU-CBI-CBE	-4.29	110.28	116.60
3	C	1202	Y01	CAU-CBI-CBE	-4.29	110.28	116.60
3	A	1202	Y01	CAU-CBI-CBE	-4.29	110.28	116.60
3	C	1203	Y01	CAV-CAZ-CBH	-4.29	110.93	116.42
3	D	1202	Y01	CAU-CBI-CBE	-4.29	110.29	116.60
3	B	1203	Y01	CAU-CBI-CBE	-4.26	110.32	116.60
3	B	1203	Y01	CBD-CAK-CAI	-4.23	106.90	112.76
3	C	1203	Y01	CBD-CAK-CAI	-4.23	106.90	112.76
3	D	1203	Y01	CBD-CAK-CAI	-4.22	106.91	112.76
3	A	1203	Y01	CBD-CAK-CAI	-4.21	106.93	112.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1203	Y01	CAS-CBF-CBH	-4.11	108.02	113.08
3	B	1203	Y01	CAS-CBF-CBH	-4.10	108.03	113.08
3	A	1203	Y01	CAS-CBF-CBH	-4.08	108.05	113.08
3	A	1203	Y01	OAW-CAY-CAM	4.07	120.28	111.48
3	B	1203	Y01	OAW-CAY-CAM	4.07	120.28	111.48
3	D	1203	Y01	CAS-CBF-CBH	-4.06	108.07	113.08
3	C	1203	Y01	OAW-CAY-CAM	4.06	120.27	111.48
3	D	1203	Y01	OAW-CAY-CAM	4.04	120.23	111.48
3	D	1202	Y01	OAW-CAY-CAM	4.01	120.16	111.48
3	C	1202	Y01	OAW-CAY-CAM	4.01	120.15	111.48
3	A	1202	Y01	OAW-CAY-CAM	4.00	120.14	111.48
3	B	1202	Y01	OAW-CAY-CAM	4.00	120.13	111.48
2	D	1201	T14	N17-C18-N29	3.95	117.45	113.22
2	A	1201	T14	N17-C18-N29	3.92	117.42	113.22
2	B	1201	T14	N17-C18-N29	3.89	117.39	113.22
2	C	1201	T14	N17-C18-N29	3.88	117.38	113.22
3	B	1202	Y01	CBI-CBE-CBB	-3.80	113.63	119.50
3	C	1202	Y01	CBI-CBE-CBB	-3.79	113.64	119.50
3	A	1202	Y01	CBI-CBE-CBB	-3.78	113.66	119.50
3	D	1202	Y01	CBI-CBE-CBB	-3.77	113.67	119.50
3	B	1204	Y01	OAW-CAY-CAM	3.74	119.56	111.48
3	A	1204	Y01	OAW-CAY-CAM	3.73	119.54	111.48
3	C	1204	Y01	OAW-CAY-CAM	3.72	119.53	111.48
3	D	1204	Y01	OAW-CAY-CAM	3.72	119.53	111.48
2	B	1201	T14	O21-N20-C19	3.72	113.25	109.33
2	C	1201	T14	O21-N20-C19	3.67	113.20	109.33
2	A	1201	T14	O21-N20-C19	3.66	113.20	109.33
2	D	1201	T14	O21-N20-C19	3.64	113.17	109.33
2	B	1201	T14	C28-C19-N20	-3.52	111.39	114.53
2	C	1201	T14	C28-C19-N20	-3.48	111.43	114.53
2	A	1201	T14	C28-C19-N20	-3.47	111.44	114.53
2	D	1201	T14	C28-C19-N20	-3.45	111.46	114.53
3	D	1203	Y01	CAU-CAS-CBF	3.36	118.84	113.14
3	A	1203	Y01	CAU-CAS-CBF	3.36	118.84	113.14
3	C	1203	Y01	CAU-CAS-CBF	3.35	118.84	113.14
3	B	1203	Y01	CAU-CAS-CBF	3.33	118.79	113.14
3	B	1204	Y01	CAU-CAS-CBF	3.28	118.71	113.14
3	C	1204	Y01	CAU-CAS-CBF	3.27	118.70	113.14
3	A	1204	Y01	CAU-CAS-CBF	3.27	118.69	113.14
3	D	1204	Y01	CAU-CAS-CBF	3.26	118.68	113.14
3	D	1204	Y01	CAV-CAZ-CBH	-3.23	112.28	116.42
3	C	1204	Y01	CAD-CBH-CAT	3.23	114.35	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1204	Y01	CAD-CBH-CAT	3.23	114.35	109.43
3	A	1204	Y01	CAD-CBH-CAT	3.23	114.34	109.43
3	A	1204	Y01	CAV-CAZ-CBH	-3.22	112.30	116.42
3	D	1204	Y01	CAD-CBH-CAT	3.22	114.32	109.43
3	B	1204	Y01	CAV-CAZ-CBH	-3.21	112.31	116.42
3	C	1204	Y01	CAV-CAZ-CBH	-3.21	112.31	116.42
4	C	1301	ULO	O11-P10-C09	-3.20	109.19	112.84
3	A	1203	Y01	CAD-CBH-CAT	3.19	114.28	109.43
3	D	1204	Y01	CAK-CBD-CBG	3.18	115.43	110.93
4	D	1301	ULO	O11-P10-C09	-3.18	109.22	112.84
3	C	1203	Y01	CAD-CBH-CAT	3.17	114.26	109.43
4	A	1301	ULO	O11-P10-C09	-3.17	109.23	112.84
3	D	1204	Y01	CAS-CBF-CBD	3.17	116.20	111.78
3	B	1203	Y01	CAD-CBH-CAT	3.17	114.25	109.43
3	D	1203	Y01	CAD-CBH-CAT	3.17	114.25	109.43
3	A	1204	Y01	CAS-CBF-CBD	3.17	116.20	111.78
3	A	1204	Y01	CAK-CBD-CBG	3.17	115.42	110.93
3	B	1204	Y01	CAK-CBD-CBG	3.17	115.42	110.93
3	B	1204	Y01	CAS-CBF-CBD	3.16	116.19	111.78
3	C	1204	Y01	CAS-CBF-CBD	3.16	116.19	111.78
3	C	1204	Y01	CAK-CBD-CBG	3.16	115.40	110.93
4	B	1301	ULO	O11-P10-C09	-3.15	109.25	112.84
3	B	1202	Y01	CAV-CAZ-CBH	-3.14	112.40	116.42
3	D	1203	Y01	CAS-CBF-CBD	3.13	116.14	111.78
3	B	1203	Y01	CAS-CBF-CBD	3.12	116.14	111.78
3	A	1203	Y01	CAS-CBF-CBD	3.12	116.13	111.78
3	A	1202	Y01	CAV-CAZ-CBH	-3.12	112.43	116.42
3	C	1202	Y01	CAV-CAZ-CBH	-3.11	112.44	116.42
4	B	1301	ULO	O11-P10-C15	-3.11	108.27	111.35
3	C	1203	Y01	CAS-CBF-CBD	3.11	116.12	111.78
3	D	1202	Y01	CAV-CAZ-CBH	-3.10	112.45	116.42
3	D	1204	Y01	CAK-CBD-CBF	-3.09	106.15	109.72
4	A	1301	ULO	O11-P10-C15	-3.09	108.29	111.35
4	C	1301	ULO	O11-P10-C15	-3.09	108.30	111.35
3	C	1202	Y01	CAD-CBH-CAT	3.08	114.11	109.43
4	D	1301	ULO	O11-P10-C15	-3.07	108.31	111.35
3	C	1204	Y01	CAK-CBD-CBF	-3.07	106.18	109.72
3	A	1202	Y01	CAD-CBH-CAT	3.06	114.09	109.43
3	D	1202	Y01	CAD-CBH-CAT	3.06	114.08	109.43
3	B	1202	Y01	CAD-CBH-CAT	3.06	114.08	109.43
3	A	1204	Y01	CAK-CBD-CBF	-3.05	106.19	109.72
3	B	1204	Y01	CAK-CBD-CBF	-3.04	106.20	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1202	Y01	CAS-CBF-CBD	2.99	115.95	111.78
3	A	1202	Y01	CAS-CBF-CBD	2.98	115.93	111.78
3	B	1202	Y01	CAS-CBF-CBD	2.96	115.91	111.78
3	C	1202	Y01	CAS-CBF-CBD	2.96	115.90	111.78
3	B	1202	Y01	CAK-CBD-CBG	2.79	114.88	110.93
3	D	1202	Y01	CAK-CBD-CBG	2.78	114.86	110.93
3	A	1202	Y01	CAK-CBD-CBG	2.76	114.83	110.93
3	C	1202	Y01	CAK-CBD-CBG	2.75	114.83	110.93
3	C	1204	Y01	CBI-CBG-CBD	-2.72	110.56	114.41
3	B	1204	Y01	CBI-CBG-CBD	-2.70	110.58	114.41
3	D	1204	Y01	CBI-CBG-CBD	-2.70	110.58	114.41
3	A	1204	Y01	CBI-CBG-CBD	-2.70	110.58	114.41
3	C	1202	Y01	CAK-CBD-CBF	-2.62	106.70	109.72
3	C	1203	Y01	CBF-CBD-CBG	-2.60	105.68	109.09
3	D	1203	Y01	CBF-CBD-CBG	-2.60	105.69	109.09
3	B	1202	Y01	CAK-CBD-CBF	-2.60	106.71	109.72
3	A	1202	Y01	CAK-CBD-CBF	-2.60	106.71	109.72
3	A	1203	Y01	CBF-CBD-CBG	-2.60	105.69	109.09
3	B	1203	Y01	CBF-CBD-CBG	-2.60	105.69	109.09
3	D	1202	Y01	CAK-CBD-CBF	-2.58	106.74	109.72
5	A	1302	NAG	C2-N2-C7	-2.49	119.57	122.90
5	B	1302	NAG	C2-N2-C7	-2.47	119.59	122.90
5	C	1302	NAG	C2-N2-C7	-2.45	119.61	122.90
4	B	1301	ULO	O11-P10-C12	-2.45	108.92	111.35
5	D	1302	NAG	C2-N2-C7	-2.45	119.62	122.90
4	D	1301	ULO	O11-P10-C12	-2.44	108.93	111.35
4	C	1301	ULO	O11-P10-C12	-2.44	108.93	111.35
5	D	1302	NAG	C8-C7-N2	2.44	120.16	116.12
4	A	1301	ULO	O11-P10-C12	-2.43	108.95	111.35
5	C	1302	NAG	C8-C7-N2	2.43	120.14	116.12
3	B	1202	Y01	CAU-CAS-CBF	2.42	117.26	113.14
5	B	1302	NAG	C8-C7-N2	2.42	120.12	116.12
3	C	1202	Y01	CAU-CAS-CBF	2.41	117.23	113.14
5	A	1302	NAG	C8-C7-N2	2.40	120.10	116.12
3	A	1202	Y01	CAU-CAS-CBF	2.40	117.21	113.14
3	D	1202	Y01	CAU-CAS-CBF	2.39	117.20	113.14
2	D	1201	T14	C16-C30-N29	-2.37	108.29	109.91
3	A	1204	Y01	CBF-CBD-CBG	-2.35	106.01	109.09
3	D	1204	Y01	CBF-CBD-CBG	-2.35	106.02	109.09
3	C	1204	Y01	CBF-CBD-CBG	-2.34	106.03	109.09
3	B	1204	Y01	CBF-CBD-CBG	-2.33	106.04	109.09
2	B	1201	T14	C16-C30-N29	-2.31	108.33	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	T14	C16-C30-N29	-2.31	108.33	109.91
2	C	1201	T14	C16-C30-N29	-2.28	108.35	109.91
3	C	1204	Y01	CAP-CBE-CBB	-2.26	108.76	112.18
3	D	1204	Y01	CAP-CBE-CBB	-2.26	108.76	112.18
3	A	1204	Y01	CAP-CBE-CBB	-2.24	108.79	112.18
3	D	1202	Y01	CAP-CBE-CBB	-2.22	108.82	112.18
3	C	1203	Y01	CAP-CBE-CBB	-2.21	108.83	112.18
3	B	1204	Y01	CAP-CBE-CBB	-2.20	108.84	112.18
2	C	1201	T14	F33-C02-C03	-2.20	108.74	112.65
3	D	1203	Y01	CAP-CBE-CBB	-2.20	108.84	112.18
3	B	1202	Y01	CAP-CBE-CBB	-2.20	108.85	112.18
3	A	1202	Y01	CAP-CBE-CBB	-2.20	108.85	112.18
3	A	1203	Y01	CAP-CBE-CBB	-2.19	108.87	112.18
2	A	1201	T14	F33-C02-C03	-2.19	108.77	112.65
3	B	1203	Y01	CAP-CBE-CBB	-2.18	108.88	112.18
3	C	1202	Y01	CAP-CBE-CBB	-2.18	108.88	112.18
2	D	1201	T14	F33-C02-C03	-2.17	108.80	112.65
2	B	1201	T14	F33-C02-C03	-2.17	108.80	112.65
3	A	1202	Y01	CBI-CBG-CBD	-2.09	111.44	114.41
3	C	1204	Y01	CBD-CAK-CAI	-2.08	109.88	112.76
2	A	1201	T14	C10-C11-C12	2.08	121.65	116.60
2	B	1201	T14	C10-C11-C12	2.08	121.65	116.60
2	C	1201	T14	C10-C11-C12	2.08	121.64	116.60
3	C	1202	Y01	CBI-CBG-CBD	-2.08	111.46	114.41
2	D	1201	T14	C10-C11-C12	2.07	121.62	116.60
3	A	1204	Y01	CBD-CAK-CAI	-2.07	109.89	112.76
3	B	1202	Y01	CBI-CBG-CBD	-2.07	111.48	114.41
3	D	1202	Y01	CBI-CBG-CBD	-2.07	111.48	114.41
3	B	1204	Y01	CBD-CAK-CAI	-2.06	109.90	112.76
3	D	1204	Y01	CBD-CAK-CAI	-2.05	109.92	112.76
3	C	1203	Y01	CAD-CBH-CBF	2.04	113.95	111.66
3	A	1203	Y01	CBG-CBI-CBE	2.03	102.43	100.10
3	D	1203	Y01	CBG-CBI-CBE	2.03	102.43	100.10
3	C	1203	Y01	CBG-CBI-CBE	2.02	102.42	100.10
3	B	1203	Y01	CAD-CBH-CBF	2.02	113.92	111.66
3	B	1203	Y01	CBG-CBI-CBE	2.01	102.41	100.10
3	D	1204	Y01	CAC-CBB-CBE	-2.01	109.87	112.88
3	A	1204	Y01	CAC-CBB-CBE	-2.00	109.88	112.88

There are no chirality outliers.

All (176) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1202	Y01	CAM-CAY-OAW-CBC
3	B	1202	Y01	CAM-CAY-OAW-CBC
3	C	1202	Y01	CAM-CAY-OAW-CBC
3	D	1202	Y01	CAM-CAY-OAW-CBC
4	A	1301	ULO	C08-C09-P10-C12
4	A	1301	ULO	C13-C12-P10-C09
4	A	1301	ULO	C13-C12-P10-C15
4	A	1301	ULO	C13-C12-P10-O11
4	A	1301	ULO	C14-C12-P10-C09
4	A	1301	ULO	C14-C12-P10-C15
4	A	1301	ULO	C14-C12-P10-O11
4	A	1301	ULO	C16-C15-P10-C09
4	A	1301	ULO	C16-C15-P10-C12
4	A	1301	ULO	C16-C15-P10-O11
4	A	1301	ULO	C17-C15-P10-C09
4	A	1301	ULO	C17-C15-P10-C12
4	A	1301	ULO	C17-C15-P10-O11
4	B	1301	ULO	C08-C09-P10-C12
4	B	1301	ULO	C13-C12-P10-C09
4	B	1301	ULO	C13-C12-P10-C15
4	B	1301	ULO	C13-C12-P10-O11
4	B	1301	ULO	C14-C12-P10-C09
4	B	1301	ULO	C14-C12-P10-C15
4	B	1301	ULO	C14-C12-P10-O11
4	B	1301	ULO	C16-C15-P10-C09
4	B	1301	ULO	C16-C15-P10-C12
4	B	1301	ULO	C16-C15-P10-O11
4	B	1301	ULO	C17-C15-P10-C09
4	B	1301	ULO	C17-C15-P10-C12
4	B	1301	ULO	C17-C15-P10-O11
4	C	1301	ULO	C08-C09-P10-C12
4	C	1301	ULO	C13-C12-P10-C09
4	C	1301	ULO	C13-C12-P10-C15
4	C	1301	ULO	C13-C12-P10-O11
4	C	1301	ULO	C14-C12-P10-C09
4	C	1301	ULO	C14-C12-P10-C15
4	C	1301	ULO	C14-C12-P10-O11
4	C	1301	ULO	C16-C15-P10-C09
4	C	1301	ULO	C16-C15-P10-C12
4	C	1301	ULO	C16-C15-P10-O11
4	C	1301	ULO	C17-C15-P10-C09
4	C	1301	ULO	C17-C15-P10-C12
4	C	1301	ULO	C17-C15-P10-O11

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Mol	Chain	Res	Type	Atoms
4	D	1301	ULO	C08-C09-P10-C12
4	D	1301	ULO	C13-C12-P10-C09
4	D	1301	ULO	C13-C12-P10-C15
4	D	1301	ULO	C13-C12-P10-O11
4	D	1301	ULO	C14-C12-P10-C09
4	D	1301	ULO	C14-C12-P10-C15
4	D	1301	ULO	C14-C12-P10-O11
4	D	1301	ULO	C16-C15-P10-C09
4	D	1301	ULO	C16-C15-P10-C12
4	D	1301	ULO	C16-C15-P10-O11
4	D	1301	ULO	C17-C15-P10-C09
4	D	1301	ULO	C17-C15-P10-C12
4	D	1301	ULO	C17-C15-P10-O11
3	A	1202	Y01	OAG-CAY-OAW-CBC
3	B	1202	Y01	OAG-CAY-OAW-CBC
3	C	1202	Y01	OAG-CAY-OAW-CBC
3	D	1202	Y01	OAG-CAY-OAW-CBC
3	A	1204	Y01	CAJ-CAO-CBB-CAC
3	B	1204	Y01	CAJ-CAO-CBB-CAC
3	C	1204	Y01	CAJ-CAO-CBB-CAC
3	D	1204	Y01	CAJ-CAO-CBB-CAC
3	A	1202	Y01	CAJ-CAO-CBB-CBE
3	A	1204	Y01	CAJ-CAO-CBB-CBE
3	B	1202	Y01	CAJ-CAO-CBB-CBE
3	B	1204	Y01	CAJ-CAO-CBB-CBE
3	C	1202	Y01	CAJ-CAO-CBB-CBE
3	C	1204	Y01	CAJ-CAO-CBB-CBE
3	D	1202	Y01	CAJ-CAO-CBB-CBE
3	D	1204	Y01	CAJ-CAO-CBB-CBE
3	A	1202	Y01	CAJ-CAO-CBB-CAC
3	B	1202	Y01	CAJ-CAO-CBB-CAC
3	C	1202	Y01	CAJ-CAO-CBB-CAC
3	D	1202	Y01	CAJ-CAO-CBB-CAC
3	A	1204	Y01	CAN-CAJ-CAO-CBB
3	B	1204	Y01	CAN-CAJ-CAO-CBB
3	C	1204	Y01	CAN-CAJ-CAO-CBB
3	D	1204	Y01	CAN-CAJ-CAO-CBB
3	A	1202	Y01	CAN-CAJ-CAO-CBB
3	B	1202	Y01	CAN-CAJ-CAO-CBB
3	C	1202	Y01	CAN-CAJ-CAO-CBB
3	D	1202	Y01	CAN-CAJ-CAO-CBB
3	A	1204	Y01	CAJ-CAN-CBA-CAB

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Mol	Chain	Res	Type	Atoms
3	B	1204	Y01	CAJ-CAN-CBA-CAB
3	C	1204	Y01	CAJ-CAN-CBA-CAB
3	D	1204	Y01	CAJ-CAN-CBA-CAB
3	A	1204	Y01	CAJ-CAN-CBA-CAA
3	B	1204	Y01	CAJ-CAN-CBA-CAA
3	C	1204	Y01	CAJ-CAN-CBA-CAA
3	D	1204	Y01	CAJ-CAN-CBA-CAA
3	A	1203	Y01	CAO-CAJ-CAN-CBA
3	B	1203	Y01	CAO-CAJ-CAN-CBA
3	C	1203	Y01	CAO-CAJ-CAN-CBA
3	D	1203	Y01	CAO-CAJ-CAN-CBA
4	A	1301	ULO	C06-C07-C08-C09
4	B	1301	ULO	C06-C07-C08-C09
4	C	1301	ULO	C06-C07-C08-C09
4	D	1301	ULO	C06-C07-C08-C09
4	A	1301	ULO	C07-C08-C09-P10
4	B	1301	ULO	C07-C08-C09-P10
4	C	1301	ULO	C07-C08-C09-P10
4	D	1301	ULO	C07-C08-C09-P10
3	D	1202	Y01	CAO-CAJ-CAN-CBA
3	A	1202	Y01	CAO-CAJ-CAN-CBA
3	B	1202	Y01	CAO-CAJ-CAN-CBA
3	C	1202	Y01	CAO-CAJ-CAN-CBA
3	A	1203	Y01	CAJ-CAO-CBB-CAC
3	B	1203	Y01	CAJ-CAO-CBB-CAC
3	C	1203	Y01	CAJ-CAO-CBB-CAC
3	D	1203	Y01	CAJ-CAO-CBB-CAC
3	A	1202	Y01	CAX-CAL-CAM-CAY
3	A	1202	Y01	CAJ-CAN-CBA-CAA
3	B	1202	Y01	CAJ-CAN-CBA-CAA
3	C	1202	Y01	CAJ-CAN-CBA-CAA
3	D	1202	Y01	CAJ-CAN-CBA-CAA
3	B	1202	Y01	CAX-CAL-CAM-CAY
3	C	1202	Y01	CAX-CAL-CAM-CAY
3	D	1202	Y01	CAX-CAL-CAM-CAY
4	A	1301	ULO	C05-C06-C07-C08
4	C	1301	ULO	C05-C06-C07-C08
4	D	1301	ULO	C05-C06-C07-C08
4	B	1301	ULO	C05-C06-C07-C08
3	A	1202	Y01	CAJ-CAN-CBA-CAB
3	B	1202	Y01	CAJ-CAN-CBA-CAB
3	C	1202	Y01	CAJ-CAN-CBA-CAB

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Mol	Chain	Res	Type	Atoms
3	D	1202	Y01	CAJ-CAN-CBA-CAB
2	A	1201	T14	C16-C11-C12-F14
2	B	1201	T14	C16-C11-C12-F14
2	C	1201	T14	C16-C11-C12-F14
2	D	1201	T14	C16-C11-C12-F14
2	A	1201	T14	C16-C11-C12-F15
2	B	1201	T14	C16-C11-C12-F15
2	D	1201	T14	C16-C11-C12-F15
2	C	1201	T14	C16-C11-C12-F15
2	A	1201	T14	C16-C11-C12-F13
2	B	1201	T14	C16-C11-C12-F13
2	C	1201	T14	C16-C11-C12-F13
2	D	1201	T14	C16-C11-C12-F13
3	A	1203	Y01	CAJ-CAN-CBA-CAA
3	B	1203	Y01	CAJ-CAN-CBA-CAA
3	C	1203	Y01	CAJ-CAN-CBA-CAA
3	D	1203	Y01	CAJ-CAN-CBA-CAA
4	C	1301	ULO	C04-C05-C06-C07
3	C	1204	Y01	CAO-CAJ-CAN-CBA
4	A	1301	ULO	C04-C05-C06-C07
4	B	1301	ULO	C04-C05-C06-C07
4	D	1301	ULO	C04-C05-C06-C07
3	A	1204	Y01	CAO-CAJ-CAN-CBA
3	B	1204	Y01	CAO-CAJ-CAN-CBA
3	D	1204	Y01	CAO-CAJ-CAN-CBA
2	B	1201	T14	C03-C08-C09-C10
2	A	1201	T14	C03-C08-C09-C10
2	D	1201	T14	C03-C08-C09-C10
2	C	1201	T14	C03-C08-C09-C10
2	B	1201	T14	C03-C08-C09-C31
2	A	1201	T14	C03-C08-C09-C31
2	C	1201	T14	C03-C08-C09-C31
2	D	1201	T14	C03-C08-C09-C31
4	D	1301	ULO	C01-C02-C03-C04
4	C	1301	ULO	C01-C02-C03-C04
4	A	1301	ULO	C01-C02-C03-C04
4	B	1301	ULO	C01-C02-C03-C04
3	A	1203	Y01	CAJ-CAO-CBB-CBE
3	B	1203	Y01	CAJ-CAO-CBB-CBE
3	C	1203	Y01	CAJ-CAO-CBB-CBE
3	D	1203	Y01	CAJ-CAO-CBB-CBE
2	D	1201	T14	C07-C08-C09-C10

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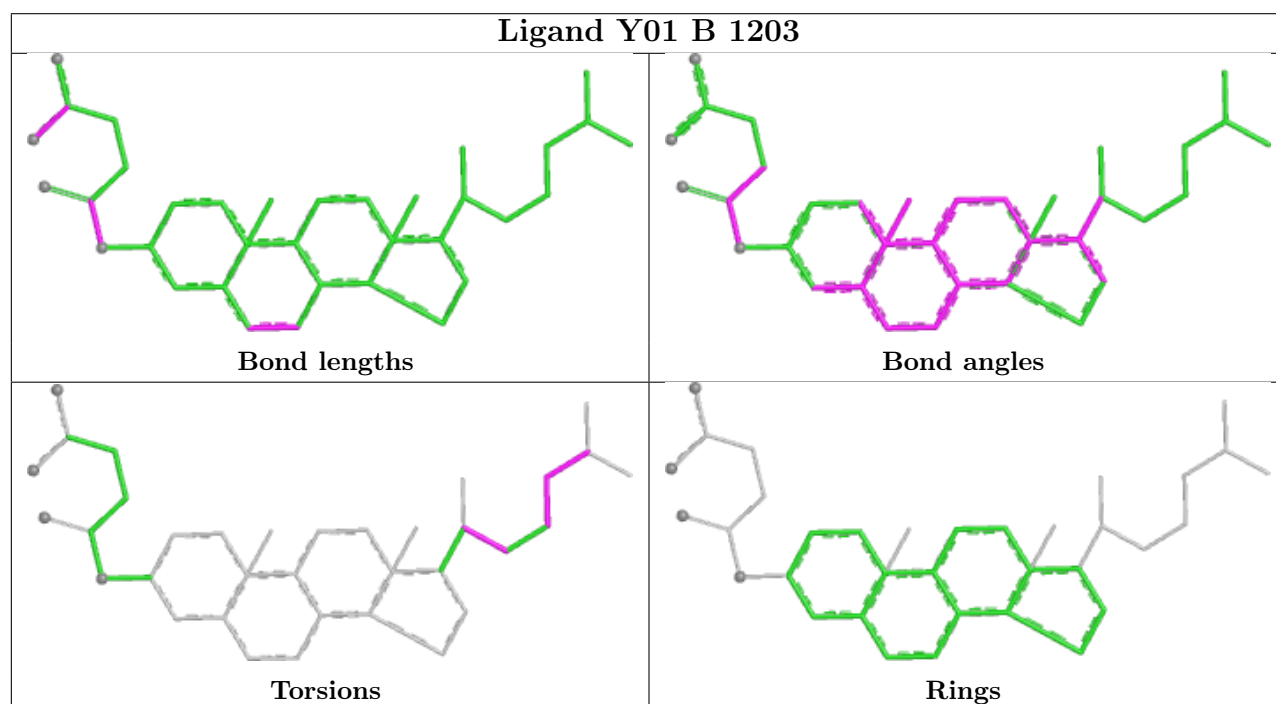
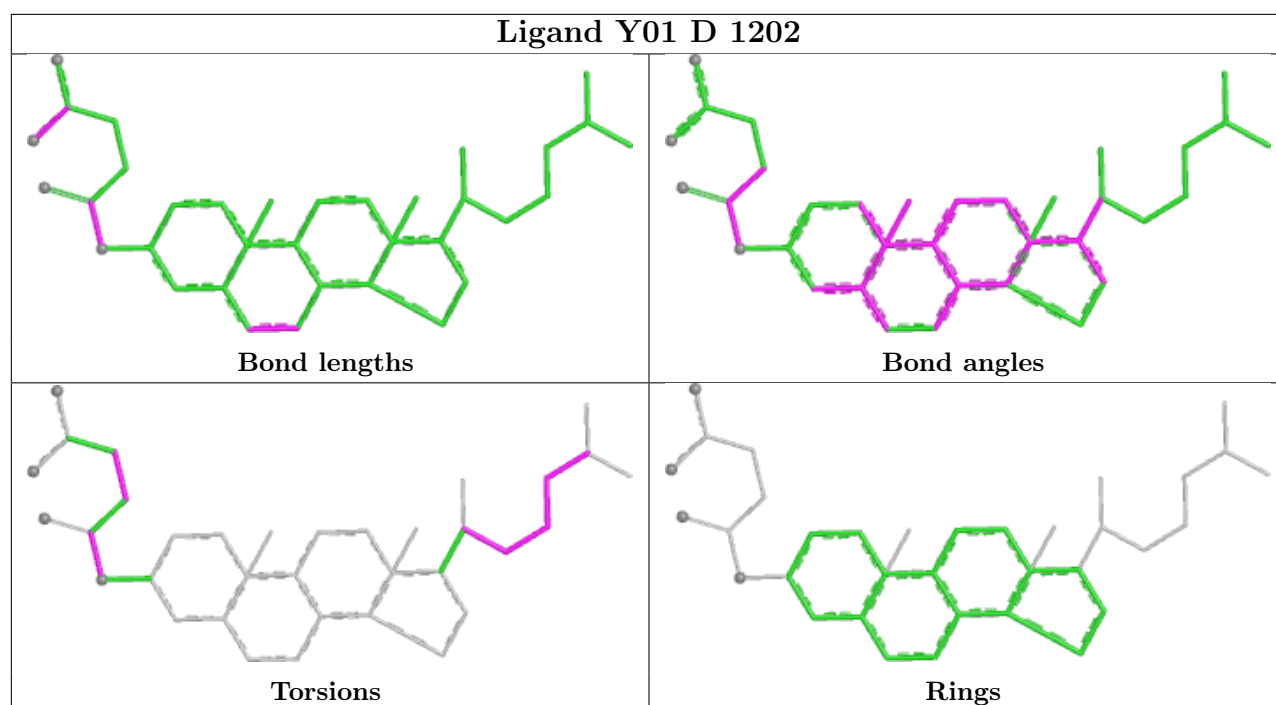
Mol	Chain	Res	Type	Atoms
2	A	1201	T14	C07-C08-C09-C10
2	B	1201	T14	C07-C08-C09-C10
2	C	1201	T14	C07-C08-C09-C10
4	A	1301	ULO	C08-C09-P10-O11
4	B	1301	ULO	C08-C09-P10-O11
4	C	1301	ULO	C08-C09-P10-O11
4	D	1301	ULO	C08-C09-P10-O11

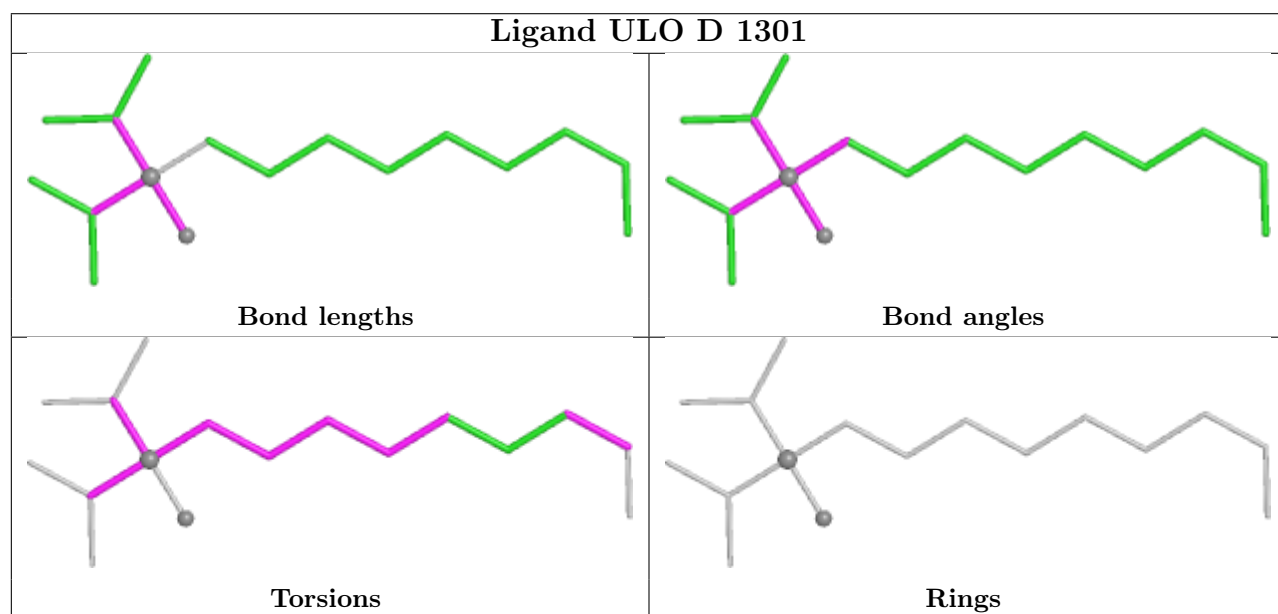
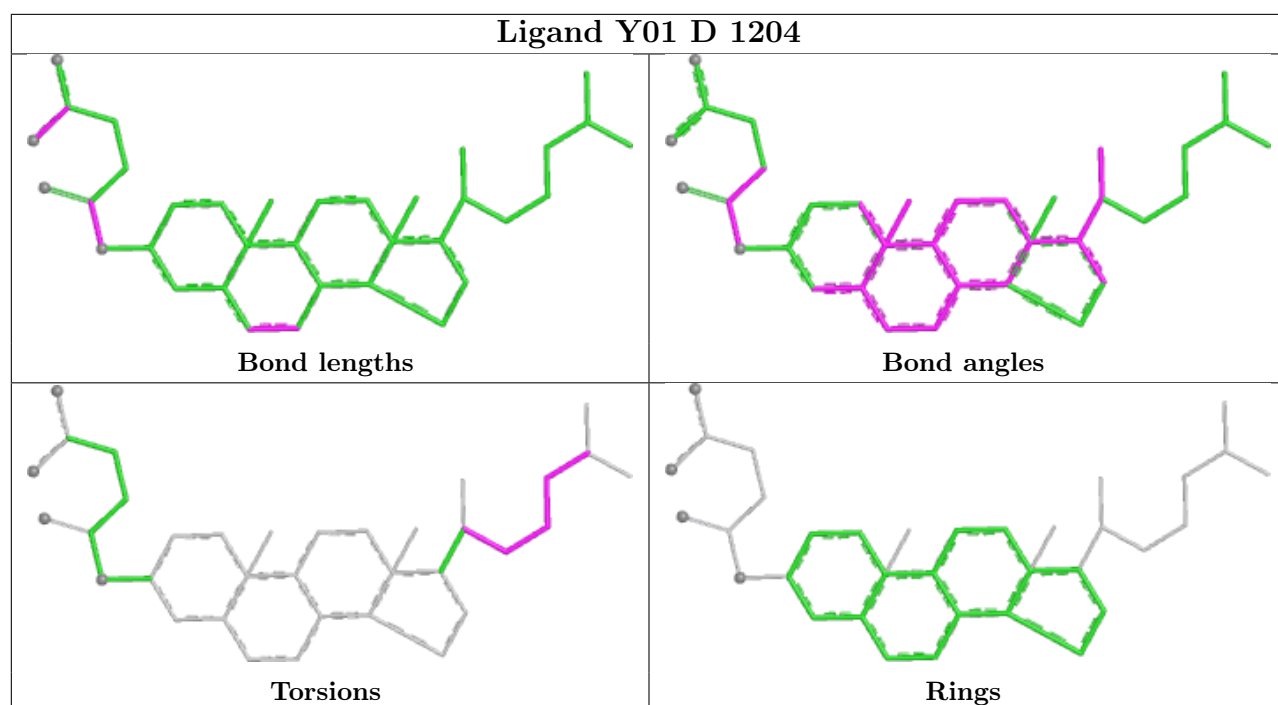
There are no ring outliers.

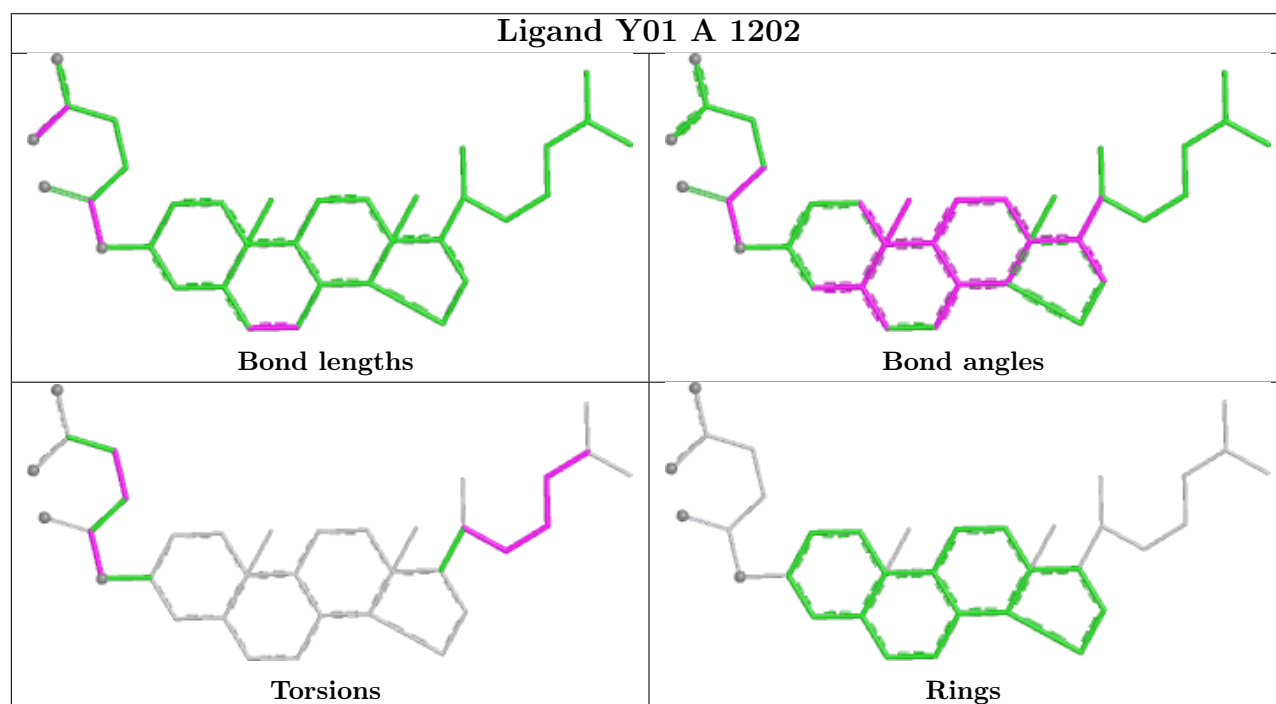
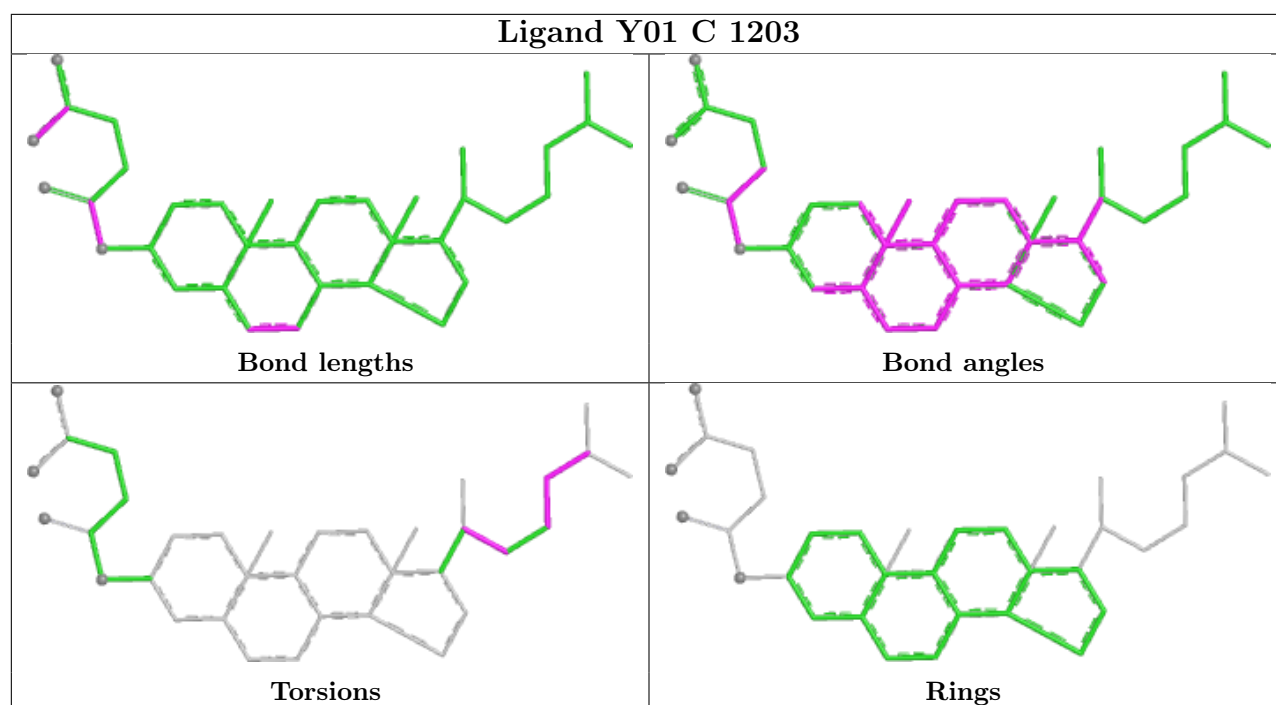
16 monomers are involved in 99 short contacts:

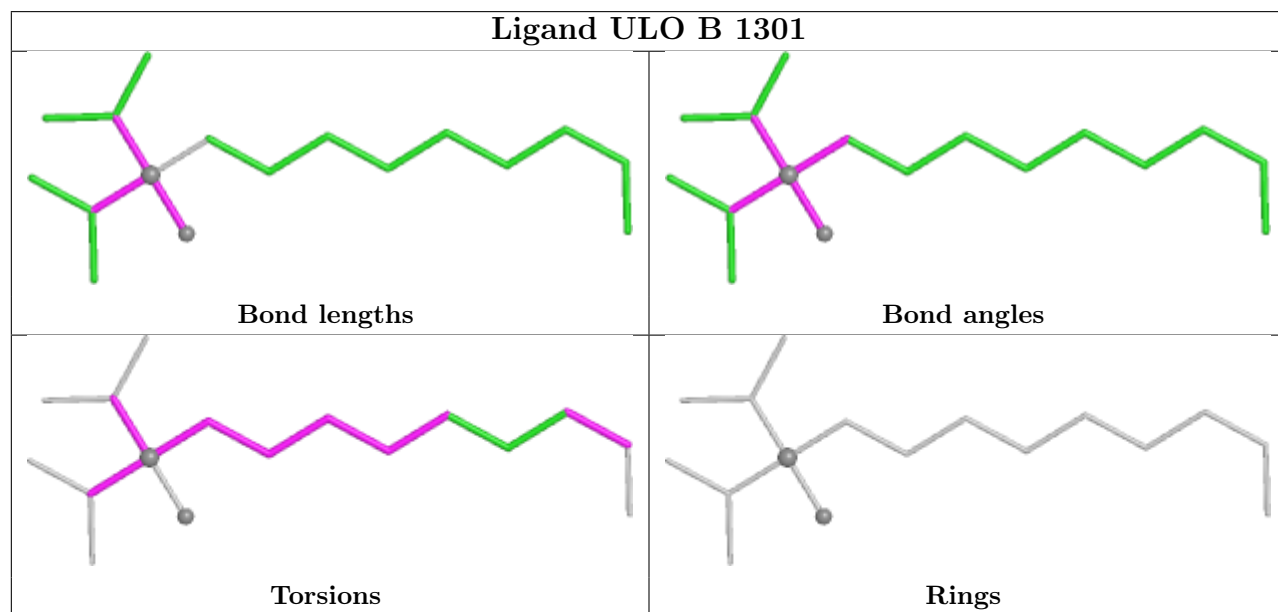
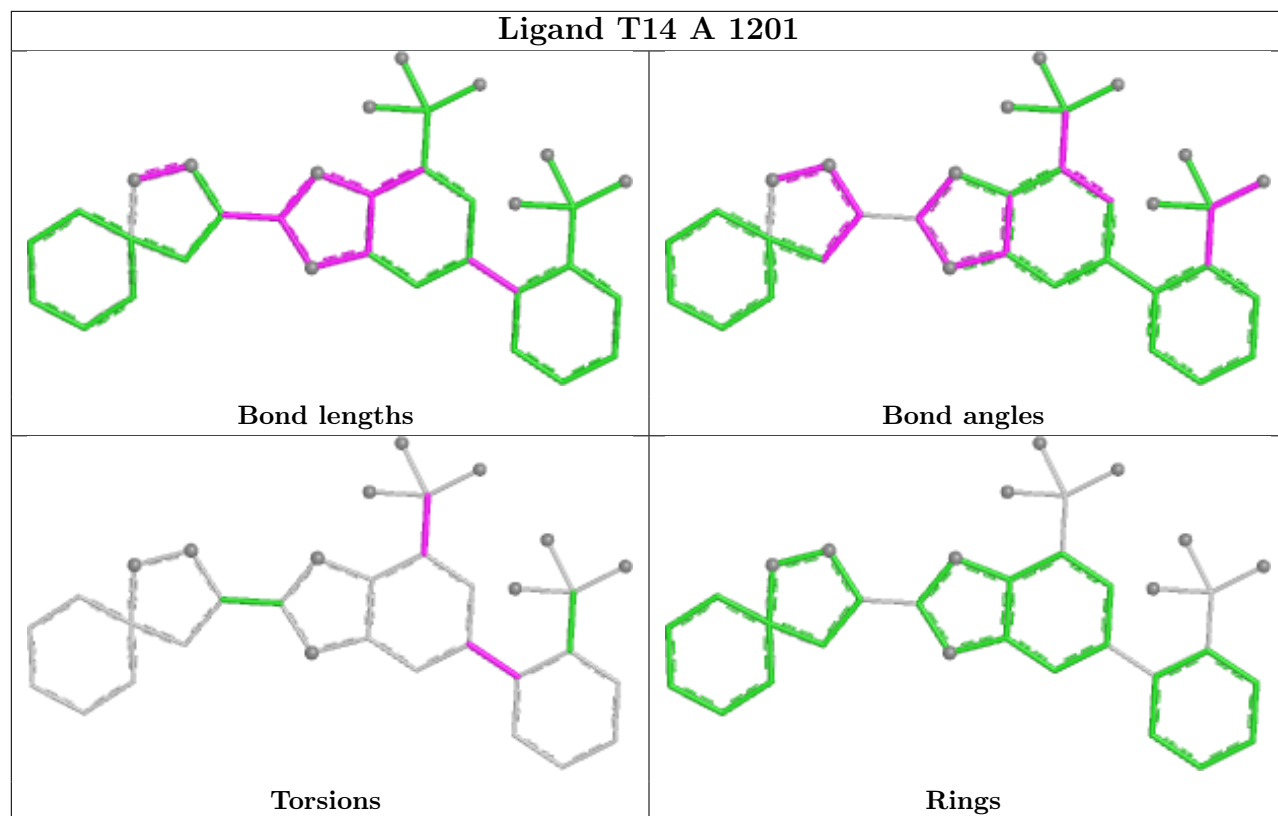
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1302	NAG	1	0
3	D	1202	Y01	5	0
3	B	1203	Y01	10	0
3	D	1204	Y01	12	0
3	C	1203	Y01	11	0
3	A	1202	Y01	7	0
5	B	1302	NAG	1	0
3	C	1204	Y01	12	0
3	A	1203	Y01	10	0
3	B	1202	Y01	4	0
3	D	1203	Y01	8	0
3	C	1202	Y01	6	0
3	B	1204	Y01	13	0
5	D	1302	NAG	1	0
3	A	1204	Y01	13	0
5	A	1302	NAG	1	0

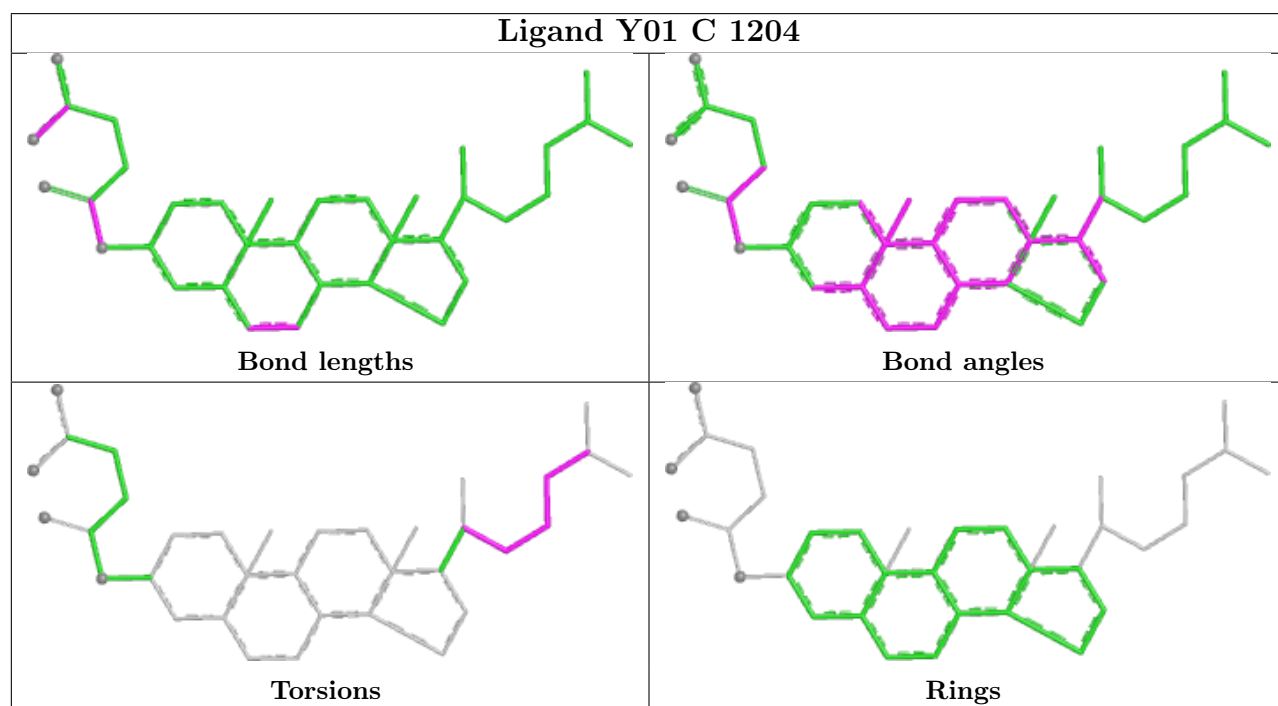
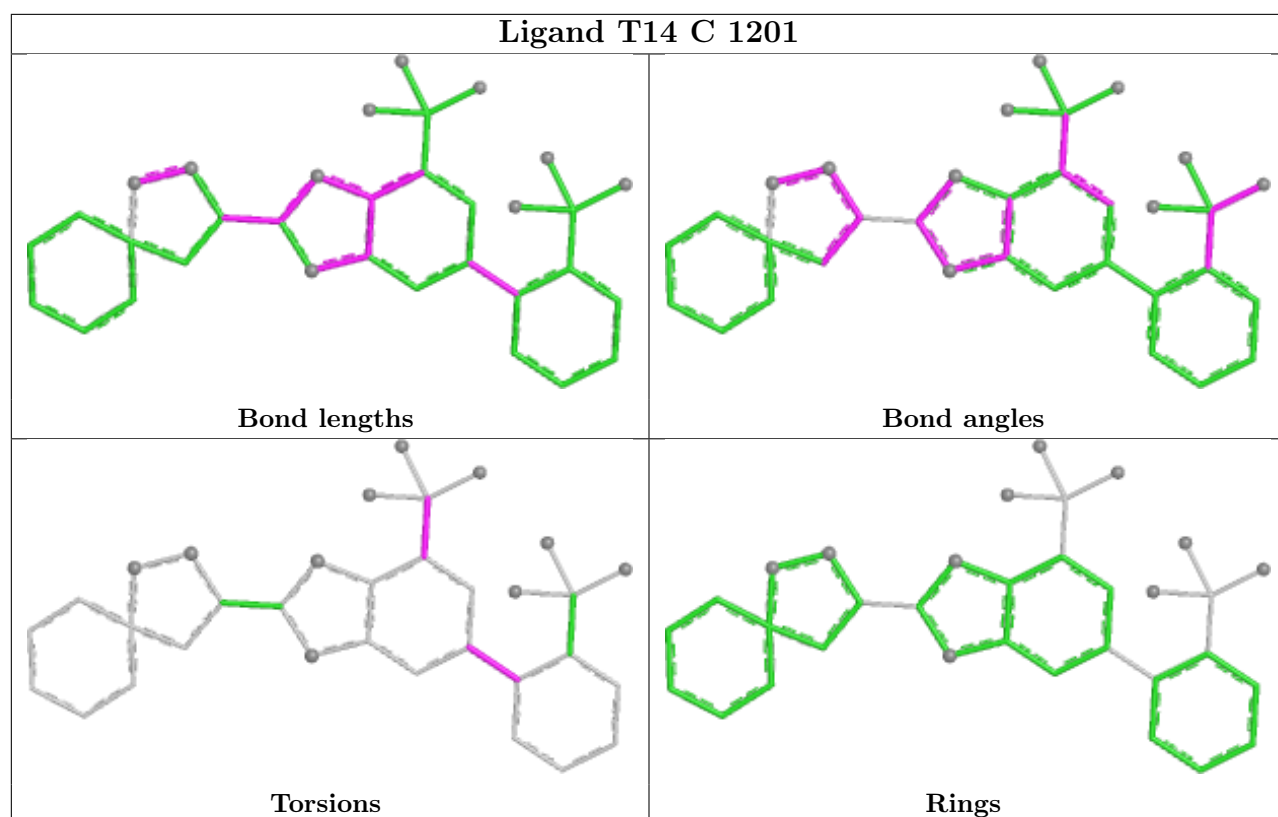
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

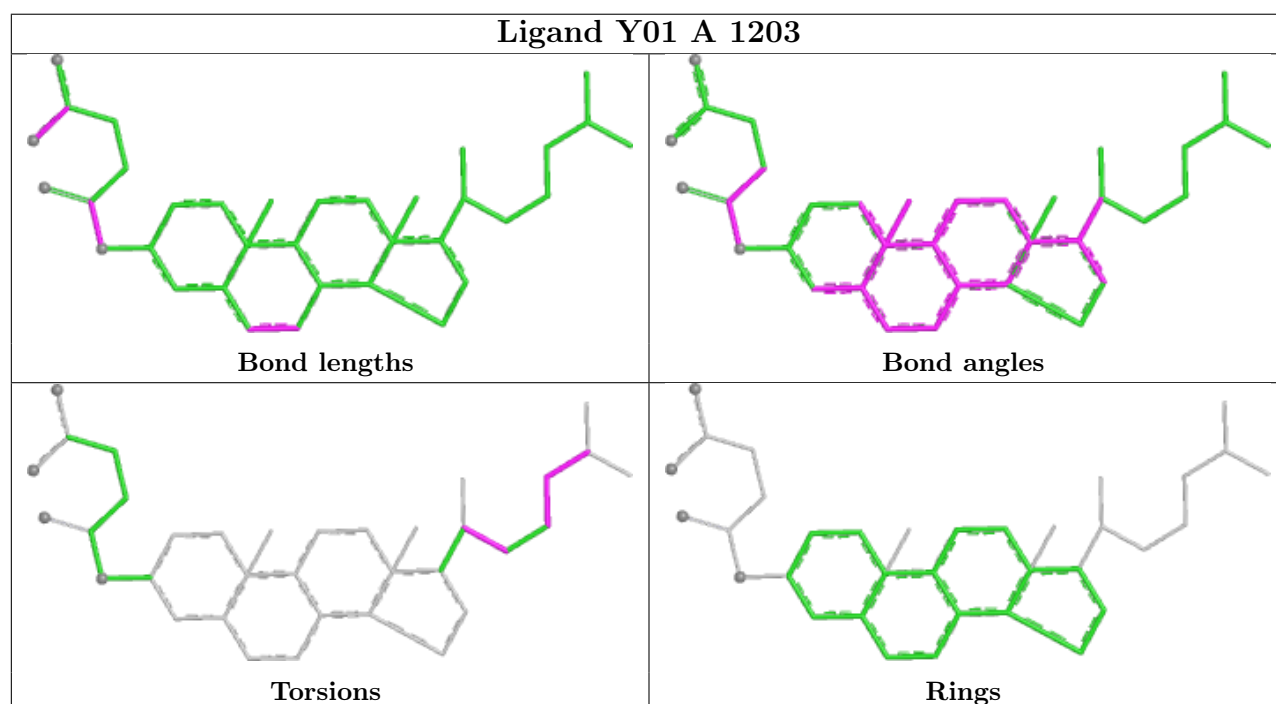
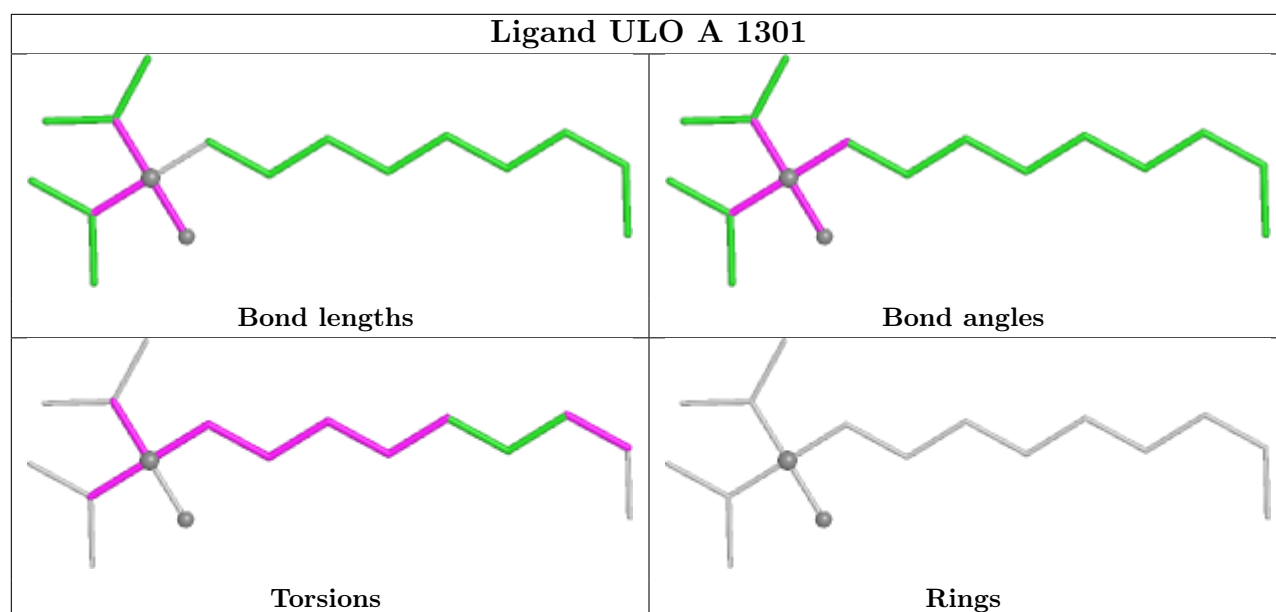


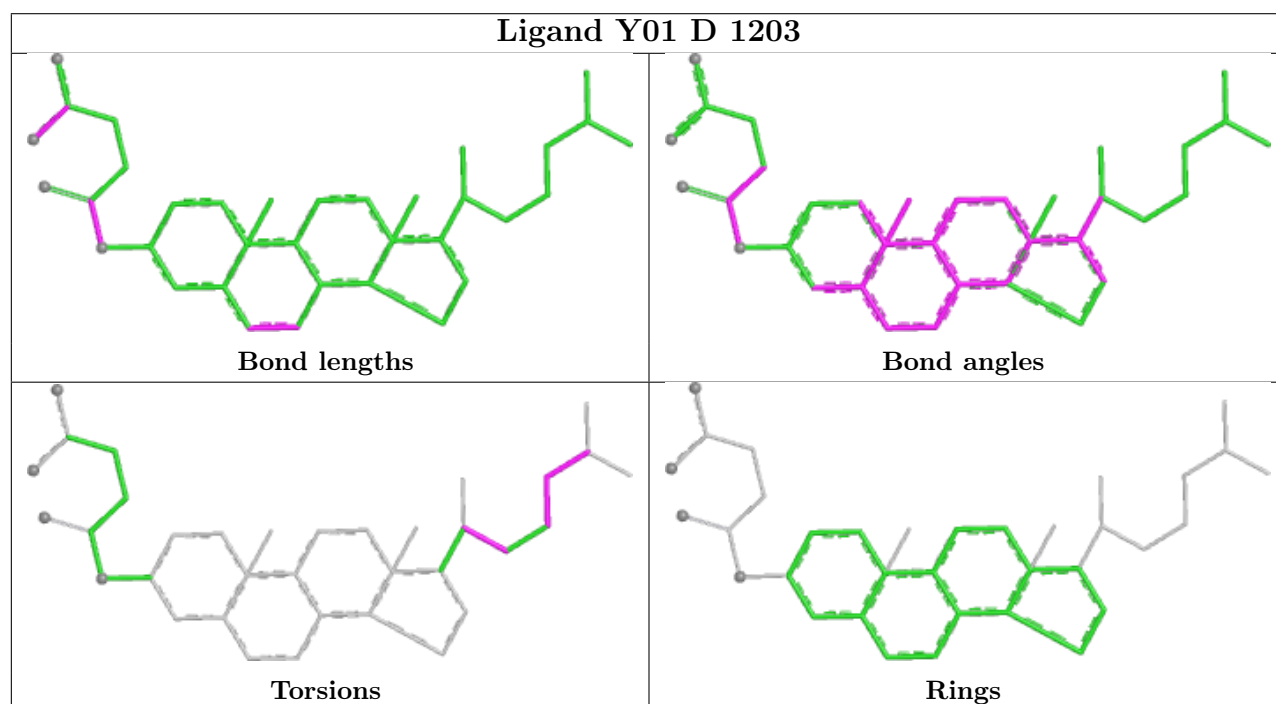
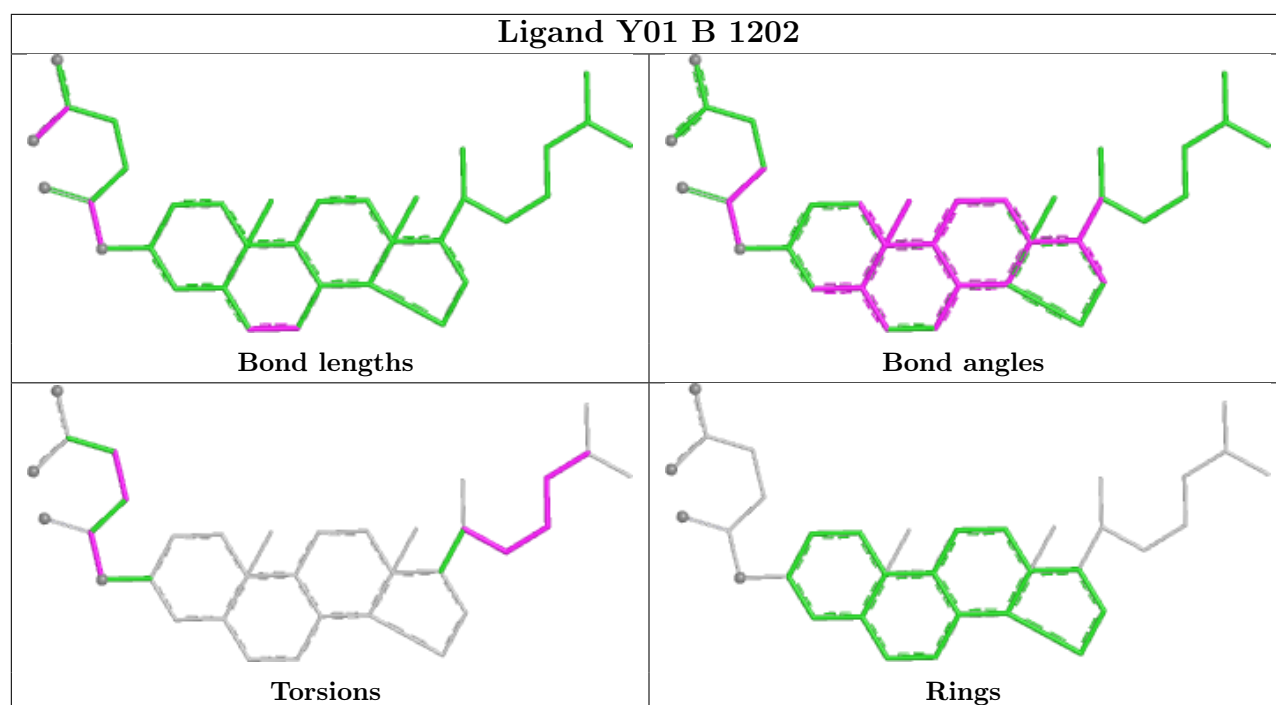


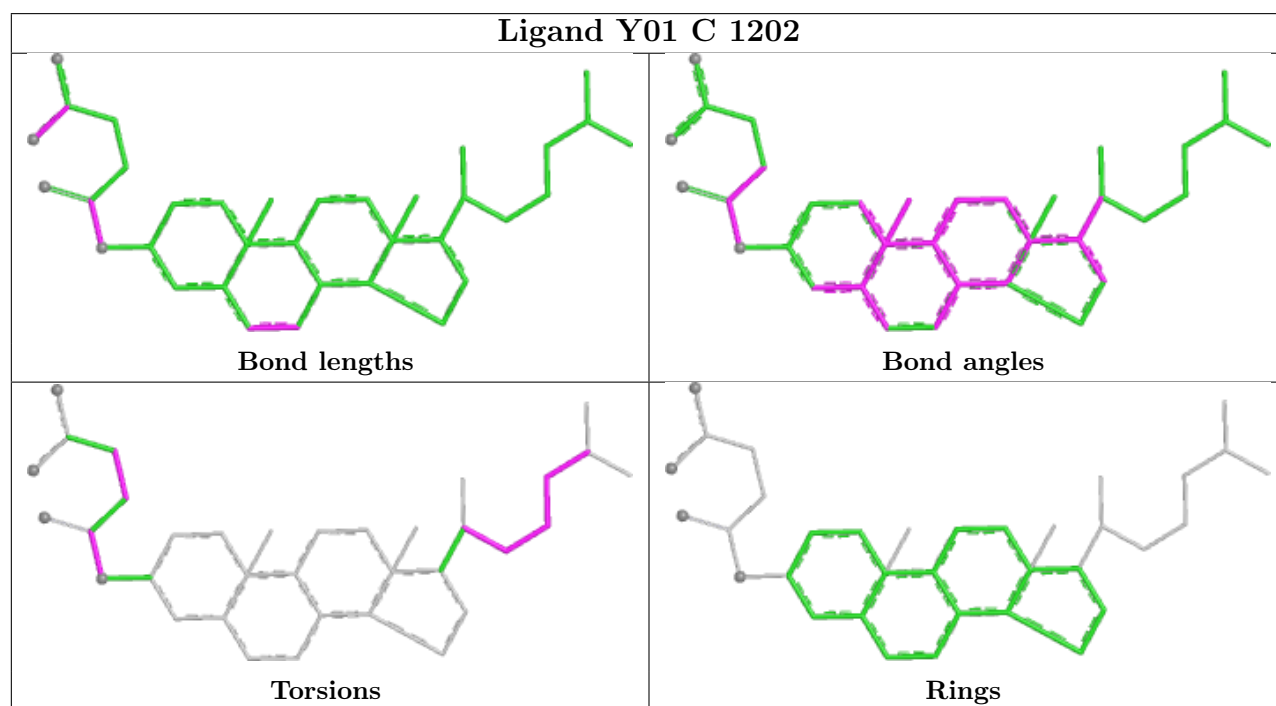
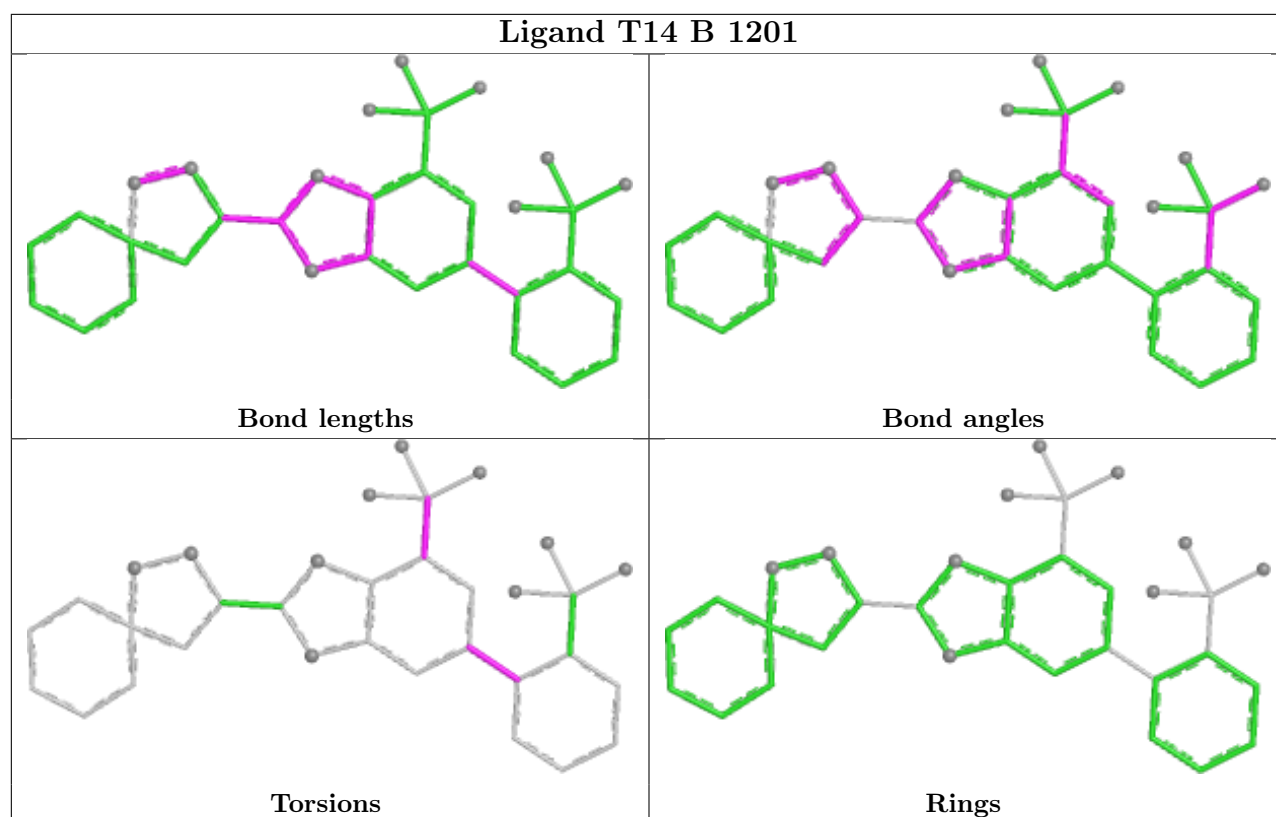


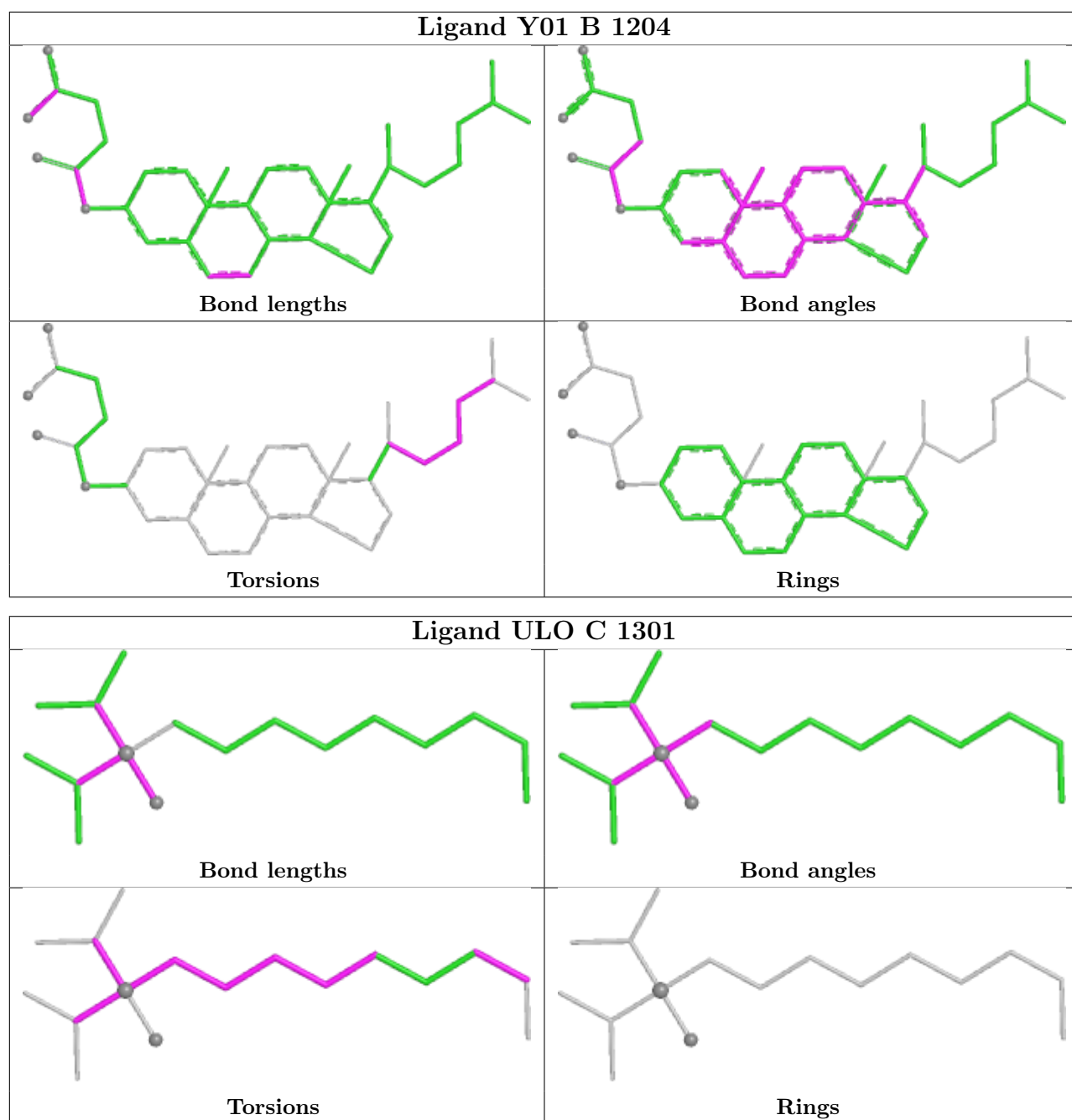


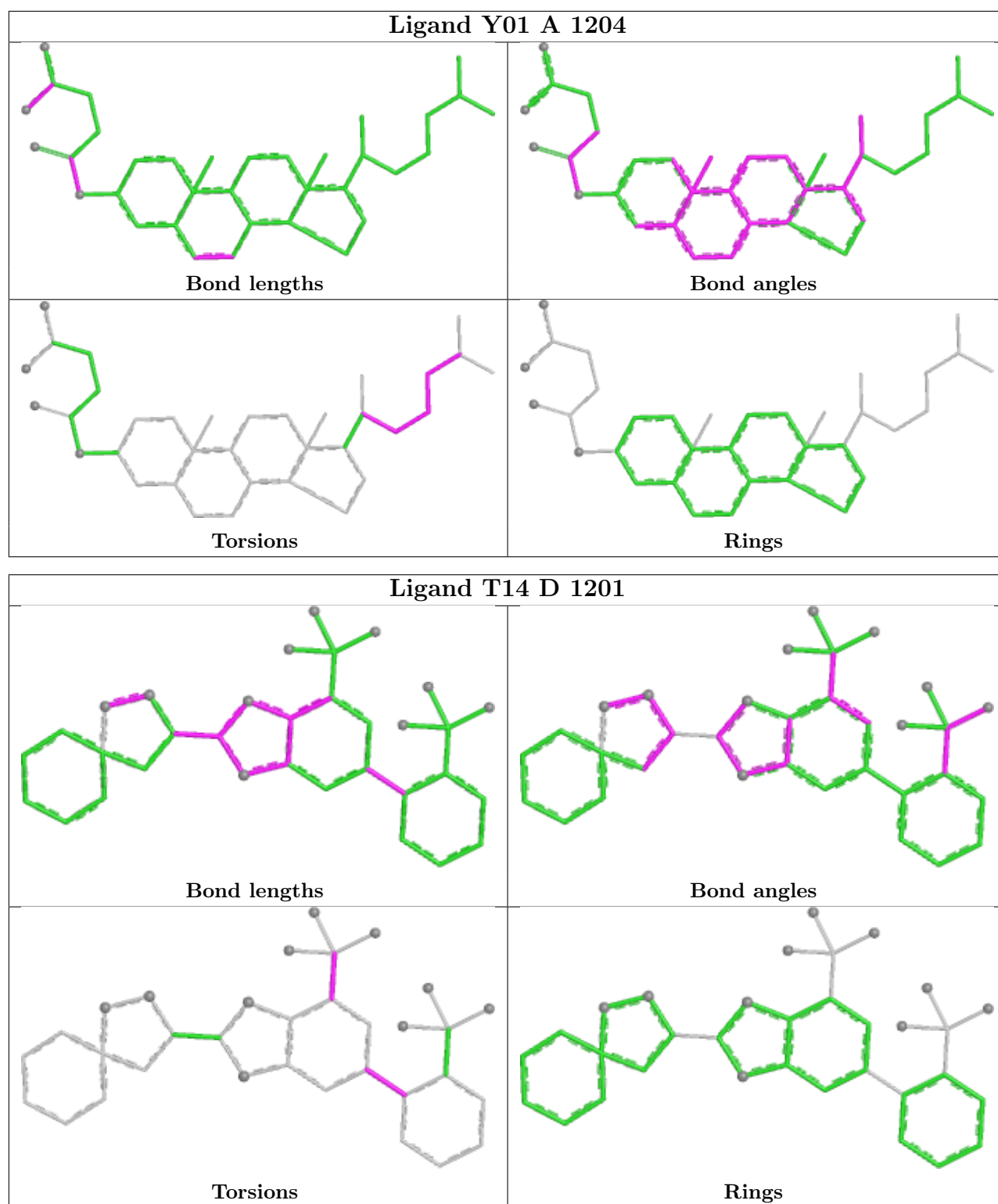












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

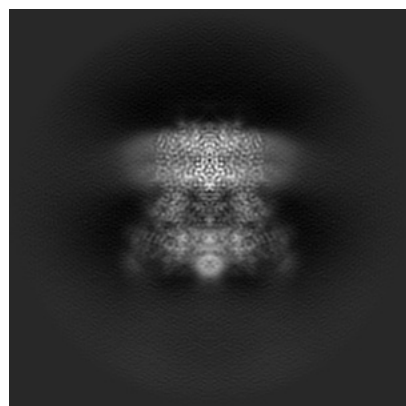
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44259. These allow visual inspection of the internal detail of the map and identification of artifacts.

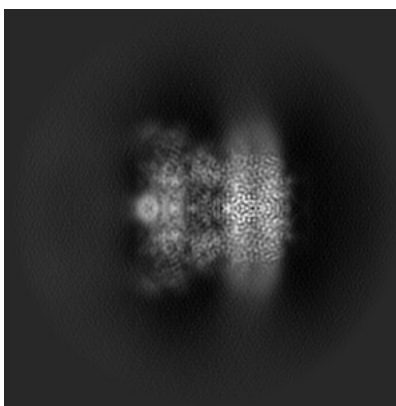
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

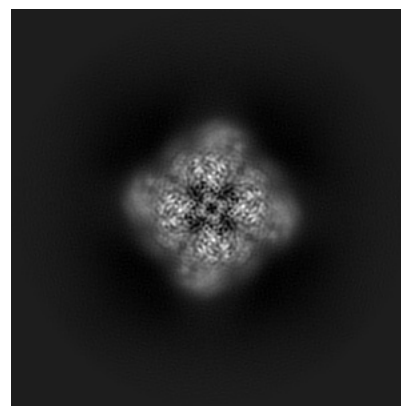
6.1.1 Primary map



X

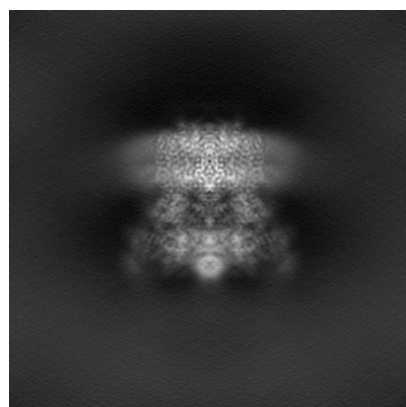


Y

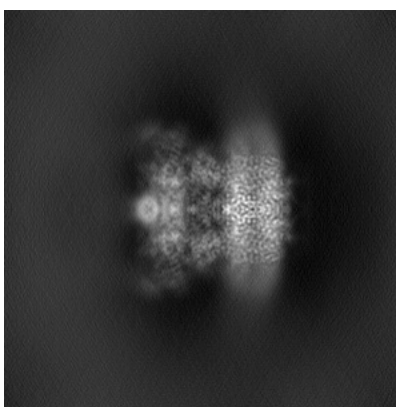


Z

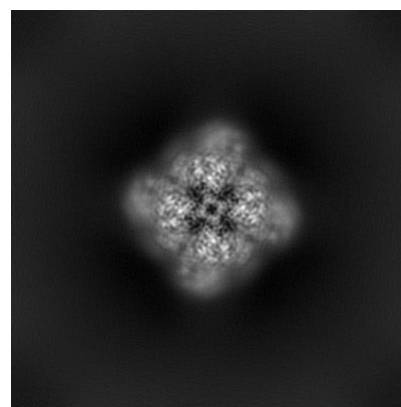
6.1.2 Raw map



X



Y

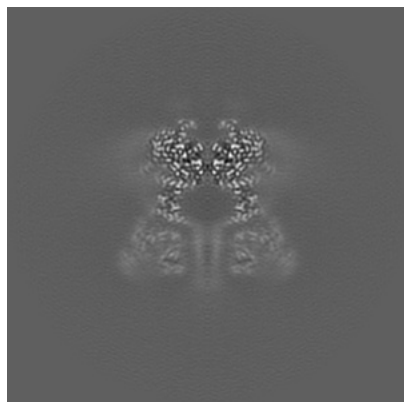


Z

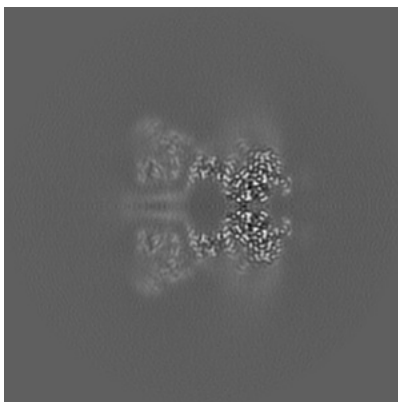
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

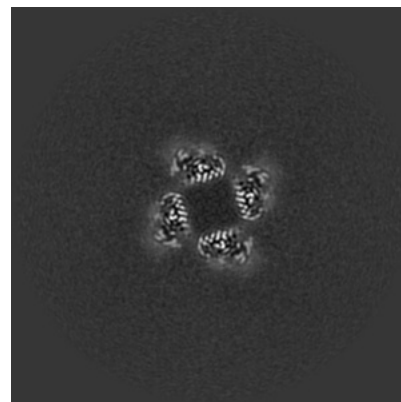
6.2.1 Primary map



X Index: 160

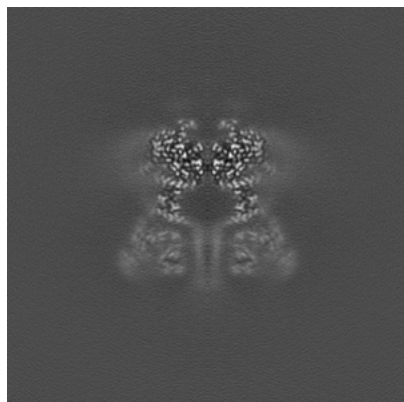


Y Index: 160

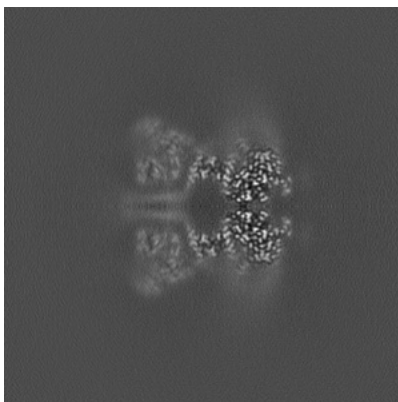


Z Index: 160

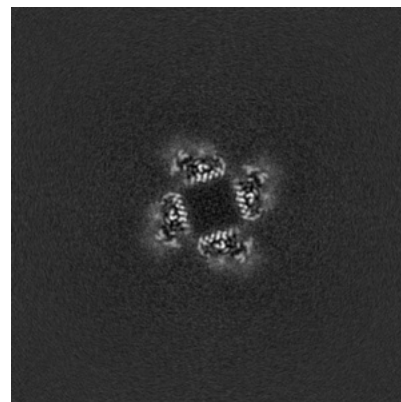
6.2.2 Raw map



X Index: 160



Y Index: 160

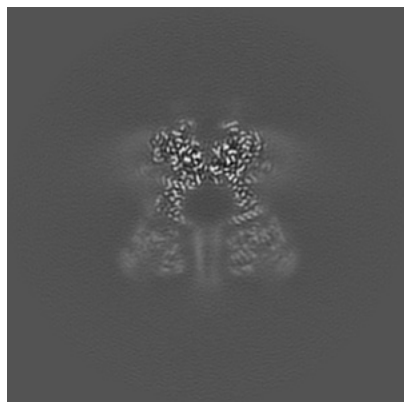


Z Index: 160

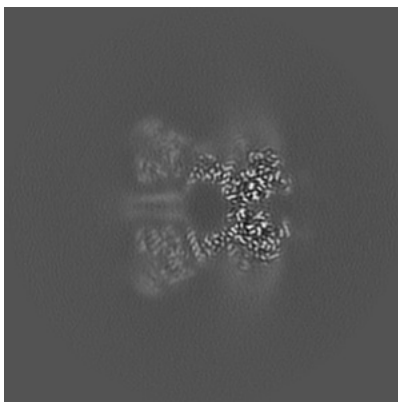
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

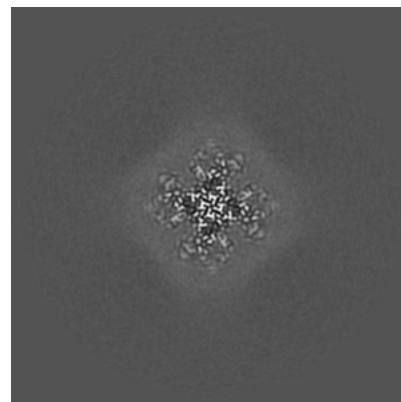
6.3.1 Primary map



X Index: 162

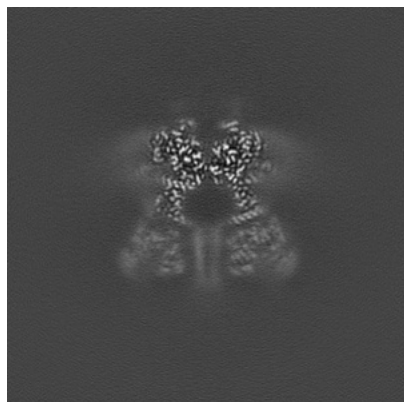


Y Index: 162

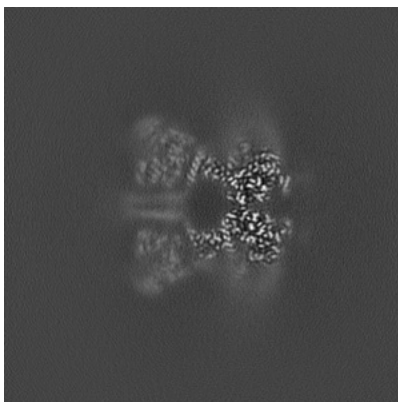


Z Index: 191

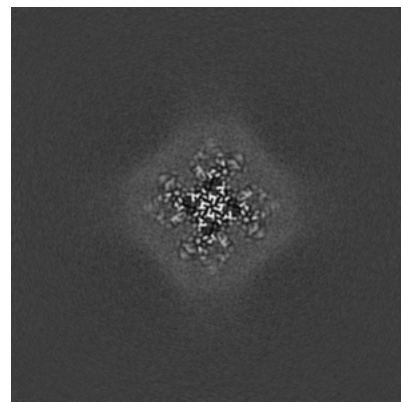
6.3.2 Raw map



X Index: 162



Y Index: 158

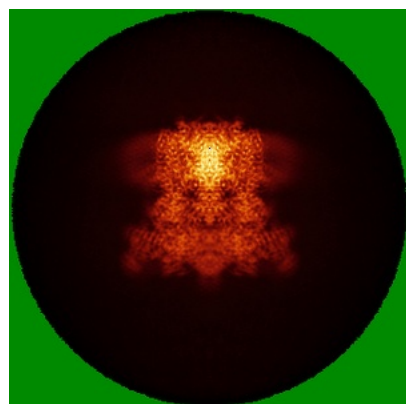


Z Index: 191

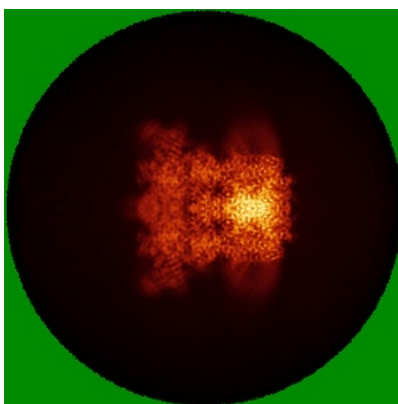
The images above show the largest variance slices of the map in three orthogonal directions.

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

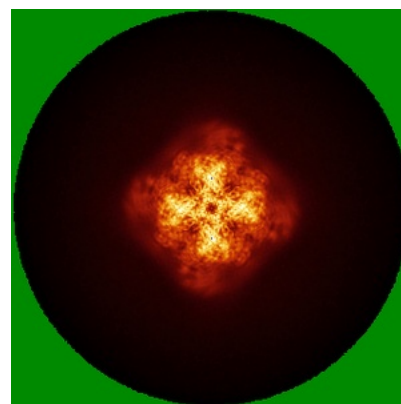
6.4.1 Primary map



X

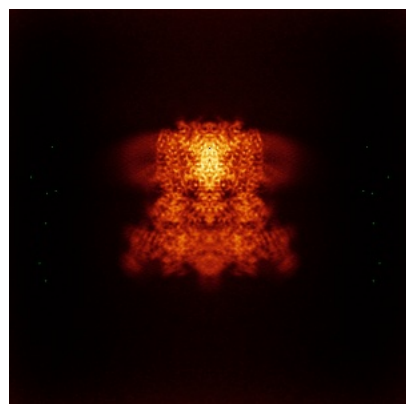


Y

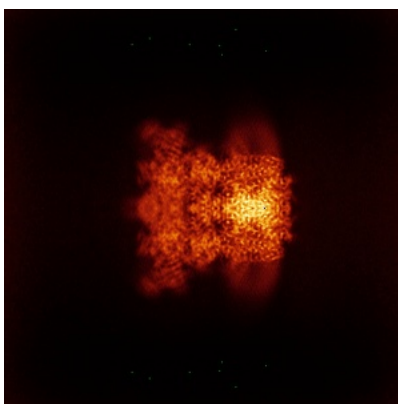


Z

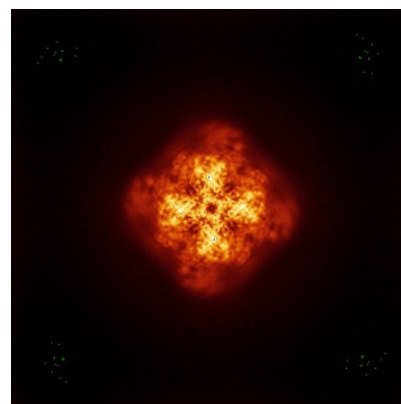
6.4.2 Raw map



X



Y

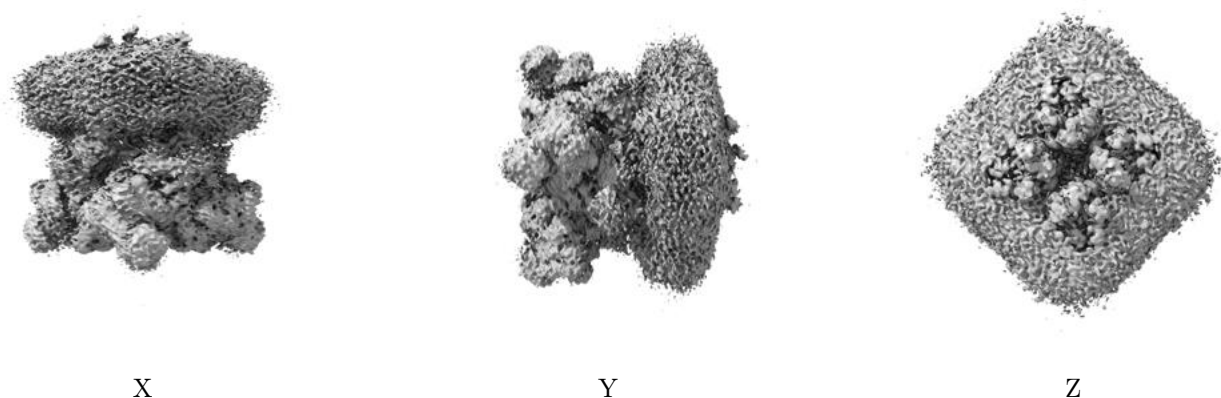


Z

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 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

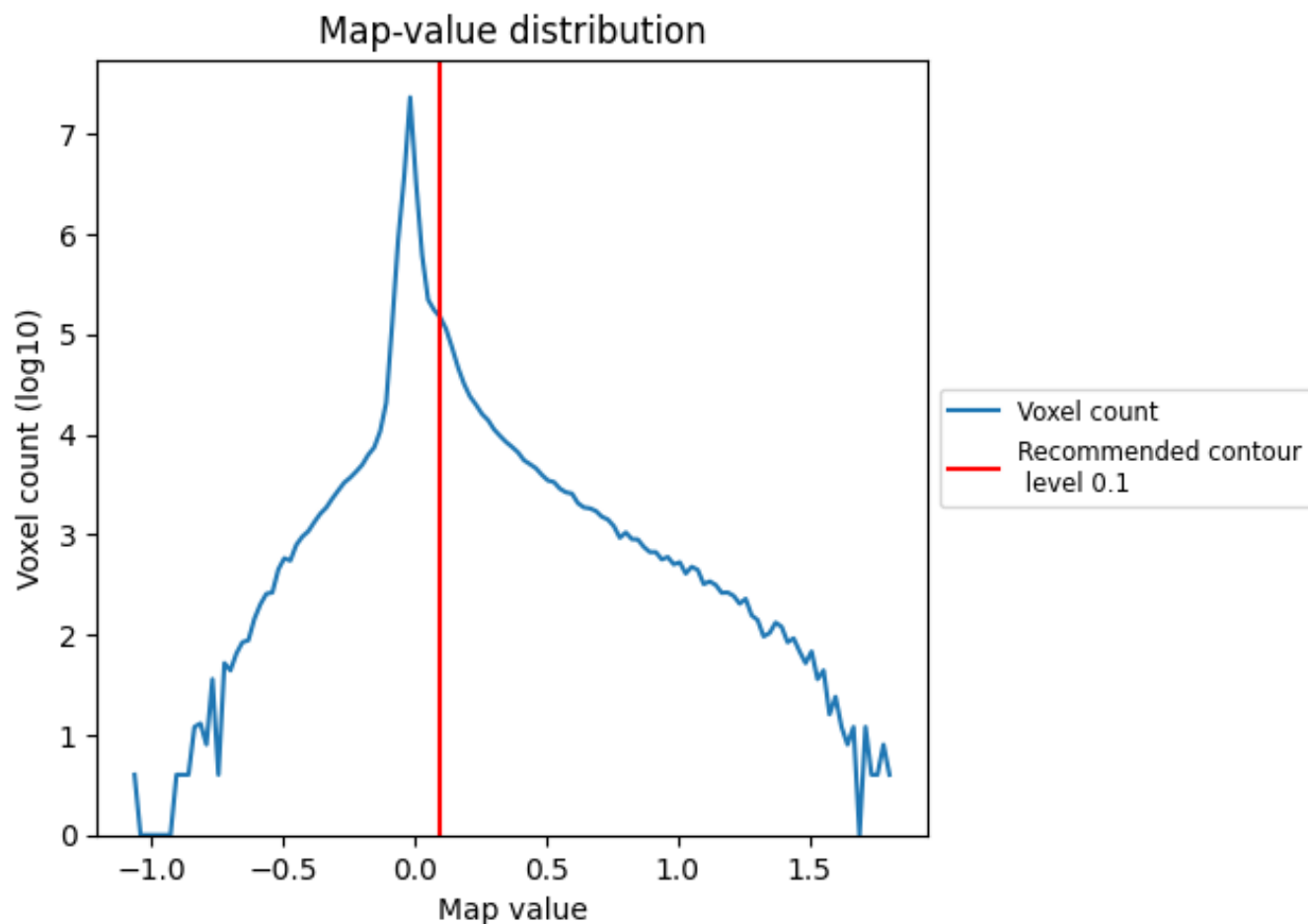
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

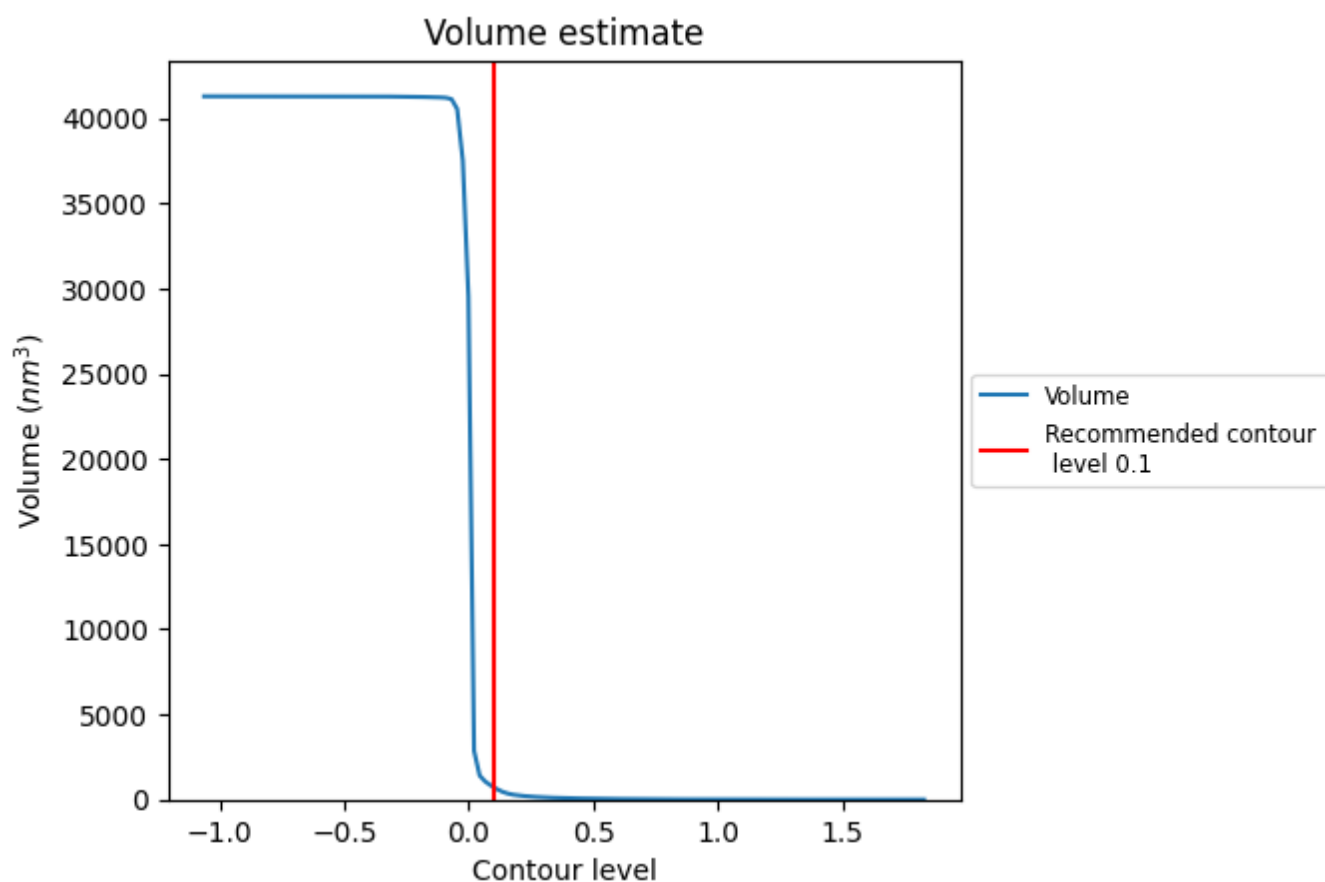
This section contains the results of statistical analysis of the map.

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.

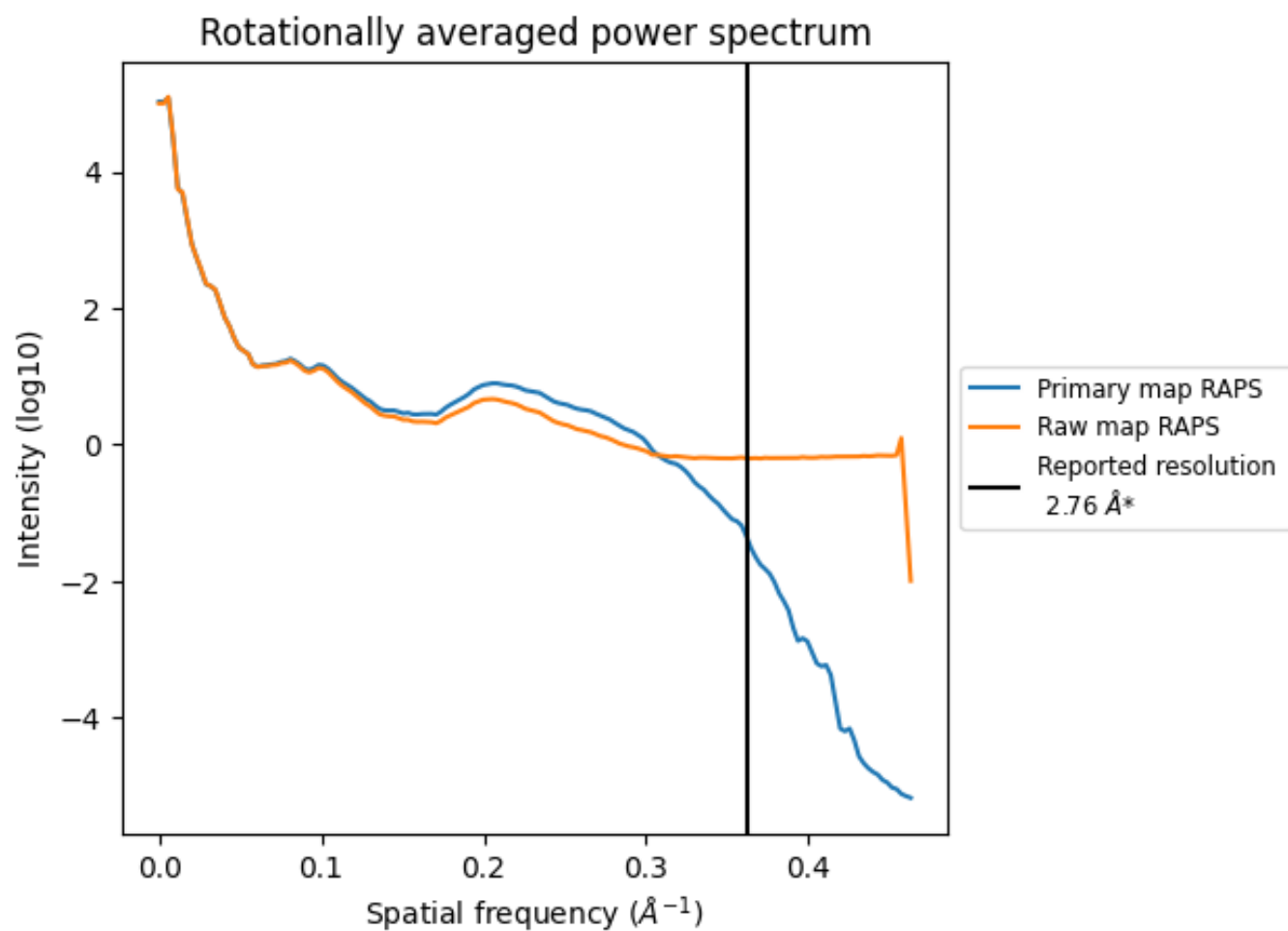
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 727 nm³; this corresponds to an approximate mass of 657 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 ⓘ

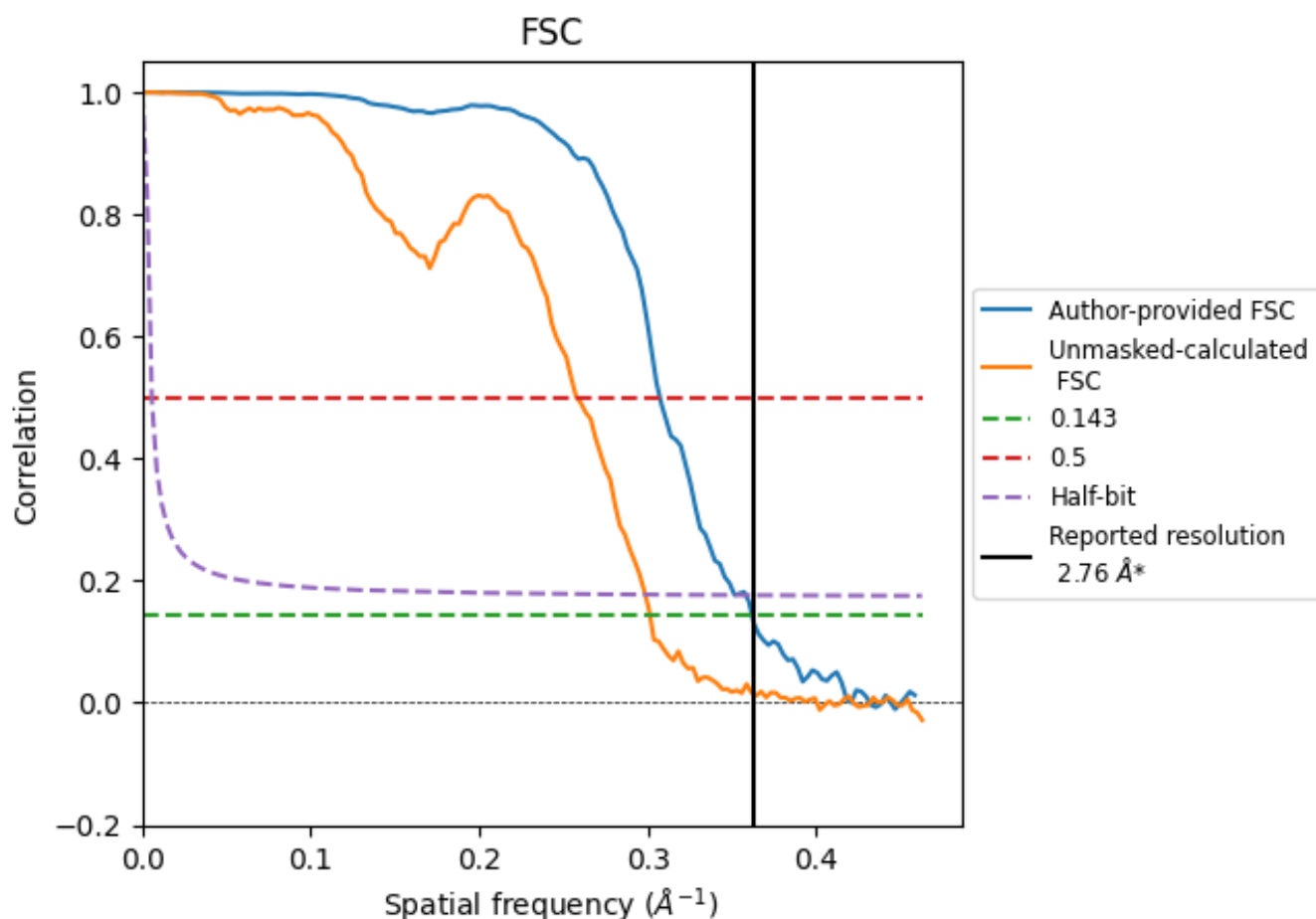


*Reported resolution corresponds to spatial frequency of 0.362 $\text{\AA}^{-1}$

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 0.362 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.76	-	-
Author-provided FSC curve	2.76	3.25	2.79
Unmasked-calculated*	3.32	3.87	3.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.32 differs from the reported value 2.76 by more than 10 %

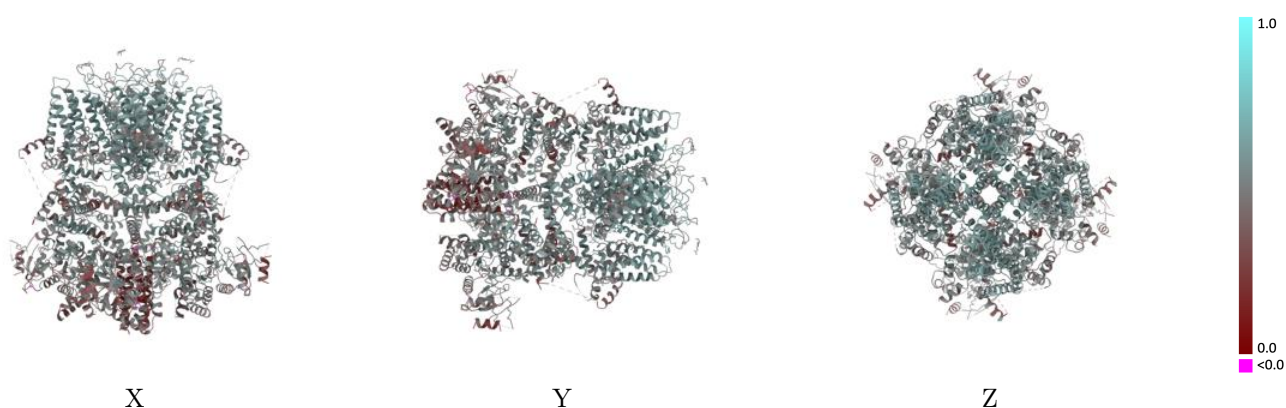
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-44259 and PDB model 9B6H. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)

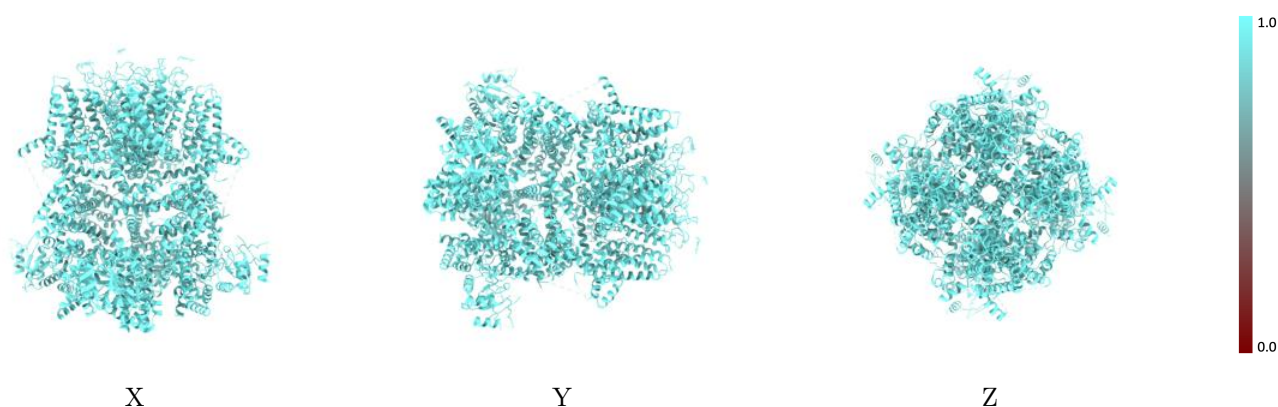
This section was not generated.

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



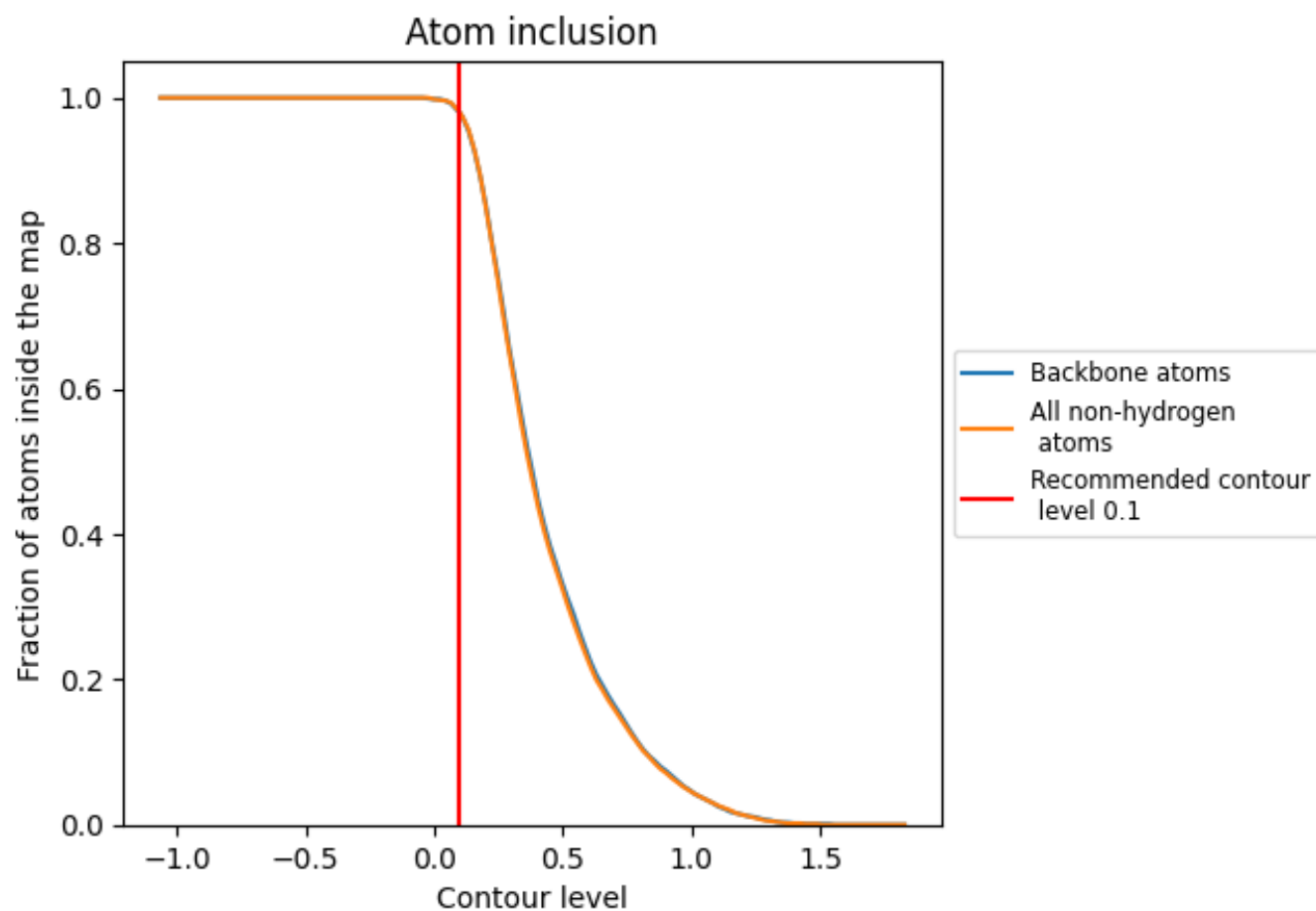
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9800	0.5020
A	0.9820	0.4990
B	0.9830	0.5040
C	0.9810	0.4970
D	0.9830	0.5060

