



Full wwPDB EM Validation Report ⓘ

Oct 26, 2024 – 04:00 PM EDT

PDB ID : 6BWI
EMDB ID : EMD-7299
Title : 3.7 angstrom cryoEM structure of full length human TRPM4
Authors : Zhang, J.; Li, Z.; Duan, J.; Li, J.; Clapham, D.E.
Deposited on : 2017-12-15
Resolution : 3.70 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

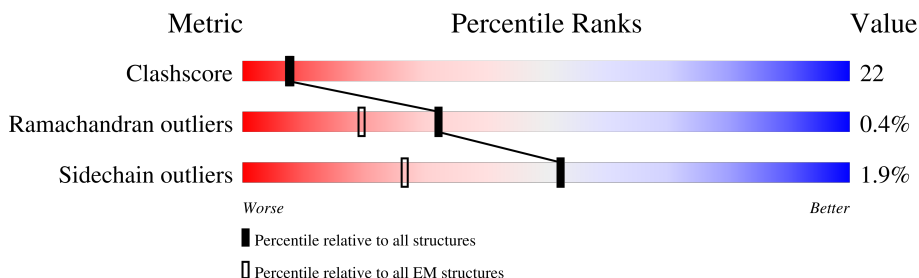
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	977	
1	B	977	
1	C	977	
1	D	977	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	Y01	A	1205	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	Y01	A	1206	-	-	X	-
3	Y01	A	1208	-	-	X	-
3	Y01	A	1209	-	-	X	-
3	Y01	B	1205	-	-	X	-
3	Y01	B	1207	-	-	X	-
3	Y01	C	1203	-	-	X	-
3	Y01	C	1205	-	-	X	-
3	Y01	D	1204	-	-	X	-
3	Y01	D	1205	-	-	X	-
3	Y01	D	1207	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23491 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.

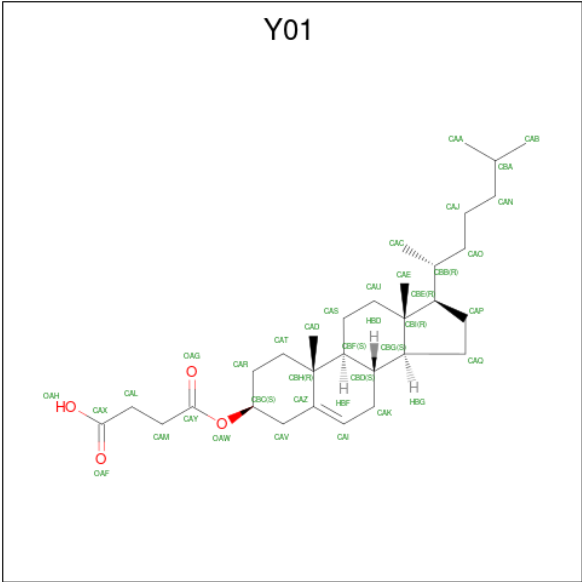
- Molecule 1 is a protein called Transient receptor potential cation channel subfamily M member 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	816	Total	C	N	O	S	0	0
			5649	3635	1016	975	23		
1	B	816	Total	C	N	O	S	0	0
			5644	3632	1014	975	23		
1	C	816	Total	C	N	O	S	0	0
			5644	3632	1014	975	23		
1	D	816	Total	C	N	O	S	0	0
			5649	3635	1016	975	23		

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
2	A	3	Total	Na	0
			3	3	
2	B	2	Total	Na	0
			2	2	

- Molecule 3 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C₃₁H₅₀O₄).



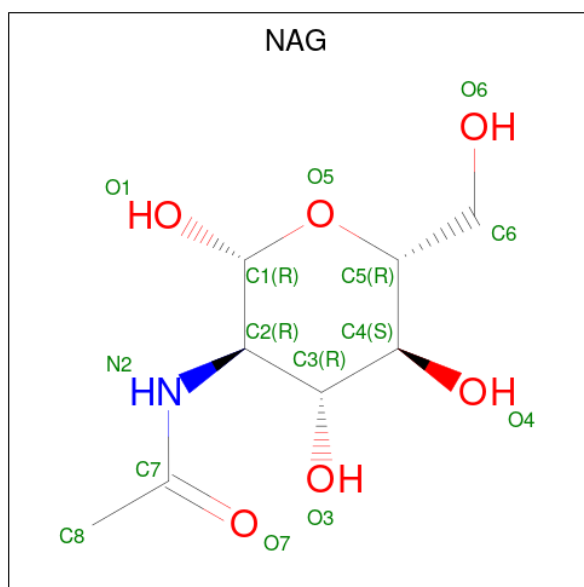
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	B	1	Total	C	O	0
			35	31	4	
3	B	1	Total	C	O	0
			35	31	4	
3	B	1	Total	C	O	0
			35	31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

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Mol	Chain	Residues	Atoms			AltConf
3	C	1	Total	C	O	0
			35	31	4	
3	C	1	Total	C	O	0
			35	31	4	
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	
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 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			15	8	1	6	

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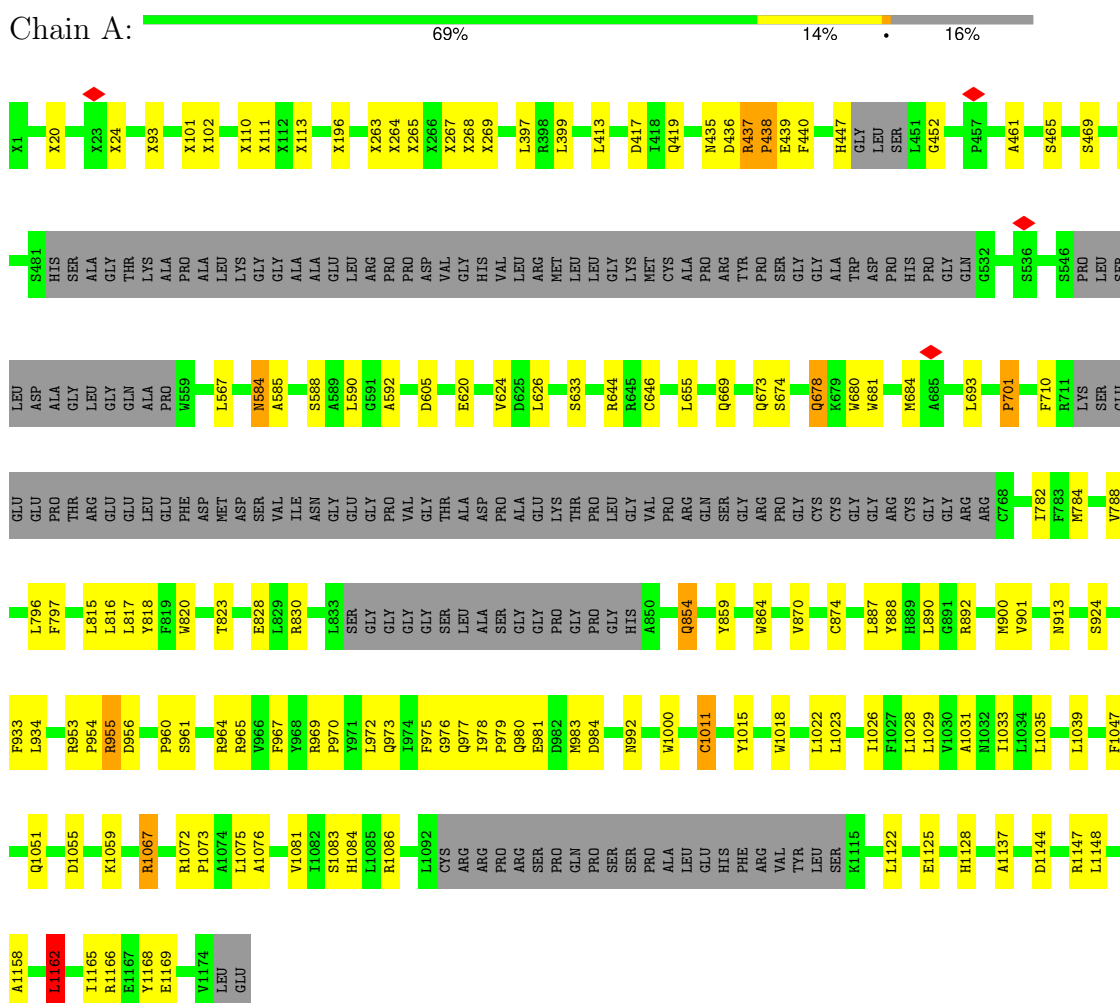
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Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			15	8	1	6	
4	C	1	Total	C	N	O	0
			15	8	1	6	
4	D	1	Total	C	N	O	0
			15	8	1	6	

3 Residue-property plots

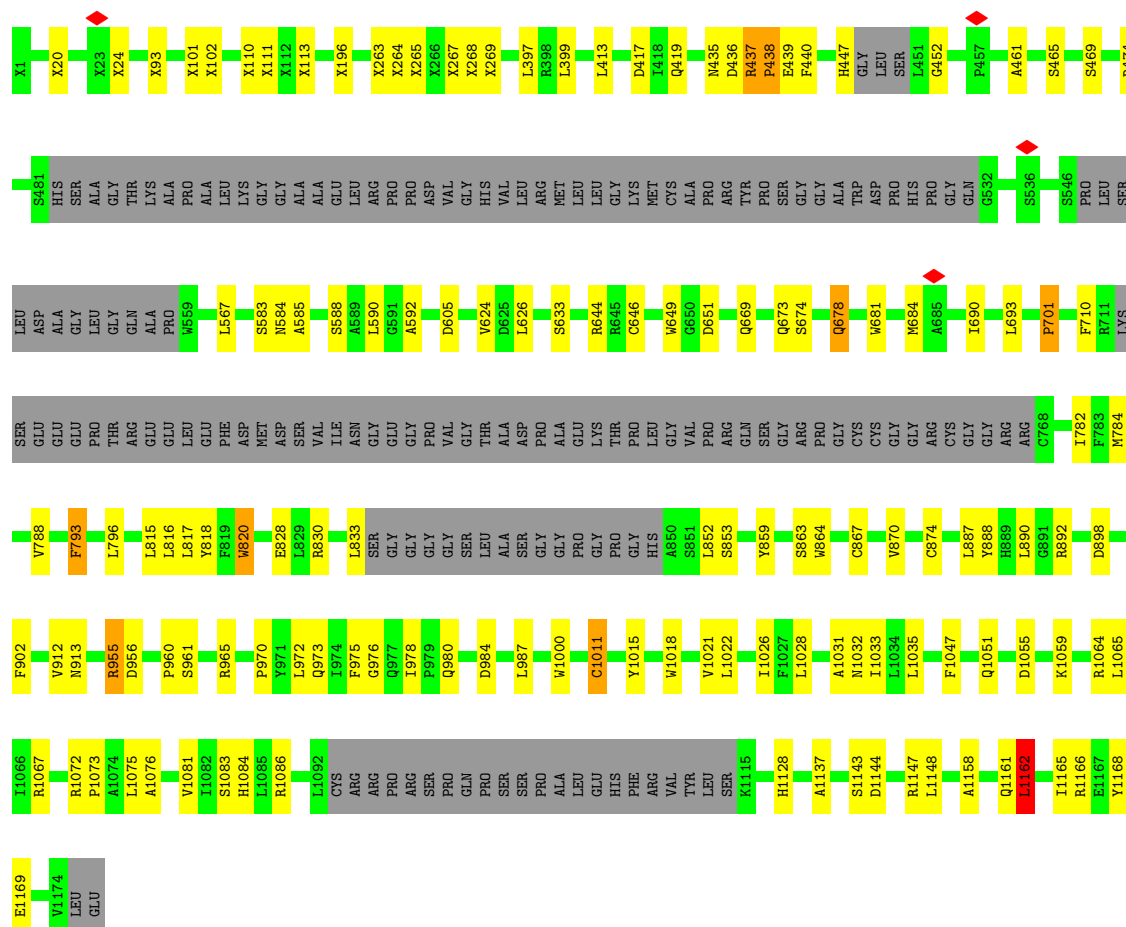
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 4



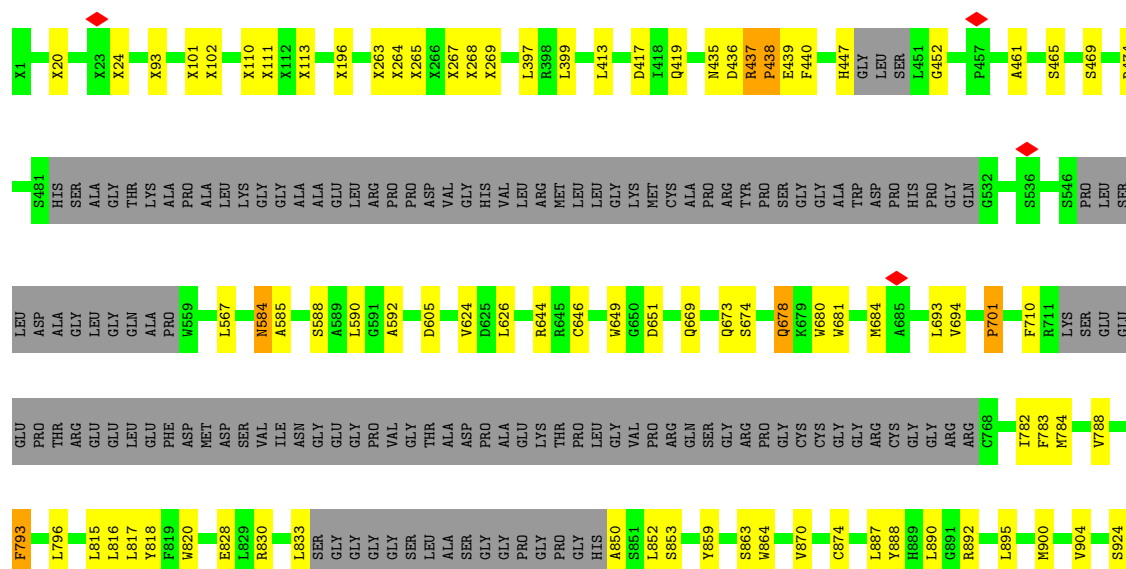
- Molecule 1: Transient receptor potential cation channel subfamily M member 4

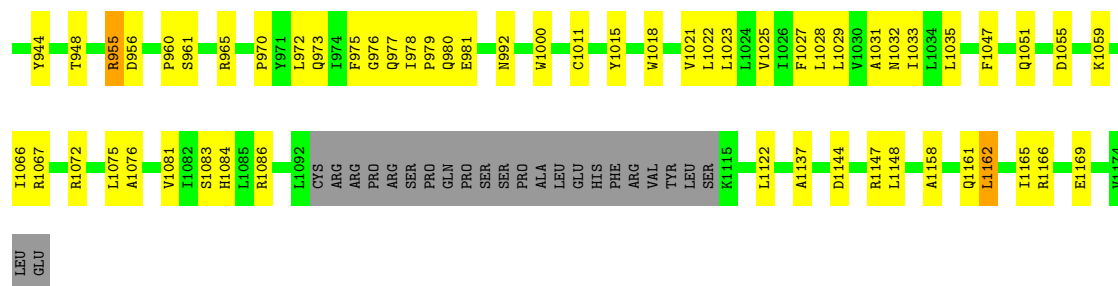




- Molecule 1: Transient receptor potential cation channel subfamily M member 4

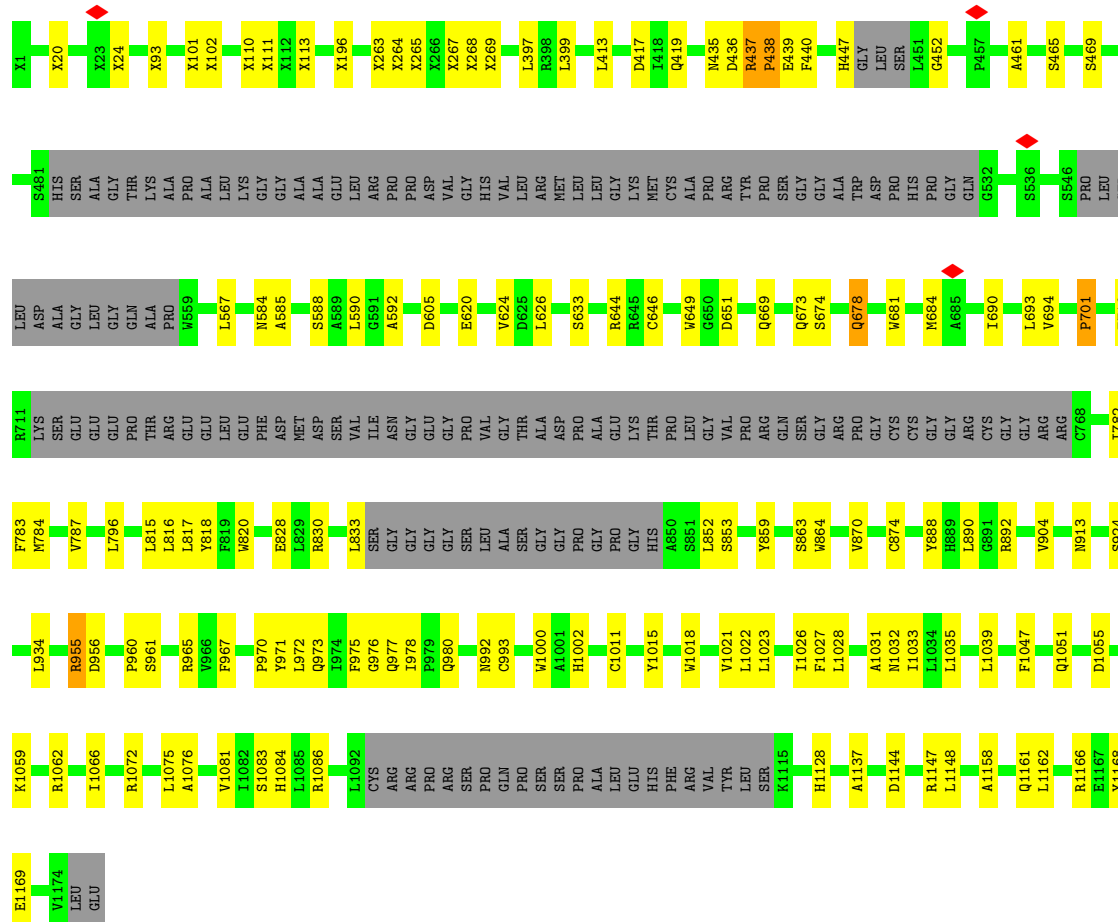
Chain C: 69% 14% 16%





- Molecule 1: Transient receptor potential cation channel subfamily M member 4

Chain D: 69% 14% 16%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	232930	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.195	Depositor
Minimum map value	-0.132	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.013	Depositor
Map size (\AA)	314.88, 314.88, 314.88	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.23, 1.23, 1.23	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: NA, Y01, NAG

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	0.50	2/4784 (0.0%)	0.70	10/6512 (0.2%)
1	B	0.50	3/4778 (0.1%)	0.68	8/6504 (0.1%)
1	C	0.43	0/4778	0.66	5/6504 (0.1%)
1	D	0.45	2/4784 (0.0%)	0.67	5/6512 (0.1%)
All	All	0.47	7/19124 (0.0%)	0.68	28/26032 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
1	C	0	4
1	D	0	4
All	All	0	17

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1162	LEU	C-N	14.55	1.59	1.33
1	B	1162	LEU	C-N	12.97	1.56	1.33
1	B	1169	GLU	C-N	11.05	1.59	1.34
1	A	1169	GLU	C-N	8.95	1.54	1.34
1	D	1169	GLU	C-N	8.29	1.53	1.34
1	D	1168	TYR	C-N	5.52	1.46	1.34
1	B	1168	TYR	C-N	5.31	1.46	1.34

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	438	PRO	CA-N-CD	-8.78	99.21	111.50
1	B	438	PRO	CA-N-CD	-8.77	99.22	111.50
1	D	438	PRO	CA-N-CD	-8.75	99.25	111.50
1	C	438	PRO	CA-N-CD	-8.74	99.26	111.50
1	C	701	PRO	N-CA-CB	8.63	113.65	103.30
1	D	701	PRO	N-CA-CB	8.62	113.64	103.30
1	A	701	PRO	N-CA-CB	8.62	113.64	103.30
1	B	701	PRO	N-CA-CB	8.60	113.61	103.30
1	A	1162	LEU	O-C-N	-8.40	108.93	123.20
1	A	1168	TYR	O-C-N	-7.78	110.25	122.70
1	A	1162	LEU	C-N-CA	7.40	137.85	122.30
1	A	1162	LEU	CA-C-N	7.29	130.77	116.20
1	B	1168	TYR	O-C-N	-7.22	111.15	122.70
1	D	590	LEU	CA-CB-CG	6.18	129.51	115.30
1	A	590	LEU	CA-CB-CG	6.17	129.50	115.30
1	C	590	LEU	CA-CB-CG	6.17	129.49	115.30
1	B	590	LEU	CA-CB-CG	6.16	129.46	115.30
1	B	1162	LEU	O-C-N	-5.89	113.19	123.20
1	A	1144	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	1168	TYR	CA-C-N	5.21	128.65	117.20
1	B	1144	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	1144	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	399	LEU	CA-CB-CG	5.17	127.18	115.30
1	D	1144	ASP	CB-CG-OD2	5.16	122.94	118.30
1	C	399	LEU	CA-CB-CG	5.15	127.15	115.30
1	D	399	LEU	CA-CB-CG	5.15	127.14	115.30
1	B	399	LEU	CA-CB-CG	5.15	127.14	115.30
1	B	1162	LEU	CA-C-N	5.00	126.21	116.20

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1067	ARG	Sidechain
1	A	1137	ALA	Peptide
1	A	435	ASN	Peptide
1	A	567	LEU	Peptide
1	A	93	UNK	Peptide
1	B	1137	ALA	Peptide
1	B	435	ASN	Peptide
1	B	567	LEU	Peptide
1	B	93	UNK	Peptide
1	C	1137	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	C	435	ASN	Peptide
1	C	567	LEU	Peptide
1	C	93	UNK	Peptide
1	D	1137	ALA	Peptide
1	D	435	ASN	Peptide
1	D	567	LEU	Peptide
1	D	93	UNK	Peptide

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	5649	0	4713	196	0
1	B	5644	0	4707	186	0
1	C	5644	0	4709	202	0
1	D	5649	0	4713	168	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
3	A	210	0	294	145	0
3	B	210	0	294	100	0
3	C	175	0	245	107	0
3	D	245	0	343	152	0
4	A	15	0	14	5	0
4	B	15	0	14	0	0
4	C	15	0	15	3	0
4	D	15	0	15	4	0
All	All	23491	0	20076	976	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 22.

All (976) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:864:TRP:CZ3	3:C:1205:Y01:HAI	1.25	1.66
1:B:864:TRP:CZ3	3:B:1207:Y01:HAT2	1.22	1.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:864:TRP:HE3	3:B:1207:Y01:CAR	1.21	1.53
1:C:864:TRP:CH2	3:C:1205:Y01:HAI	1.45	1.49
1:B:864:TRP:CE3	3:B:1207:Y01:CAR	1.98	1.47
1:A:436:ASP:C	1:A:438:PRO:HD3	1.36	1.46
1:A:864:TRP:CZ3	3:A:1208:Y01:HAT2	1.52	1.45
1:B:864:TRP:CZ3	3:B:1207:Y01:CAT	1.97	1.44
1:C:436:ASP:C	1:C:438:PRO:HD3	1.36	1.44
1:D:436:ASP:C	1:D:438:PRO:HD3	1.36	1.43
1:B:436:ASP:C	1:B:438:PRO:HD3	1.36	1.41
1:C:864:TRP:CE3	3:C:1205:Y01:HAV2	1.55	1.39
1:C:864:TRP:CZ3	3:C:1205:Y01:CAI	2.07	1.38
1:B:1015:TYR:OH	3:B:1205:Y01:CAT	1.79	1.30
1:C:1161:GLN:NE2	1:D:1162:LEU:HB3	1.46	1.29
1:A:1029:LEU:HD13	3:A:1206:Y01:CAB	1.66	1.25
3:A:1205:Y01:CAS	1:D:890:LEU:HD11	1.66	1.24
1:A:864:TRP:CE3	3:A:1208:Y01:CAR	2.22	1.23
1:A:864:TRP:HE3	3:A:1208:Y01:CAR	1.52	1.23
1:B:1015:TYR:OH	3:B:1205:Y01:HAT2	1.06	1.22
1:A:864:TRP:CZ3	3:A:1208:Y01:CAT	2.26	1.17
1:A:1015:TYR:OH	3:A:1205:Y01:HAD2	1.42	1.17
1:A:1029:LEU:HD13	3:A:1206:Y01:HAB2	1.21	1.17
1:B:864:TRP:CE3	3:B:1207:Y01:CAT	2.25	1.17
1:B:864:TRP:CE3	3:B:1207:Y01:HAT2	1.78	1.17
1:A:1015:TYR:OH	3:A:1205:Y01:CAD	1.94	1.16
1:A:436:ASP:CB	1:A:438:PRO:HG3	1.76	1.16
1:C:436:ASP:CB	1:C:438:PRO:HG3	1.76	1.15
1:B:436:ASP:CB	1:B:438:PRO:HG3	1.76	1.15
1:B:436:ASP:CA	1:B:438:PRO:HD3	1.78	1.14
1:B:864:TRP:HE3	3:B:1207:Y01:HAR2	1.09	1.14
1:A:436:ASP:CA	1:A:438:PRO:HD3	1.77	1.14
1:D:436:ASP:CB	1:D:438:PRO:HG3	1.76	1.14
1:C:864:TRP:CZ3	3:C:1205:Y01:HAV2	1.83	1.14
1:D:436:ASP:CA	1:D:438:PRO:HD3	1.77	1.13
3:C:1201:Y01:HAO2	3:C:1201:Y01:HAA1	1.24	1.12
1:C:436:ASP:CA	1:C:438:PRO:HD3	1.78	1.12
1:B:864:TRP:CE3	3:B:1207:Y01:HAR1	1.74	1.11
3:B:1204:Y01:HAQ2	1:C:1021:VAL:CG1	1.81	1.10
1:C:904:VAL:HG11	3:C:1205:Y01:HAQ1	1.22	1.09
3:A:1205:Y01:HAS1	1:D:890:LEU:HD11	1.13	1.09
1:A:864:TRP:CE3	3:A:1208:Y01:HAR1	1.87	1.08
1:B:436:ASP:C	1:B:438:PRO:CD	2.22	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:ASP:C	1:D:438:PRO:CD	2.22	1.08
1:A:864:TRP:HE3	3:A:1208:Y01:HAR1	1.15	1.08
1:B:890:LEU:HD11	3:C:1203:Y01:CAU	1.84	1.07
1:C:436:ASP:C	1:C:438:PRO:CD	2.22	1.07
1:C:436:ASP:CB	1:C:438:PRO:HD3	1.84	1.07
3:D:1207:Y01:HAN1	3:D:1207:Y01:HAC3	1.32	1.07
1:A:436:ASP:C	1:A:438:PRO:CD	2.22	1.06
1:A:854:GLN:HE21	1:A:854:GLN:HA	1.17	1.06
1:B:864:TRP:HZ3	3:B:1207:Y01:CAT	1.49	1.06
1:D:436:ASP:CB	1:D:438:PRO:HD3	1.84	1.06
3:D:1207:Y01:HAA2	3:D:1207:Y01:HAO2	1.37	1.06
1:A:436:ASP:CB	1:A:438:PRO:HD3	1.84	1.05
1:C:436:ASP:CB	1:C:438:PRO:CG	2.34	1.05
1:B:436:ASP:CB	1:B:438:PRO:HD3	1.84	1.05
1:C:864:TRP:CZ3	3:C:1205:Y01:CAV	2.39	1.05
1:C:890:LEU:HD11	3:D:1204:Y01:CAU	1.87	1.05
1:D:436:ASP:CB	1:D:438:PRO:CG	2.34	1.04
1:C:1161:GLN:HE21	1:D:1162:LEU:HB3	0.94	1.04
1:A:1029:LEU:CD1	3:A:1206:Y01:HAB2	1.87	1.04
1:B:864:TRP:HE3	3:B:1207:Y01:HAR1	1.08	1.04
1:A:436:ASP:CB	1:A:438:PRO:CG	2.34	1.04
1:B:436:ASP:CB	1:B:438:PRO:CG	2.34	1.04
3:A:1205:Y01:HAS1	1:D:890:LEU:CD1	1.87	1.04
1:C:904:VAL:HG11	3:C:1205:Y01:CAQ	1.87	1.04
3:A:1205:Y01:HAV2	3:A:1205:Y01:HAM2	1.38	1.03
1:B:955:ARG:CZ	1:B:955:ARG:HA	1.89	1.03
1:D:955:ARG:HA	1:D:955:ARG:CZ	1.89	1.03
1:A:992:ASN:ND2	4:A:1210:NAG:O1	1.92	1.02
3:B:1208:Y01:HAB3	3:B:1208:Y01:HAO2	1.36	1.02
1:A:955:ARG:HA	1:A:955:ARG:CZ	1.90	1.02
1:C:864:TRP:CH2	3:C:1205:Y01:CAI	2.35	1.02
3:D:1204:Y01:CAB	3:D:1204:Y01:HAC3	1.90	1.01
3:C:1204:Y01:HAC2	3:C:1204:Y01:HAE2	1.39	1.01
1:D:975:PHE:O	1:D:977:GLN:N	1.92	1.01
1:C:890:LEU:HD11	3:D:1204:Y01:CAS	1.90	1.01
3:C:1203:Y01:CAB	3:C:1203:Y01:HAC3	1.91	1.01
1:C:955:ARG:CZ	1:C:955:ARG:HA	1.89	1.01
1:A:864:TRP:HZ3	3:A:1208:Y01:HAT2	1.21	0.99
1:C:890:LEU:HD11	3:D:1204:Y01:HAS1	1.40	0.99
1:A:969:ARG:HH22	1:A:983:MET:HE2	1.28	0.99
1:D:913:ASN:OD1	3:D:1205:Y01:HAL2	1.62	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1205:Y01:HAO2	3:B:1205:Y01:HAU2	1.44	0.98
1:D:436:ASP:CB	1:D:438:PRO:CD	2.42	0.98
1:A:436:ASP:CB	1:A:438:PRO:CD	2.42	0.97
1:A:1026:ILE:CD1	3:A:1206:Y01:CAC	2.41	0.97
1:B:436:ASP:CB	1:B:438:PRO:CD	2.42	0.97
1:A:969:ARG:HH22	1:A:983:MET:CE	1.78	0.97
1:C:436:ASP:CB	1:C:438:PRO:CD	2.42	0.97
1:C:1165:ILE:O	1:C:1169:GLU:HG2	1.64	0.97
3:A:1208:Y01:CAB	3:A:1208:Y01:HBB	1.95	0.96
3:A:1208:Y01:HAE2	3:A:1208:Y01:HAC1	1.44	0.96
1:A:864:TRP:HZ3	3:A:1208:Y01:CAT	1.73	0.96
3:A:1205:Y01:HAE2	3:A:1205:Y01:HAC2	1.48	0.96
3:A:1206:Y01:HAD1	3:D:1207:Y01:CAD	1.95	0.96
3:D:1203:Y01:HAB1	3:D:1203:Y01:HBB	1.44	0.96
3:D:1207:Y01:HAU2	3:D:1207:Y01:HAC1	1.46	0.96
3:A:1207:Y01:HAE2	3:A:1207:Y01:HAC2	1.48	0.95
1:D:992:ASN:ND2	4:D:1208:NAG:O1	1.99	0.95
1:D:864:TRP:CZ3	3:D:1207:Y01:HAV2	2.02	0.95
3:C:1205:Y01:HAE2	3:C:1205:Y01:HAC2	1.45	0.95
1:D:783:PHE:HE2	3:D:1205:Y01:HAM2	1.31	0.94
1:C:864:TRP:CE3	3:C:1205:Y01:CAV	2.49	0.94
3:C:1203:Y01:HAE2	3:C:1203:Y01:HAC2	1.50	0.93
3:D:1204:Y01:HAE2	3:D:1204:Y01:HAC2	1.50	0.93
1:A:1015:TYR:HH	3:A:1205:Y01:HAD2	1.25	0.93
3:B:1204:Y01:HAC2	3:B:1204:Y01:HAN2	1.47	0.93
1:C:1161:GLN:NE2	1:D:1162:LEU:CB	2.32	0.93
3:B:1205:Y01:HAC2	3:B:1205:Y01:HAE2	1.47	0.93
1:C:1032:ASN:C	1:C:1033:ILE:HD12	1.89	0.93
1:B:1015:TYR:OH	3:B:1205:Y01:CAR	2.16	0.93
1:D:1032:ASN:C	1:D:1033:ILE:HD12	1.89	0.93
1:B:898:ASP:O	1:B:902:PHE:HD1	1.51	0.93
3:D:1204:Y01:HAC3	3:D:1204:Y01:HAB3	1.51	0.93
1:B:438:PRO:HD2	1:B:439:GLU:H	1.35	0.92
1:A:438:PRO:HD2	1:A:439:GLU:H	1.35	0.92
1:B:1015:TYR:HH	3:B:1205:Y01:HAT2	1.12	0.92
1:C:438:PRO:HD2	1:C:439:GLU:H	1.35	0.91
3:D:1205:Y01:HAC2	3:D:1205:Y01:HAE2	1.50	0.91
3:D:1205:Y01:HAO2	3:D:1205:Y01:HAU2	1.50	0.91
3:A:1209:Y01:CAP	3:A:1209:Y01:HAJ2	1.98	0.91
1:D:904:VAL:HG11	3:D:1207:Y01:HAK1	1.51	0.91
1:D:438:PRO:HD2	1:D:439:GLU:H	1.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1162:LEU:HB3	1:D:1161:GLN:NE2	1.86	0.90
1:A:992:ASN:CG	4:A:1210:NAG:O1	2.09	0.90
3:A:1206:Y01:CAD	3:D:1207:Y01:HAD2	2.02	0.90
1:C:864:TRP:HE3	3:C:1205:Y01:HAV2	1.23	0.90
3:A:1205:Y01:CAU	1:D:890:LEU:HD11	2.01	0.90
3:A:1209:Y01:HAJ2	3:A:1209:Y01:HAP2	1.51	0.89
3:D:1206:Y01:HAJ2	3:D:1206:Y01:CAP	2.03	0.89
3:B:1207:Y01:HAC1	3:B:1207:Y01:HAU2	1.53	0.89
1:C:1015:TYR:OH	3:C:1203:Y01:HAD2	1.74	0.88
3:C:1203:Y01:HAC3	3:C:1203:Y01:HAB3	1.54	0.88
1:A:967:PHE:HB3	3:A:1204:Y01:HAB1	1.54	0.88
3:D:1203:Y01:HAB1	3:D:1203:Y01:CAC	2.02	0.88
1:B:890:LEU:HD11	3:C:1203:Y01:CAS	2.03	0.88
1:A:1162:LEU:HD12	1:D:1161:GLN:HG2	1.55	0.87
3:A:1206:Y01:CAD	3:D:1207:Y01:CAD	2.52	0.87
3:B:1204:Y01:HAQ2	1:C:1021:VAL:HG11	1.55	0.87
3:D:1203:Y01:HAB1	3:D:1203:Y01:CBB	2.03	0.87
3:A:1205:Y01:HAC3	3:A:1205:Y01:CBA	2.03	0.87
1:A:588:SER:O	1:A:592:ALA:HB2	1.74	0.87
1:A:864:TRP:HE3	3:A:1208:Y01:HAR2	1.39	0.87
1:D:588:SER:O	1:D:592:ALA:HB2	1.74	0.87
1:A:1026:ILE:HD11	3:A:1206:Y01:CAC	2.04	0.87
1:C:1032:ASN:O	1:C:1033:ILE:HD12	1.75	0.86
3:C:1201:Y01:HAU2	3:C:1201:Y01:HAC1	1.57	0.86
1:D:1032:ASN:O	1:D:1033:ILE:HD12	1.75	0.86
1:A:864:TRP:CE3	3:A:1208:Y01:HAR2	2.09	0.86
1:B:588:SER:O	1:B:592:ALA:HB2	1.74	0.86
3:A:1208:Y01:HBB	3:A:1208:Y01:HAB1	1.58	0.86
1:B:1032:ASN:C	1:B:1033:ILE:HD12	1.96	0.86
1:C:850:ALA:N	1:C:853:SER:HG	1.74	0.86
1:B:864:TRP:CE3	3:B:1207:Y01:HAR2	1.90	0.86
1:C:588:SER:O	1:C:592:ALA:HB2	1.74	0.85
1:A:1029:LEU:CD1	3:A:1206:Y01:CAB	2.48	0.85
1:D:1015:TYR:OH	3:D:1204:Y01:HAD2	1.74	0.85
1:D:913:ASN:OD1	3:D:1205:Y01:CAL	2.23	0.85
1:C:1161:GLN:HE21	1:D:1162:LEU:CB	1.86	0.85
1:A:1015:TYR:OH	3:A:1205:Y01:HAD1	1.76	0.85
1:B:864:TRP:HZ3	3:B:1207:Y01:HAT1	1.41	0.85
3:B:1205:Y01:HAO1	3:B:1205:Y01:HAB3	1.56	0.84
3:B:1204:Y01:HAA1	3:B:1204:Y01:HAO1	1.58	0.84
1:A:1026:ILE:CD1	3:A:1206:Y01:HAC2	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1204:Y01:HAU2	3:D:1204:Y01:HAO2	1.59	0.84
3:D:1205:Y01:HAO1	3:D:1205:Y01:HAB1	1.59	0.84
3:B:1203:Y01:HAC1	3:B:1203:Y01:HAU2	1.59	0.84
1:B:890:LEU:HD11	3:C:1203:Y01:HAS1	1.58	0.83
1:C:864:TRP:CZ3	3:C:1205:Y01:CAZ	2.60	0.83
3:B:1204:Y01:HAQ2	1:C:1021:VAL:HG12	1.60	0.83
3:A:1205:Y01:HAC3	3:A:1205:Y01:HAA1	1.61	0.82
1:B:816:LEU:O	1:B:820:TRP:HB2	1.77	0.82
3:B:1203:Y01:HAN1	3:B:1203:Y01:HAC3	1.61	0.82
3:A:1205:Y01:HAM2	3:A:1205:Y01:CAV	2.08	0.82
1:A:864:TRP:CE3	3:A:1208:Y01:HAT2	2.14	0.82
1:A:1026:ILE:HG12	3:A:1206:Y01:HAC2	1.62	0.81
3:C:1203:Y01:HAU2	3:C:1203:Y01:HAO2	1.60	0.81
1:A:955:ARG:NH2	1:A:1000:TRP:CZ3	2.49	0.81
3:B:1208:Y01:HAC1	3:B:1208:Y01:HAU2	1.64	0.80
3:D:1204:Y01:HAC3	3:D:1204:Y01:HAB1	1.64	0.79
1:C:864:TRP:HZ3	3:C:1205:Y01:CAV	1.93	0.79
3:D:1201:Y01:HAC1	3:D:1201:Y01:HAU2	1.64	0.79
3:D:1205:Y01:HBB	3:D:1205:Y01:HBA	1.65	0.79
3:C:1203:Y01:HAC3	3:C:1203:Y01:HAB1	1.61	0.79
3:D:1203:Y01:HAC2	3:D:1203:Y01:HAE2	1.64	0.79
3:B:1203:Y01:HAN1	3:B:1203:Y01:CAC	2.12	0.78
1:D:955:ARG:HA	1:D:955:ARG:NE	1.99	0.78
1:B:955:ARG:HA	1:B:955:ARG:NE	1.98	0.78
1:C:955:ARG:HA	1:C:955:ARG:NE	1.98	0.78
3:D:1203:Y01:HBB	3:D:1203:Y01:CAB	2.12	0.78
1:A:864:TRP:CE3	3:A:1208:Y01:CAT	2.60	0.78
3:B:1205:Y01:HAC2	3:B:1205:Y01:CAE	2.14	0.78
3:A:1205:Y01:HAC3	3:A:1205:Y01:CAN	2.13	0.78
3:B:1206:Y01:HAC1	3:B:1206:Y01:HAE2	1.65	0.78
3:A:1205:Y01:HAC2	3:A:1205:Y01:CAE	2.13	0.78
3:B:1206:Y01:HAE2	3:B:1206:Y01:CAC	2.13	0.78
1:A:972:LEU:O	1:A:977:GLN:HB2	1.84	0.78
3:B:1205:Y01:CAB	3:B:1205:Y01:HBB	2.14	0.78
3:B:1204:Y01:HAN2	3:B:1204:Y01:CAC	2.14	0.78
1:A:584:ASN:OD1	1:A:1122:LEU:HD22	1.82	0.78
1:C:796:LEU:O	1:C:796:LEU:HD13	1.84	0.78
1:C:972:LEU:CD1	1:D:980:GLN:NE2	2.47	0.78
3:C:1205:Y01:HAE1	3:D:1206:Y01:HAD2	1.66	0.78
3:A:1205:Y01:HAC3	3:A:1205:Y01:CAA	2.14	0.77
3:D:1205:Y01:HAC2	3:D:1205:Y01:CAE	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:980:GLN:O	1:B:987:LEU:HD23	1.84	0.77
1:C:973:GLN:HE22	1:C:978:ILE:HG23	1.48	0.77
1:A:969:ARG:NH2	1:A:983:MET:CE	2.46	0.77
3:A:1207:Y01:HAC2	3:A:1207:Y01:CAE	2.14	0.77
3:D:1204:Y01:HAC2	3:D:1204:Y01:CAE	2.14	0.77
3:B:1205:Y01:HAB3	3:B:1205:Y01:CAO	2.14	0.77
3:D:1206:Y01:HAJ2	3:D:1206:Y01:HAP2	1.66	0.77
3:A:1209:Y01:HAC1	3:A:1209:Y01:HAE2	1.66	0.77
1:A:1026:ILE:HD13	3:A:1206:Y01:CAC	2.15	0.76
1:B:796:LEU:HD13	1:B:796:LEU:O	1.84	0.76
3:B:1208:Y01:HAB2	1:C:1029:LEU:HD13	1.67	0.76
1:D:904:VAL:CG1	3:D:1207:Y01:HAK1	2.16	0.76
3:D:1205:Y01:HAB1	3:D:1205:Y01:CAO	2.15	0.76
1:B:960:PRO:HB2	3:B:1204:Y01:CAR	2.16	0.76
1:A:854:GLN:HA	1:A:854:GLN:NE2	1.99	0.76
1:B:890:LEU:HD11	3:C:1203:Y01:HAU2	1.68	0.76
3:C:1203:Y01:HAC2	3:C:1203:Y01:CAE	2.14	0.76
3:A:1208:Y01:HAE2	3:A:1208:Y01:CAC	2.15	0.76
1:A:972:LEU:CD1	1:B:980:GLN:NE2	2.49	0.76
1:A:1023:LEU:HD21	3:D:1207:Y01:HAJ2	1.68	0.75
1:A:973:GLN:HE22	1:A:978:ILE:HG23	1.52	0.75
3:D:1203:Y01:HAC2	3:D:1203:Y01:CAE	2.15	0.75
1:B:1161:GLN:HG2	1:C:1162:LEU:HD12	1.69	0.75
1:C:890:LEU:CD1	3:D:1204:Y01:HAS1	2.16	0.75
1:D:796:LEU:HD13	1:D:796:LEU:O	1.85	0.75
3:A:1206:Y01:HAC1	3:A:1206:Y01:HAU2	1.67	0.75
1:D:992:ASN:CG	4:D:1208:NAG:O1	2.25	0.74
3:C:1202:Y01:HAC1	3:C:1202:Y01:HAU2	1.68	0.74
3:D:1206:Y01:HAC1	3:D:1206:Y01:HAU2	1.68	0.74
3:D:1207:Y01:HAA1	3:D:1207:Y01:CAC	2.17	0.74
1:A:1026:ILE:CG1	3:A:1206:Y01:HAC2	2.17	0.74
1:B:972:LEU:CD1	1:C:980:GLN:NE2	2.50	0.74
1:A:1026:ILE:HD11	3:A:1206:Y01:HAC3	1.66	0.74
3:A:1209:Y01:CAO	3:A:1209:Y01:HAB3	2.18	0.74
1:C:437:ARG:N	1:C:438:PRO:HD3	2.02	0.74
1:A:924:SER:HB3	3:A:1209:Y01:OAF	1.88	0.74
1:A:438:PRO:HD2	1:A:439:GLU:N	2.03	0.73
3:D:1205:Y01:HBB	3:D:1205:Y01:CBA	2.18	0.73
1:B:437:ARG:N	1:B:438:PRO:HD3	2.02	0.73
1:B:438:PRO:HD2	1:B:439:GLU:N	2.03	0.73
1:D:864:TRP:CZ3	3:D:1207:Y01:CAV	2.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1205:Y01:HBB	3:D:1205:Y01:CAB	2.18	0.73
1:A:437:ARG:N	1:A:438:PRO:HD3	2.02	0.73
1:C:793:PHE:O	1:C:793:PHE:CD1	2.41	0.73
3:C:1201:Y01:HAO2	3:C:1201:Y01:CAA	2.08	0.73
1:D:438:PRO:HD2	1:D:439:GLU:N	2.04	0.73
1:D:783:PHE:CE2	3:D:1205:Y01:HAM2	2.21	0.73
1:C:904:VAL:CG1	3:C:1205:Y01:CAQ	2.66	0.72
3:C:1204:Y01:HAC2	3:C:1204:Y01:CAE	2.16	0.72
1:D:437:ARG:N	1:D:438:PRO:HD3	2.02	0.72
3:D:1201:Y01:HAU2	3:D:1201:Y01:CAC	2.20	0.72
3:D:1207:Y01:HAC3	3:D:1207:Y01:CAN	2.13	0.72
1:B:955:ARG:NH2	1:B:1000:TRP:CZ3	2.58	0.72
1:D:783:PHE:HE2	3:D:1205:Y01:CAM	2.02	0.72
3:D:1201:Y01:HAB3	3:D:1201:Y01:HAO1	1.72	0.72
3:B:1205:Y01:HBB	3:B:1205:Y01:HAB1	1.71	0.72
3:B:1208:Y01:HAD1	3:B:1208:Y01:OAW	1.90	0.72
3:C:1205:Y01:HAC2	3:C:1205:Y01:CAE	2.20	0.72
3:D:1201:Y01:HAO1	3:D:1201:Y01:CAB	2.19	0.71
1:B:1148:LEU:HD13	1:B:1148:LEU:O	1.89	0.71
3:C:1205:Y01:HAO1	3:C:1205:Y01:HAU2	1.72	0.71
3:A:1205:Y01:HAC3	3:A:1205:Y01:HAN2	1.72	0.71
3:D:1206:Y01:HAU2	3:D:1206:Y01:CAC	2.20	0.71
1:A:969:ARG:NH2	1:A:983:MET:HE2	2.05	0.71
3:C:1201:Y01:CAP	3:C:1201:Y01:HAJ2	2.21	0.70
3:D:1202:Y01:HAC1	3:D:1202:Y01:HAU2	1.72	0.70
1:C:900:MET:CE	3:C:1205:Y01:HAB1	2.21	0.70
1:D:436:ASP:O	1:D:438:PRO:CD	2.40	0.70
1:A:436:ASP:O	1:A:438:PRO:CD	2.40	0.70
1:A:1026:ILE:HD12	3:D:1207:Y01:HAN2	1.74	0.70
1:C:783:PHE:CE2	3:C:1204:Y01:OAG	2.45	0.70
1:A:955:ARG:HA	1:A:955:ARG:NE	2.03	0.69
3:A:1204:Y01:HAC1	3:A:1204:Y01:HAU2	1.73	0.69
3:D:1207:Y01:HAO2	3:D:1207:Y01:CAA	2.17	0.69
1:B:436:ASP:O	1:B:438:PRO:CD	2.40	0.69
1:B:960:PRO:HB2	3:B:1204:Y01:HAT2	1.75	0.69
1:C:955:ARG:NH2	1:C:1000:TRP:CZ3	2.61	0.69
1:A:864:TRP:CZ3	3:A:1208:Y01:CAR	2.64	0.69
1:C:436:ASP:O	1:C:438:PRO:CD	2.40	0.69
1:A:644:ARG:NH2	1:A:646:CYS:SG	2.66	0.69
1:B:644:ARG:NH2	1:B:646:CYS:SG	2.66	0.69
3:D:1205:Y01:HAB1	3:D:1205:Y01:CBB	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1205:Y01:CAO	3:A:1205:Y01:HAU2	2.23	0.69
3:B:1204:Y01:HAJ2	3:B:1204:Y01:HAP2	1.73	0.69
1:C:644:ARG:NH2	1:C:646:CYS:SG	2.66	0.68
1:B:436:ASP:O	1:B:438:PRO:HD3	1.93	0.68
3:A:1206:Y01:HAD2	3:D:1207:Y01:HAD2	1.74	0.68
3:B:1207:Y01:HAA1	1:C:1023:LEU:HD21	1.74	0.68
1:C:438:PRO:HD2	1:C:439:GLU:N	2.03	0.68
1:D:644:ARG:NH2	1:D:646:CYS:SG	2.66	0.68
1:B:633:SER:OG	1:B:1128:HIS:NE2	2.27	0.68
1:C:436:ASP:O	1:C:438:PRO:HD3	1.93	0.68
3:D:1201:Y01:HAB3	3:D:1201:Y01:CAO	2.24	0.68
1:D:955:ARG:NH1	1:D:1000:TRP:CZ3	2.61	0.67
1:A:1018:TRP:O	1:A:1022:LEU:HB2	1.95	0.67
1:C:1018:TRP:O	1:C:1022:LEU:HB2	1.94	0.67
1:D:1018:TRP:O	1:D:1022:LEU:HB2	1.94	0.67
1:D:1158:ALA:O	1:D:1162:LEU:HD23	1.94	0.67
1:A:1162:LEU:HD11	1:D:1162:LEU:HD22	1.76	0.67
1:D:993:CYS:HB2	1:D:1002:HIS:HB2	1.76	0.67
1:A:633:SER:OG	1:A:1128:HIS:NE2	2.27	0.67
3:A:1209:Y01:CAC	3:A:1209:Y01:HAU2	2.25	0.67
3:B:1204:Y01:HAO1	3:B:1204:Y01:CAA	2.25	0.67
1:B:972:LEU:CD1	1:C:980:GLN:HE21	2.07	0.66
1:B:1018:TRP:O	1:B:1022:LEU:HB2	1.94	0.66
1:A:1033:ILE:HD11	1:D:975:PHE:HE1	1.58	0.66
3:D:1207:Y01:HAA1	3:D:1207:Y01:HAC2	1.74	0.66
3:B:1208:Y01:HAB3	3:B:1208:Y01:CAO	2.18	0.66
1:D:633:SER:OG	1:D:1128:HIS:NE2	2.28	0.66
1:A:796:LEU:HD13	1:A:796:LEU:O	1.95	0.66
3:B:1208:Y01:HAU2	3:B:1208:Y01:CAC	2.25	0.66
1:A:976:GLY:O	1:A:977:GLN:OE1	2.14	0.66
3:D:1203:Y01:CAO	3:D:1203:Y01:HAU2	2.26	0.66
3:B:1204:Y01:HAJ2	3:B:1204:Y01:CAP	2.24	0.65
3:C:1205:Y01:CAD	3:D:1206:Y01:HAD1	2.25	0.65
1:C:793:PHE:O	1:C:793:PHE:HD1	1.78	0.65
3:B:1208:Y01:HAO2	3:B:1208:Y01:CAB	2.21	0.65
1:D:796:LEU:HD13	1:D:796:LEU:C	2.17	0.65
1:A:955:ARG:HB2	1:A:1011:CYS:HB3	1.77	0.65
1:D:864:TRP:CE3	3:D:1207:Y01:HAV2	2.30	0.65
1:A:796:LEU:HD13	1:A:796:LEU:C	2.17	0.65
1:A:979:PRO:O	1:A:981:GLU:N	2.28	0.65
3:A:1208:Y01:HBG	3:A:1209:Y01:CAD	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1205:Y01:HAN2	3:B:1205:Y01:HAC3	1.79	0.65
1:A:975:PHE:CE2	1:B:1028:LEU:HB3	2.31	0.65
1:A:796:LEU:HD12	1:A:817:LEU:CD2	2.27	0.65
3:A:1208:Y01:HBB	3:A:1208:Y01:HAB3	1.76	0.65
1:D:436:ASP:O	1:D:438:PRO:HD3	1.93	0.65
1:D:973:GLN:HE22	1:D:978:ILE:HG23	1.61	0.64
3:D:1207:Y01:HAA2	3:D:1207:Y01:CAO	2.20	0.64
1:A:633:SER:HG	1:A:1128:HIS:HE2	1.46	0.64
1:C:890:LEU:HD11	3:D:1204:Y01:HAU2	1.77	0.64
1:C:796:LEU:HD13	1:C:796:LEU:C	2.18	0.64
3:C:1204:Y01:HAO2	3:C:1204:Y01:HAU2	1.80	0.64
1:A:955:ARG:HA	1:A:955:ARG:NH2	2.11	0.64
1:A:973:GLN:NE2	1:A:978:ILE:HG23	2.12	0.64
3:D:1206:Y01:HAV1	3:D:1206:Y01:OAG	1.98	0.64
3:B:1203:Y01:HAC3	3:B:1203:Y01:CAN	2.28	0.64
3:C:1202:Y01:HAU2	3:C:1202:Y01:CAC	2.28	0.63
1:A:674:SER:O	1:A:678:GLN:HB2	1.99	0.63
1:C:864:TRP:CE3	3:C:1205:Y01:HAI	2.17	0.63
1:B:796:LEU:HD13	1:B:796:LEU:C	2.18	0.63
1:D:1026:ILE:HD13	3:D:1206:Y01:HAC2	1.81	0.63
3:A:1208:Y01:HAB1	3:A:1208:Y01:CBB	2.28	0.63
1:B:960:PRO:HB2	3:B:1204:Y01:CAT	2.29	0.63
3:A:1206:Y01:OAG	3:A:1206:Y01:HAV1	1.99	0.63
1:B:436:ASP:CA	1:B:438:PRO:CD	2.68	0.63
1:B:674:SER:O	1:B:678:GLN:HB2	1.98	0.63
1:B:913:ASN:OD1	3:B:1206:Y01:OAF	2.16	0.63
1:D:674:SER:O	1:D:678:GLN:HB2	1.98	0.63
1:C:624:VAL:HG13	1:C:669:GLN:HE21	1.64	0.63
1:C:955:ARG:HG3	1:C:956:ASP:H	1.64	0.62
1:D:624:VAL:HG13	1:D:669:GLN:HE21	1.64	0.62
1:D:796:LEU:HD12	1:D:817:LEU:CD2	2.28	0.62
1:A:978:ILE:HD13	1:A:1028:LEU:HD11	1.81	0.62
1:A:1033:ILE:CD1	1:D:975:PHE:HE1	2.13	0.62
1:D:955:ARG:HG3	1:D:956:ASP:H	1.64	0.62
3:A:1209:Y01:HAC1	3:A:1209:Y01:HAU2	1.80	0.62
1:C:992:ASN:ND2	4:C:1206:NAG:O1	2.32	0.62
1:A:693:LEU:O	1:A:693:LEU:HD13	1.98	0.62
3:D:1203:Y01:HAE2	3:D:1203:Y01:HAO2	1.80	0.62
3:D:1207:Y01:HAN1	3:D:1207:Y01:CAC	2.11	0.62
3:A:1209:Y01:CAC	1:B:1026:ILE:HD13	2.29	0.62
1:B:1033:ILE:HD12	1:B:1033:ILE:N	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1205:Y01:HAO2	3:B:1205:Y01:CAU	2.19	0.62
1:C:674:SER:O	1:C:678:GLN:HB2	1.98	0.62
3:D:1204:Y01:HAU2	3:D:1204:Y01:CAO	2.29	0.62
1:C:796:LEU:HD12	1:C:817:LEU:CD2	2.29	0.62
1:C:900:MET:CE	3:C:1205:Y01:CAB	2.78	0.62
3:D:1205:Y01:HAB1	3:D:1205:Y01:HBB	1.81	0.62
1:A:624:VAL:HG13	1:A:669:GLN:HE21	1.64	0.62
1:B:624:VAL:HG13	1:B:669:GLN:HE21	1.64	0.62
1:C:904:VAL:CG1	3:C:1205:Y01:HAQ2	2.30	0.62
3:B:1204:Y01:HAC2	3:B:1204:Y01:CAN	2.23	0.61
1:A:1026:ILE:HD13	3:A:1206:Y01:HAC1	1.82	0.61
1:D:972:LEU:O	1:D:977:GLN:O	2.18	0.61
1:B:864:TRP:CZ3	3:B:1207:Y01:CAR	2.52	0.61
3:C:1203:Y01:CAX	3:C:1203:Y01:HAV2	2.30	0.61
3:A:1204:Y01:HAU2	3:A:1204:Y01:CAC	2.31	0.61
1:C:1148:LEU:HD13	1:C:1148:LEU:O	2.01	0.61
1:B:796:LEU:HD12	1:B:817:LEU:CD2	2.30	0.61
1:A:436:ASP:CA	1:A:438:PRO:CD	2.68	0.61
1:B:890:LEU:CD1	3:C:1203:Y01:HAS1	2.30	0.61
1:B:955:ARG:HG3	1:B:956:ASP:H	1.65	0.61
3:C:1201:Y01:HAU2	3:C:1201:Y01:CAC	2.30	0.61
3:A:1206:Y01:HBA	1:D:934:LEU:HD11	1.83	0.61
1:B:1018:TRP:HB3	3:B:1203:Y01:HAD2	1.83	0.61
3:C:1203:Y01:HAU2	3:C:1203:Y01:CAO	2.30	0.61
1:A:1148:LEU:HD12	1:D:1147:ARG:HD2	1.83	0.60
1:B:633:SER:HG	1:B:1128:HIS:HE2	1.45	0.60
1:B:1148:LEU:HD13	1:B:1148:LEU:C	2.22	0.60
1:B:793:PHE:CD1	1:B:793:PHE:C	2.75	0.60
1:B:1015:TYR:CE1	3:B:1205:Y01:HAR1	2.37	0.60
1:D:864:TRP:CH2	3:D:1207:Y01:HAI	2.37	0.60
3:A:1209:Y01:HAC2	1:B:1026:ILE:CD1	2.32	0.60
3:A:1209:Y01:HAC2	1:B:1026:ILE:HD13	1.84	0.60
1:B:1162:LEU:HD22	1:C:1162:LEU:HD21	1.82	0.60
1:A:655:LEU:HD13	1:A:1067:ARG:NH1	2.17	0.60
1:C:904:VAL:HG11	3:C:1205:Y01:HAQ2	1.82	0.60
1:D:633:SER:HG	1:D:1128:HIS:HE2	1.48	0.60
1:C:904:VAL:CG1	3:C:1205:Y01:HAQ1	2.15	0.60
3:A:1204:Y01:HAC1	3:A:1204:Y01:HAE2	1.83	0.60
3:A:1205:Y01:HAU2	1:D:890:LEU:HD11	1.82	0.60
1:D:992:ASN:ND2	4:D:1208:NAG:C1	2.64	0.60
1:A:900:MET:CE	3:A:1208:Y01:HAJ1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:955:ARG:NH2	1:A:1000:TRP:HZ3	1.95	0.60
1:A:1026:ILE:CD1	3:D:1207:Y01:HAN2	2.32	0.59
1:C:1047:PHE:O	1:C:1051:GLN:HB2	2.02	0.59
1:C:693:LEU:HD13	1:C:693:LEU:O	2.02	0.59
1:C:783:PHE:HE2	3:C:1204:Y01:OAG	1.85	0.59
1:D:1015:TYR:OH	3:D:1204:Y01:CAD	2.49	0.59
1:B:955:ARG:NH2	1:B:1000:TRP:HZ3	1.99	0.59
1:A:693:LEU:HD13	1:A:693:LEU:C	2.23	0.59
3:C:1201:Y01:HAJ2	3:C:1201:Y01:HAP1	1.83	0.59
1:D:1047:PHE:O	1:D:1051:GLN:HB2	2.02	0.59
1:B:898:ASP:O	1:B:902:PHE:CD1	2.43	0.59
3:B:1207:Y01:HAU2	3:B:1207:Y01:CAC	2.29	0.59
1:A:1047:PHE:O	1:A:1051:GLN:HB2	2.02	0.59
3:B:1208:Y01:CAB	1:C:1029:LEU:HD13	2.33	0.59
1:D:693:LEU:HD13	1:D:693:LEU:C	2.23	0.59
3:A:1209:Y01:CAC	1:B:1026:ILE:CD1	2.80	0.59
1:B:693:LEU:HD13	1:B:693:LEU:O	2.02	0.59
1:D:693:LEU:HD13	1:D:693:LEU:O	2.02	0.59
1:A:796:LEU:HD12	1:A:817:LEU:HD23	1.85	0.59
1:D:796:LEU:HD12	1:D:817:LEU:HD23	1.85	0.59
3:D:1205:Y01:HAU2	3:D:1205:Y01:CAO	2.26	0.59
3:A:1209:Y01:HAB3	3:A:1209:Y01:HAO2	1.85	0.58
1:A:1162:LEU:HD21	1:D:1162:LEU:HD21	1.85	0.58
3:A:1208:Y01:HAC2	3:A:1208:Y01:HAU2	1.84	0.58
1:A:438:PRO:CD	1:A:439:GLU:H	2.13	0.58
1:C:900:MET:SD	3:C:1205:Y01:HAB3	2.43	0.58
3:D:1207:Y01:HAC1	3:D:1207:Y01:CAU	2.22	0.58
1:B:693:LEU:HD13	1:B:693:LEU:C	2.24	0.58
3:C:1205:Y01:HAE2	3:C:1205:Y01:CAC	2.28	0.58
3:D:1201:Y01:HAC1	3:D:1201:Y01:HAE2	1.86	0.58
1:B:690:ILE:HD13	3:B:1206:Y01:HAM2	1.84	0.58
1:B:1161:GLN:CG	1:C:1162:LEU:HD12	2.33	0.58
1:C:680:TRP:CE3	1:C:1066:ILE:CD1	2.87	0.58
1:D:1148:LEU:O	1:D:1148:LEU:HD13	2.04	0.58
1:A:969:ARG:NH2	1:A:983:MET:HE3	2.18	0.58
1:C:693:LEU:HD13	1:C:693:LEU:C	2.24	0.58
1:C:904:VAL:HB	3:C:1205:Y01:HAQ2	1.86	0.58
3:D:1203:Y01:HAU2	3:D:1203:Y01:HAO2	1.85	0.58
1:B:438:PRO:CD	1:B:439:GLU:H	2.13	0.58
1:B:1047:PHE:O	1:B:1051:GLN:HB2	2.02	0.58
1:C:436:ASP:CA	1:C:438:PRO:CD	2.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:788:VAL:HG22	3:B:1206:Y01:CAU	2.34	0.57
3:C:1204:Y01:OAG	3:C:1204:Y01:HAR1	2.04	0.57
1:D:783:PHE:CE2	3:D:1205:Y01:CAM	2.84	0.57
3:D:1206:Y01:HAC1	3:D:1206:Y01:HAE2	1.85	0.57
1:C:975:PHE:CE2	1:D:1028:LEU:HB3	2.39	0.57
1:A:900:MET:HE1	3:A:1208:Y01:CAJ	2.34	0.57
1:A:1023:LEU:HD21	3:D:1207:Y01:CAJ	2.34	0.57
1:A:1162:LEU:HB3	1:D:1161:GLN:HE21	1.63	0.57
3:D:1202:Y01:OAG	3:D:1202:Y01:HAV2	2.05	0.57
1:A:979:PRO:O	1:A:980:GLN:HB2	2.02	0.57
1:A:788:VAL:HG22	3:A:1207:Y01:CAU	2.34	0.57
3:A:1205:Y01:HAU2	3:A:1205:Y01:HAO2	1.86	0.57
1:B:788:VAL:HG22	3:B:1206:Y01:HAS1	1.86	0.56
1:C:1051:GLN:O	1:C:1055:ASP:HB2	2.05	0.56
1:B:972:LEU:HD13	1:C:980:GLN:HE21	1.70	0.56
1:C:864:TRP:HZ3	3:C:1205:Y01:CAI	2.04	0.56
1:D:438:PRO:CD	1:D:439:GLU:H	2.13	0.56
1:D:955:ARG:NH1	1:D:1000:TRP:HZ3	2.03	0.56
1:D:1018:TRP:O	1:D:1022:LEU:CB	2.53	0.56
1:D:1026:ILE:CD1	3:D:1206:Y01:HAC2	2.35	0.56
1:B:264:UNK:O	1:B:268:UNK:CB	2.53	0.56
1:B:960:PRO:HB2	3:B:1204:Y01:HAR1	1.87	0.56
1:C:796:LEU:HD12	1:C:817:LEU:HD23	1.88	0.56
3:C:1201:Y01:HAA1	3:C:1201:Y01:CAO	2.15	0.56
3:D:1207:Y01:HAU2	3:D:1207:Y01:CAC	2.30	0.56
1:A:113:UNK:O	1:A:196:UNK:N	2.39	0.56
1:A:977:GLN:O	1:A:978:ILE:HG12	2.06	0.56
3:A:1204:Y01:HAV2	3:A:1204:Y01:OAG	2.04	0.56
1:B:863:SER:OG	3:B:1207:Y01:HAM1	2.06	0.56
1:A:264:UNK:O	1:A:268:UNK:CB	2.54	0.56
1:A:900:MET:HE1	3:A:1208:Y01:HAJ1	1.87	0.56
3:A:1207:Y01:CAO	3:A:1207:Y01:HAU2	2.36	0.56
1:C:1018:TRP:O	1:C:1022:LEU:CB	2.53	0.56
1:D:436:ASP:CA	1:D:438:PRO:CD	2.68	0.56
1:A:1051:GLN:O	1:A:1055:ASP:HB2	2.05	0.56
3:D:1205:Y01:HAO2	3:D:1205:Y01:CAU	2.23	0.56
1:B:113:UNK:O	1:B:196:UNK:N	2.39	0.56
1:B:796:LEU:HD12	1:B:817:LEU:HD23	1.88	0.56
1:D:1051:GLN:O	1:D:1055:ASP:HB2	2.05	0.56
1:C:438:PRO:CD	1:C:439:GLU:H	2.13	0.56
1:D:264:UNK:O	1:D:268:UNK:CB	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1158:ALA:O	1:A:1162:LEU:HB2	2.05	0.55
3:A:1208:Y01:HAC1	3:A:1208:Y01:CAE	2.28	0.55
1:B:397:LEU:HD11	1:B:413:LEU:HD21	1.87	0.55
1:C:113:UNK:O	1:C:196:UNK:N	2.39	0.55
1:C:924:SER:HB3	3:D:1206:Y01:OAH	2.06	0.55
1:A:972:LEU:HD12	1:B:980:GLN:HE22	1.71	0.55
1:A:1018:TRP:O	1:A:1022:LEU:CB	2.54	0.55
1:A:1148:LEU:HD23	1:B:1148:LEU:HD21	1.87	0.55
1:B:890:LEU:HD11	3:C:1203:Y01:HAU1	1.81	0.55
1:C:397:LEU:HD11	1:C:413:LEU:HD21	1.87	0.55
3:C:1205:Y01:HAO1	3:C:1205:Y01:CAU	2.35	0.55
1:A:397:LEU:HD11	1:A:413:LEU:HD21	1.87	0.55
1:B:1051:GLN:O	1:B:1055:ASP:HB2	2.05	0.55
1:C:438:PRO:CD	1:C:439:GLU:N	2.70	0.55
1:C:694:VAL:HG21	3:C:1204:Y01:HAK2	1.87	0.55
1:C:680:TRP:CE3	1:C:1066:ILE:HD12	2.42	0.55
1:C:960:PRO:HB2	3:C:1202:Y01:HAI	1.88	0.55
1:D:397:LEU:HD11	1:D:413:LEU:HD21	1.87	0.55
3:A:1206:Y01:OAF	1:D:924:SER:HB3	2.07	0.55
3:A:1207:Y01:HAU2	3:A:1207:Y01:HAO2	1.89	0.55
1:B:438:PRO:CD	1:B:439:GLU:N	2.70	0.55
1:C:1076:ALA:HB1	1:C:1081:VAL:HG13	1.89	0.55
1:D:113:UNK:O	1:D:196:UNK:N	2.39	0.55
1:A:972:LEU:CD1	1:B:980:GLN:HE22	2.20	0.55
1:B:1018:TRP:O	1:B:1022:LEU:CB	2.53	0.55
1:C:264:UNK:O	1:C:268:UNK:CB	2.54	0.55
1:C:904:VAL:CB	3:C:1205:Y01:HAQ2	2.36	0.55
3:D:1207:Y01:HAC3	3:D:1207:Y01:HAA1	1.88	0.55
3:B:1206:Y01:CAC	3:B:1206:Y01:CAE	2.84	0.55
1:C:864:TRP:HZ3	3:C:1205:Y01:HAV1	1.71	0.55
3:D:1204:Y01:HAB3	3:D:1204:Y01:CAC	2.32	0.55
3:A:1205:Y01:HAU2	3:A:1205:Y01:HAO1	1.87	0.55
1:B:1076:ALA:HB1	1:B:1081:VAL:HG13	1.89	0.55
1:A:1076:ALA:HB1	1:A:1081:VAL:HG13	1.89	0.55
1:C:1018:TRP:CE3	3:C:1201:Y01:HAQ2	2.42	0.55
1:D:913:ASN:OD1	3:D:1205:Y01:HAL1	2.05	0.55
3:A:1209:Y01:CAO	3:A:1209:Y01:CAB	2.85	0.55
1:D:438:PRO:CD	1:D:439:GLU:N	2.70	0.55
1:D:694:VAL:HG21	3:D:1205:Y01:HAK2	1.88	0.55
3:A:1205:Y01:CAE	3:A:1205:Y01:CAC	2.85	0.54
1:C:793:PHE:CD1	1:C:793:PHE:C	2.77	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:960:PRO:HB2	3:D:1202:Y01:HAI	1.88	0.54
1:C:992:ASN:CG	4:C:1206:NAG:O1	2.45	0.54
1:D:1076:ALA:HB1	1:D:1081:VAL:HG13	1.89	0.54
3:B:1204:Y01:HAA1	3:B:1204:Y01:CAO	2.35	0.54
3:C:1201:Y01:CAP	3:C:1201:Y01:CAJ	2.86	0.54
3:C:1203:Y01:CAU	3:C:1203:Y01:HAO2	2.35	0.54
3:C:1204:Y01:HAU2	3:C:1204:Y01:CAO	2.36	0.54
1:A:782:ILE:HD13	1:A:1075:LEU:H	1.72	0.54
3:B:1205:Y01:CAB	3:B:1205:Y01:CAO	2.85	0.54
3:B:1207:Y01:HAC1	3:B:1207:Y01:CAU	2.28	0.54
1:C:900:MET:HE2	3:C:1205:Y01:HAB1	1.89	0.54
1:C:955:ARG:HG3	1:C:956:ASP:N	2.23	0.54
3:C:1205:Y01:CAE	3:D:1206:Y01:HAD2	2.36	0.54
1:B:1015:TYR:OH	3:B:1205:Y01:HAR1	2.06	0.54
1:C:970:PRO:HA	1:C:973:GLN:HG2	1.90	0.54
1:B:970:PRO:HA	1:B:973:GLN:HG2	1.90	0.54
3:B:1205:Y01:CAB	3:B:1205:Y01:CBB	2.86	0.54
3:B:1207:Y01:CAC	3:B:1207:Y01:CAU	2.85	0.54
1:C:955:ARG:NH2	1:C:1000:TRP:HZ3	2.03	0.54
1:D:782:ILE:HD13	1:D:1075:LEU:H	1.72	0.54
3:D:1207:Y01:OAG	3:D:1207:Y01:HAR2	2.08	0.54
3:B:1203:Y01:HAC1	3:B:1203:Y01:CAU	2.37	0.54
1:C:1018:TRP:CD2	3:C:1201:Y01:HAQ2	2.43	0.54
3:B:1205:Y01:HAB3	3:B:1205:Y01:CBB	2.37	0.54
1:D:870:VAL:O	1:D:874:CYS:CB	2.56	0.54
3:A:1205:Y01:CAU	3:A:1205:Y01:CAO	2.86	0.54
3:C:1205:Y01:HAB2	1:D:1023:LEU:CD2	2.38	0.54
3:A:1206:Y01:HAD1	3:D:1207:Y01:HAD3	1.87	0.53
1:B:975:PHE:CE1	1:C:1028:LEU:HD13	2.43	0.53
3:A:1207:Y01:CAE	3:A:1207:Y01:CAC	2.85	0.53
1:B:583:SER:HB2	1:B:584:ASN:OD1	2.08	0.53
1:C:782:ILE:HD13	1:C:1075:LEU:H	1.72	0.53
3:C:1202:Y01:HAC1	3:C:1202:Y01:HAE2	1.89	0.53
1:B:782:ILE:HD13	1:B:1075:LEU:H	1.72	0.53
1:B:1158:ALA:O	1:B:1162:LEU:HB2	2.08	0.53
3:D:1205:Y01:HBA	3:D:1205:Y01:CBB	2.36	0.53
3:D:1207:Y01:CAC	3:D:1207:Y01:CAA	2.86	0.53
1:A:1147:ARG:CD	1:B:1148:LEU:HD12	2.38	0.53
3:B:1205:Y01:HAU2	3:B:1205:Y01:CAO	2.26	0.53
3:D:1201:Y01:CAC	3:D:1201:Y01:CAU	2.85	0.53
3:D:1207:Y01:CAC	3:D:1207:Y01:CAU	2.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:870:VAL:O	1:C:874:CYS:CB	2.56	0.53
1:C:1032:ASN:C	1:C:1033:ILE:CD1	2.70	0.53
1:A:870:VAL:O	1:A:874:CYS:CB	2.56	0.53
3:C:1205:Y01:CAE	3:C:1205:Y01:CAC	2.85	0.53
1:A:970:PRO:HA	1:A:973:GLN:HG2	1.90	0.53
1:A:973:GLN:HA	1:A:977:GLN:O	2.09	0.53
1:B:1147:ARG:HD2	1:C:1148:LEU:HD12	1.91	0.53
1:D:970:PRO:HA	1:D:973:GLN:HG2	1.90	0.53
1:A:900:MET:CE	3:A:1208:Y01:CAJ	2.86	0.53
1:A:913:ASN:OD1	3:A:1207:Y01:HAL2	2.07	0.53
3:C:1201:Y01:HAP1	3:C:1201:Y01:CAJ	2.39	0.53
1:A:438:PRO:CD	1:A:439:GLU:N	2.70	0.52
1:B:955:ARG:HG3	1:B:956:ASP:N	2.24	0.52
1:B:975:PHE:CE1	1:C:1028:LEU:HB3	2.44	0.52
1:C:680:TRP:HE3	1:C:1066:ILE:HD12	1.74	0.52
1:B:870:VAL:O	1:B:874:CYS:CB	2.56	0.52
1:C:1148:LEU:HD13	1:C:1148:LEU:C	2.28	0.52
1:A:1029:LEU:HD13	3:A:1206:Y01:HAB1	1.78	0.52
1:D:828:GLU:OE1	1:D:859:TYR:OH	2.28	0.52
1:A:680:TRP:NE1	3:A:1207:Y01:OAF	2.39	0.52
1:A:890:LEU:HD11	3:B:1205:Y01:HAU1	1.91	0.52
3:A:1205:Y01:CAN	3:A:1205:Y01:CAC	2.85	0.52
1:B:1033:ILE:N	1:B:1033:ILE:CD1	2.73	0.52
3:B:1208:Y01:CAO	3:B:1208:Y01:CAB	2.85	0.52
1:C:1033:ILE:CD1	1:C:1033:ILE:N	2.73	0.52
3:C:1203:Y01:HAV2	3:C:1203:Y01:OAF	2.10	0.52
1:D:1033:ILE:N	1:D:1033:ILE:CD1	2.73	0.52
3:A:1205:Y01:HAC3	3:A:1205:Y01:HBA	1.88	0.52
3:C:1205:Y01:CAB	1:D:1023:LEU:HD21	2.39	0.52
1:C:890:LEU:HD11	3:D:1204:Y01:HAU1	1.87	0.52
1:D:955:ARG:HG3	1:D:956:ASP:N	2.24	0.52
1:A:955:ARG:O	1:A:956:ASP:C	2.47	0.52
3:B:1205:Y01:CAE	3:B:1205:Y01:CAC	2.85	0.52
1:A:102:UNK:HA	1:A:110:UNK:HA	1.92	0.52
1:C:828:GLU:OE1	1:C:859:TYR:OH	2.28	0.52
3:D:1205:Y01:CAO	3:D:1205:Y01:CAU	2.85	0.52
1:C:1158:ALA:O	1:C:1162:LEU:HB2	2.10	0.51
3:D:1205:Y01:OAG	3:D:1205:Y01:HAV1	2.10	0.51
3:A:1205:Y01:HAV2	3:A:1205:Y01:CAM	2.24	0.51
1:C:979:PRO:O	1:C:980:GLN:HB2	2.09	0.51
1:B:1161:GLN:HG2	1:C:1162:LEU:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:LEU:CD1	1:A:784:MET:SD	2.98	0.51
1:B:102:UNK:HA	1:B:110:UNK:HA	1.92	0.51
1:C:904:VAL:HG12	3:C:1205:Y01:HAK1	1.91	0.51
3:C:1205:Y01:HAD3	3:D:1206:Y01:HAD1	1.92	0.51
1:A:934:LEU:HD21	3:A:1209:Y01:HAN1	1.92	0.51
1:C:1033:ILE:HD12	1:C:1033:ILE:N	2.23	0.51
3:C:1204:Y01:CAE	3:C:1204:Y01:CAC	2.85	0.51
3:B:1208:Y01:CAC	3:B:1208:Y01:CAU	2.85	0.51
3:D:1204:Y01:CAE	3:D:1204:Y01:CAC	2.85	0.51
1:B:469:SER:HA	1:B:474:ARG:HG2	1.93	0.51
3:B:1205:Y01:CAO	3:B:1205:Y01:CAU	2.87	0.51
1:C:890:LEU:CD1	3:D:1204:Y01:CAU	2.76	0.51
1:D:1148:LEU:HD13	1:D:1148:LEU:C	2.31	0.51
3:D:1206:Y01:CAC	3:D:1206:Y01:CAU	2.86	0.51
1:A:1033:ILE:HD11	1:D:975:PHE:CE1	2.43	0.51
1:B:1147:ARG:CD	1:C:1148:LEU:HD12	2.41	0.51
1:C:830:ARG:HH22	1:C:1072:ARG:HD3	1.76	0.51
1:A:1033:ILE:CD1	1:D:975:PHE:CE1	2.92	0.51
1:B:436:ASP:O	1:B:438:PRO:HD2	2.11	0.51
1:C:469:SER:HA	1:C:474:ARG:HG2	1.92	0.51
1:C:783:PHE:CD2	3:C:1204:Y01:OAG	2.64	0.51
1:A:992:ASN:OD1	4:A:1210:NAG:O1	2.29	0.51
1:A:469:SER:HA	1:A:474:ARG:HG2	1.92	0.50
1:C:102:UNK:HA	1:C:110:UNK:HA	1.92	0.50
1:C:979:PRO:C	1:C:981:GLU:H	2.14	0.50
3:D:1203:Y01:HAU2	3:D:1203:Y01:HAO1	1.94	0.50
3:A:1205:Y01:HAN2	3:A:1205:Y01:CAC	2.41	0.50
1:B:828:GLU:OE1	1:B:859:TYR:OH	2.28	0.50
1:C:972:LEU:HD12	1:D:980:GLN:NE2	2.23	0.50
1:D:1032:ASN:C	1:D:1033:ILE:CD1	2.70	0.50
1:B:584:ASN:OD1	1:B:584:ASN:N	2.44	0.50
1:D:870:VAL:O	1:D:874:CYS:HB3	2.11	0.50
1:A:955:ARG:NH2	1:A:1000:TRP:CH2	2.79	0.50
1:B:870:VAL:O	1:B:874:CYS:HB3	2.11	0.50
1:B:955:ARG:NE	1:B:955:ARG:CA	2.74	0.50
1:C:900:MET:SD	3:C:1205:Y01:CAB	3.00	0.50
1:A:828:GLU:OE1	1:A:859:TYR:OH	2.28	0.50
1:A:890:LEU:HD11	3:B:1205:Y01:HBF	1.94	0.50
1:C:900:MET:HE1	3:C:1205:Y01:CAB	2.41	0.50
1:D:469:SER:HA	1:D:474:ARG:HG2	1.92	0.50
1:A:1148:LEU:HD12	1:D:1147:ARG:CD	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1209:Y01:HAB3	3:A:1209:Y01:HAO1	1.92	0.50
1:B:830:ARG:HH22	1:B:1072:ARG:HD3	1.76	0.50
1:C:1147:ARG:HD2	1:D:1148:LEU:HD12	1.93	0.50
1:D:436:ASP:O	1:D:438:PRO:HD2	2.11	0.50
1:D:830:ARG:HH22	1:D:1072:ARG:HD3	1.76	0.50
1:C:955:ARG:NE	1:C:955:ARG:CA	2.73	0.49
3:C:1203:Y01:HAB3	3:C:1203:Y01:CAC	2.34	0.49
1:D:102:UNK:HA	1:D:110:UNK:HA	1.92	0.49
3:D:1205:Y01:CAB	3:D:1205:Y01:CBB	2.86	0.49
3:D:1207:Y01:CAA	3:D:1207:Y01:CAO	2.85	0.49
1:C:870:VAL:O	1:C:874:CYS:HB3	2.11	0.49
1:A:870:VAL:O	1:A:874:CYS:HB3	2.11	0.49
1:A:1147:ARG:HD2	1:B:1148:LEU:HD12	1.94	0.49
3:A:1205:Y01:CBA	3:A:1205:Y01:CAC	2.85	0.49
1:B:588:SER:O	1:B:592:ALA:CB	2.55	0.49
1:C:788:VAL:HG22	3:C:1204:Y01:CAU	2.43	0.49
1:C:888:TYR:OH	1:C:892:ARG:NH1	2.46	0.49
3:D:1204:Y01:CAU	3:D:1204:Y01:CAO	2.91	0.49
1:D:693:LEU:CD1	1:D:784:MET:SD	3.01	0.49
1:A:815:LEU:HA	1:A:818:TYR:HD2	1.77	0.49
1:A:830:ARG:HH22	1:A:1072:ARG:HD3	1.76	0.49
1:C:436:ASP:O	1:C:438:PRO:HD2	2.11	0.49
1:C:972:LEU:HD12	1:D:980:GLN:HE22	1.77	0.49
1:A:888:TYR:OH	1:A:892:ARG:NH1	2.46	0.49
1:C:461:ALA:O	1:C:465:SER:HB3	2.13	0.49
1:D:992:ASN:OD1	4:D:1208:NAG:O1	2.29	0.49
1:B:20:UNK:O	1:B:24:UNK:CB	2.61	0.49
1:D:461:ALA:O	1:D:465:SER:HB3	2.13	0.49
1:D:815:LEU:HA	1:D:818:TYR:HD2	1.77	0.49
3:B:1206:Y01:HAE2	3:B:1206:Y01:HAC2	1.95	0.49
1:C:20:UNK:O	1:C:24:UNK:CB	2.61	0.49
1:A:20:UNK:O	1:A:24:UNK:CB	2.61	0.49
1:D:20:UNK:O	1:D:24:UNK:CB	2.61	0.49
1:B:461:ALA:O	1:B:465:SER:HB3	2.13	0.48
1:C:417:ASP:HB3	1:C:419:GLN:HG2	1.95	0.48
1:D:955:ARG:NE	1:D:955:ARG:CA	2.74	0.48
1:D:690:ILE:HG21	3:D:1205:Y01:HAV2	1.95	0.48
1:A:263:UNK:O	1:A:267:UNK:CB	2.62	0.48
1:A:816:LEU:O	1:A:820:TRP:HB2	2.14	0.48
1:B:417:ASP:HB3	1:B:419:GLN:HG2	1.95	0.48
3:D:1201:Y01:CAB	3:D:1201:Y01:CAO	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:SER:O	1:A:592:ALA:CB	2.55	0.48
1:A:901:VAL:HG22	3:A:1208:Y01:CAC	2.42	0.48
1:C:263:UNK:O	1:C:267:UNK:CB	2.62	0.48
1:C:815:LEU:HA	1:C:818:TYR:HD2	1.78	0.48
3:D:1205:Y01:CAO	3:D:1205:Y01:CAB	2.86	0.48
1:A:436:ASP:O	1:A:438:PRO:HD2	2.11	0.48
1:B:263:UNK:O	1:B:267:UNK:CB	2.62	0.48
1:C:693:LEU:CD1	1:C:784:MET:SD	3.02	0.48
3:A:1209:Y01:CAB	3:A:1209:Y01:HAO1	2.43	0.48
1:B:888:TYR:OH	1:B:892:ARG:NH1	2.46	0.48
3:B:1204:Y01:OAG	3:B:1204:Y01:HAV1	2.13	0.48
3:B:1208:Y01:HAB2	1:C:1029:LEU:CD1	2.42	0.48
1:A:417:ASP:HB3	1:A:419:GLN:HG2	1.95	0.48
1:B:955:ARG:HB2	1:B:1011:CYS:HB3	1.96	0.48
1:B:960:PRO:CB	3:B:1204:Y01:HAT2	2.43	0.48
3:C:1202:Y01:CAC	3:C:1202:Y01:CAU	2.90	0.48
1:D:263:UNK:O	1:D:267:UNK:CB	2.62	0.48
1:A:1162:LEU:C	1:D:1161:GLN:NE2	2.67	0.48
1:B:815:LEU:HA	1:B:818:TYR:HD2	1.78	0.48
3:A:1205:Y01:CAU	3:A:1205:Y01:HAO1	2.44	0.47
1:B:1047:PHE:O	1:B:1051:GLN:CB	2.62	0.47
3:C:1203:Y01:CAE	3:C:1203:Y01:CAC	2.85	0.47
1:A:681:TRP:HB3	1:A:684:MET:HB2	1.96	0.47
1:C:960:PRO:HB2	3:C:1202:Y01:CAI	2.44	0.47
3:C:1203:Y01:HAC1	3:C:1203:Y01:HAP1	1.72	0.47
1:D:417:ASP:HB3	1:D:419:GLN:HG2	1.95	0.47
1:D:585:ALA:HB2	1:D:626:LEU:HD23	1.96	0.47
1:D:888:TYR:OH	1:D:892:ARG:NH1	2.46	0.47
3:A:1204:Y01:CAE	1:B:1021:VAL:HG11	2.44	0.47
1:B:693:LEU:CD1	1:B:784:MET:SD	3.02	0.47
1:C:588:SER:O	1:C:592:ALA:CB	2.55	0.47
1:C:816:LEU:O	1:C:820:TRP:HB2	2.14	0.47
3:D:1204:Y01:HAN1	3:D:1204:Y01:HBB	1.75	0.47
1:A:1047:PHE:O	1:A:1051:GLN:CB	2.62	0.47
1:C:673:GLN:HE22	1:C:1059:LYS:HB3	1.80	0.47
1:C:1047:PHE:O	1:C:1051:GLN:CB	2.62	0.47
3:C:1204:Y01:CAO	3:C:1204:Y01:CAU	2.92	0.47
1:D:863:SER:OG	3:D:1207:Y01:HAL1	2.15	0.47
1:A:461:ALA:O	1:A:465:SER:HB3	2.13	0.47
1:A:684:MET:HG3	1:A:710:PHE:HB3	1.96	0.47
1:A:1162:LEU:HD22	1:B:1162:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1209:Y01:CAC	3:A:1209:Y01:CAU	2.91	0.47
1:B:585:ALA:HB2	1:B:626:LEU:HD23	1.96	0.47
1:B:1162:LEU:CD2	1:C:1162:LEU:HD21	2.45	0.47
3:C:1203:Y01:CAU	3:C:1203:Y01:CAO	2.92	0.47
1:D:588:SER:O	1:D:592:ALA:CB	2.55	0.47
1:D:681:TRP:HB3	1:D:684:MET:HB2	1.96	0.47
1:D:816:LEU:O	1:D:820:TRP:HB2	2.13	0.47
1:D:1047:PHE:O	1:D:1051:GLN:CB	2.62	0.47
3:A:1205:Y01:CAC	3:A:1205:Y01:HBA	2.44	0.47
1:C:904:VAL:CG1	3:C:1205:Y01:HAK1	2.45	0.47
1:D:904:VAL:HG21	3:D:1207:Y01:HAQ1	1.96	0.47
1:A:1162:LEU:C	1:D:1161:GLN:HE21	2.17	0.47
1:C:961:SER:OG	1:C:965:ARG:NH1	2.48	0.47
1:D:673:GLN:HE22	1:D:1059:LYS:HB3	1.80	0.47
1:D:961:SER:OG	1:D:965:ARG:NH1	2.48	0.47
1:B:673:GLN:HE22	1:B:1059:LYS:HB3	1.80	0.47
1:D:684:MET:HG3	1:D:710:PHE:HB3	1.96	0.47
3:D:1205:Y01:CBA	3:D:1205:Y01:CBB	2.86	0.46
1:A:585:ALA:HB2	1:A:626:LEU:HD23	1.96	0.46
3:A:1206:Y01:HAC1	3:A:1206:Y01:CAU	2.40	0.46
3:A:1207:Y01:CAU	3:A:1207:Y01:CAO	2.94	0.46
3:A:1209:Y01:HAC3	1:B:1026:ILE:CD1	2.45	0.46
1:B:681:TRP:HB3	1:B:684:MET:HB2	1.96	0.46
3:B:1204:Y01:HAQ2	1:C:1021:VAL:CB	2.44	0.46
3:D:1206:Y01:HAJ2	3:D:1206:Y01:HAP1	1.94	0.46
1:B:684:MET:HG3	1:B:710:PHE:HB3	1.96	0.46
1:B:788:VAL:HG22	3:B:1206:Y01:CAS	2.45	0.46
3:B:1204:Y01:CAP	3:B:1204:Y01:CAJ	2.88	0.46
1:C:681:TRP:HB3	1:C:684:MET:HB2	1.96	0.46
3:D:1201:Y01:OAG	3:D:1201:Y01:HAV2	2.16	0.46
1:A:796:LEU:CD1	1:A:817:LEU:CD2	2.93	0.46
1:C:585:ALA:HB2	1:C:626:LEU:HD23	1.96	0.46
1:C:863:SER:OG	3:C:1205:Y01:HAM2	2.15	0.46
1:C:955:ARG:O	1:C:956:ASP:C	2.54	0.46
1:D:971:TYR:CE2	1:D:975:PHE:HE2	2.34	0.46
3:D:1205:Y01:HAO1	3:D:1205:Y01:CAB	2.38	0.46
1:A:673:GLN:HE22	1:A:1059:LYS:HB3	1.80	0.46
1:A:1148:LEU:HD13	1:A:1148:LEU:O	2.16	0.46
1:C:1083:SER:HA	1:C:1086:ARG:HB3	1.98	0.46
1:C:944:TYR:O	1:C:948:THR:OG1	2.29	0.46
3:A:1207:Y01:HAN1	3:A:1207:Y01:HBB	1.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:UNK:O	1:B:111:UNK:N	2.49	0.46
1:C:684:MET:HG3	1:C:710:PHE:HB3	1.96	0.46
1:D:1015:TYR:HH	3:D:1204:Y01:HAD2	1.80	0.46
3:D:1205:Y01:HAC3	3:D:1205:Y01:HAJ2	1.74	0.46
1:A:955:ARG:NE	1:A:955:ARG:CA	2.78	0.45
1:C:101:UNK:O	1:C:111:UNK:N	2.49	0.45
3:C:1204:Y01:HAN1	3:C:1204:Y01:HBB	1.64	0.45
3:C:1205:Y01:HAB2	1:D:1023:LEU:HD21	1.98	0.45
1:D:101:UNK:O	1:D:111:UNK:N	2.49	0.45
1:D:1083:SER:HA	1:D:1086:ARG:HB3	1.98	0.45
3:A:1206:Y01:HAD1	3:D:1207:Y01:HAD1	1.93	0.45
3:A:1209:Y01:HAE2	3:A:1209:Y01:CAC	2.37	0.45
1:B:955:ARG:O	1:B:956:ASP:C	2.54	0.45
1:C:850:ALA:N	1:C:853:SER:OG	2.44	0.45
3:D:1203:Y01:CAO	3:D:1203:Y01:CAU	2.89	0.45
1:A:961:SER:OG	1:A:965:ARG:NH1	2.48	0.45
1:B:793:PHE:HD2	1:B:820:TRP:CD1	2.34	0.45
1:B:961:SER:OG	1:B:965:ARG:NH1	2.48	0.45
1:A:960:PRO:HB2	3:A:1204:Y01:HAI	1.99	0.45
1:B:1015:TYR:CZ	3:B:1205:Y01:HAR1	2.52	0.45
3:C:1201:Y01:HAJ2	3:C:1201:Y01:HAP2	1.95	0.45
1:D:955:ARG:O	1:D:956:ASP:C	2.54	0.45
1:A:101:UNK:O	1:A:111:UNK:N	2.49	0.45
1:A:1083:SER:HA	1:A:1086:ARG:HB3	1.98	0.45
1:B:1031:ALA:HA	1:B:1035:LEU:HD12	1.99	0.45
1:A:820:TRP:O	1:A:823:THR:OG1	2.28	0.45
3:A:1208:Y01:HAB1	3:A:1208:Y01:CAC	2.46	0.45
1:C:864:TRP:CE3	3:C:1205:Y01:CAI	2.87	0.45
3:C:1202:Y01:HAJ2	3:C:1202:Y01:HAA2	1.76	0.45
1:A:788:VAL:HG22	3:A:1207:Y01:HAU2	1.99	0.45
1:A:972:LEU:HD11	1:B:980:GLN:NE2	2.28	0.45
1:C:1147:ARG:CD	1:D:1148:LEU:HD12	2.46	0.45
1:A:975:PHE:CD2	1:B:1028:LEU:HD13	2.52	0.45
3:A:1204:Y01:CAC	3:A:1204:Y01:CAU	2.92	0.45
1:B:1028:LEU:O	1:B:1032:ASN:HB2	2.17	0.45
1:C:1031:ALA:HA	1:C:1035:LEU:HD12	1.99	0.45
1:D:796:LEU:C	1:D:796:LEU:CD1	2.86	0.45
1:A:864:TRP:CZ3	3:A:1208:Y01:HAR1	2.37	0.44
1:C:265:UNK:O	1:C:269:UNK:CB	2.66	0.44
3:A:1206:Y01:CAD	3:D:1207:Y01:HAD3	2.44	0.44
3:A:1206:Y01:HAD2	3:D:1207:Y01:CAD	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1162:LEU:O	1:B:1165:ILE:HG13	2.17	0.44
3:D:1205:Y01:HAC1	3:D:1205:Y01:HAP1	1.73	0.44
1:B:833:LEU:HD22	1:B:852:LEU:HD22	1.98	0.44
1:D:833:LEU:HD22	1:D:852:LEU:HD22	1.98	0.44
3:D:1203:Y01:CAC	3:D:1203:Y01:CAB	2.87	0.44
1:A:1148:LEU:HD13	1:A:1148:LEU:C	2.38	0.44
1:B:265:UNK:O	1:B:269:UNK:CB	2.65	0.44
1:B:796:LEU:HD12	1:B:817:LEU:HD21	2.00	0.44
1:B:973:GLN:HE22	1:B:978:ILE:HG23	1.81	0.44
3:D:1201:Y01:HAJ2	3:D:1201:Y01:HAC3	1.72	0.44
3:B:1208:Y01:HAA3	1:C:1025:VAL:HG12	1.99	0.44
1:C:833:LEU:HD22	1:C:852:LEU:HD22	1.98	0.44
1:D:1081:VAL:HG12	1:D:1084:HIS:H	1.82	0.44
1:A:265:UNK:O	1:A:269:UNK:CB	2.65	0.44
1:B:1081:VAL:HG12	1:B:1084:HIS:H	1.82	0.44
1:C:796:LEU:C	1:C:796:LEU:CD1	2.86	0.44
3:D:1203:Y01:CAC	3:D:1203:Y01:CAE	2.85	0.44
1:A:901:VAL:HG22	3:A:1208:Y01:HAC3	2.00	0.44
1:B:1083:SER:HA	1:B:1086:ARG:HB3	1.98	0.44
1:C:796:LEU:HD12	1:C:817:LEU:HD21	1.99	0.44
1:C:975:PHE:CD2	1:D:1028:LEU:HD13	2.52	0.44
3:D:1205:Y01:CAE	3:D:1205:Y01:CAC	2.85	0.44
1:A:978:ILE:O	1:A:979:PRO:C	2.57	0.44
1:A:1081:VAL:HG12	1:A:1084:HIS:H	1.82	0.44
3:A:1209:Y01:HAD2	3:A:1209:Y01:HAS2	1.78	0.44
4:A:1210:NAG:O7	4:A:1210:NAG:H3	2.16	0.44
1:C:1161:GLN:NE2	1:D:1162:LEU:C	2.71	0.44
1:D:796:LEU:HD12	1:D:817:LEU:HD21	1.99	0.44
1:A:796:LEU:HD12	1:A:817:LEU:HD21	1.97	0.44
1:A:1031:ALA:HA	1:A:1035:LEU:HD12	1.99	0.44
1:B:1148:LEU:C	1:B:1148:LEU:CD1	2.85	0.44
1:D:796:LEU:CD1	1:D:817:LEU:CD2	2.95	0.44
1:B:447:HIS:HA	1:B:452:GLY:HA2	2.00	0.43
1:D:1031:ALA:HA	1:D:1035:LEU:HD12	1.99	0.43
3:A:1205:Y01:HAC1	3:A:1205:Y01:HAP1	1.75	0.43
1:B:1015:TYR:HE1	3:B:1205:Y01:HAR1	1.82	0.43
1:C:977:GLN:NE2	1:D:978:ILE:HB	2.33	0.43
1:A:933:PHE:CE2	1:B:1033:ILE:HG21	2.54	0.43
1:A:934:LEU:CD2	3:A:1209:Y01:HAN1	2.48	0.43
1:A:976:GLY:C	1:A:977:GLN:HG2	2.38	0.43
3:A:1206:Y01:CAS	3:D:1207:Y01:CAE	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:867:CYS:SG	3:B:1207:Y01:HAE1	2.58	0.43
1:C:447:HIS:HA	1:C:452:GLY:HA2	2.00	0.43
1:C:904:VAL:CB	3:C:1205:Y01:CAQ	2.96	0.43
1:C:955:ARG:CG	1:C:956:ASP:H	2.30	0.43
3:C:1203:Y01:HAN1	3:C:1203:Y01:HBB	1.75	0.43
1:A:796:LEU:C	1:A:796:LEU:CD1	2.86	0.43
3:A:1206:Y01:HAE2	3:A:1206:Y01:HBB	1.87	0.43
3:A:1209:Y01:HAC2	1:B:1026:ILE:HG12	2.00	0.43
1:C:975:PHE:CE2	1:D:1028:LEU:HD13	2.53	0.43
3:D:1203:Y01:CAC	3:D:1203:Y01:HAE2	2.39	0.43
1:C:437:ARG:HA	1:C:440:PHE:HD2	1.84	0.43
3:D:1206:Y01:HAD2	3:D:1206:Y01:HAS2	1.80	0.43
1:A:854:GLN:HE21	1:A:854:GLN:CA	2.00	0.43
1:A:1162:LEU:O	1:A:1165:ILE:HG13	2.18	0.43
3:A:1207:Y01:HAB1	3:A:1207:Y01:HAJ2	1.83	0.43
1:C:1081:VAL:HG12	1:C:1084:HIS:H	1.83	0.43
1:D:265:UNK:O	1:D:269:UNK:CB	2.65	0.43
1:A:1039:LEU:CD1	1:B:1033:ILE:HG23	2.49	0.43
3:B:1206:Y01:HAA2	3:B:1206:Y01:HAJ2	1.77	0.43
3:D:1206:Y01:CAP	3:D:1206:Y01:CAJ	2.85	0.43
1:B:437:ARG:HA	1:B:440:PHE:HD2	1.84	0.43
3:B:1205:Y01:HAC3	3:B:1205:Y01:CAN	2.44	0.43
1:A:605:ASP:N	1:A:605:ASP:OD1	2.52	0.43
3:B:1207:Y01:HAA1	1:C:1023:LEU:CD2	2.47	0.43
3:C:1202:Y01:CAE	1:D:1021:VAL:HG11	2.49	0.43
1:A:447:HIS:HA	1:A:452:GLY:HA2	2.00	0.43
3:B:1204:Y01:HBB	3:B:1204:Y01:HAE2	1.68	0.43
1:C:992:ASN:OD1	4:C:1206:NAG:O1	2.37	0.43
3:C:1201:Y01:CAC	3:C:1201:Y01:CAU	2.96	0.43
3:D:1207:Y01:HAJ2	3:D:1207:Y01:HAB3	1.79	0.43
1:B:955:ARG:CG	1:B:956:ASP:H	2.32	0.42
1:D:437:ARG:HA	1:D:440:PHE:HD2	1.84	0.42
3:D:1202:Y01:HAC1	3:D:1202:Y01:CAU	2.46	0.42
3:D:1206:Y01:HAC1	3:D:1206:Y01:CAU	2.39	0.42
1:C:955:ARG:HA	1:C:955:ARG:NH2	2.32	0.42
1:A:584:ASN:HB3	1:A:1125:GLU:OE1	2.20	0.42
3:A:1204:Y01:HAE2	1:B:1021:VAL:HG11	2.01	0.42
3:A:1206:Y01:HAS2	3:D:1207:Y01:HAE1	2.01	0.42
3:A:1209:Y01:HAC2	1:B:1026:ILE:CG1	2.50	0.42
1:B:633:SER:HG	1:B:1128:HIS:CE1	2.31	0.42
1:A:437:ARG:HA	1:A:440:PHE:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:976:GLY:O	1:A:977:GLN:CD	2.57	0.42
1:A:983:MET:O	1:A:984:ASP:C	2.57	0.42
1:B:1032:ASN:HB3	1:B:1033:ILE:HD12	2.02	0.42
3:C:1205:Y01:HAO2	3:C:1205:Y01:HBA	1.81	0.42
1:D:447:HIS:HA	1:D:452:GLY:HA2	2.00	0.42
3:D:1206:Y01:HAD3	3:D:1206:Y01:HBD	1.84	0.42
1:B:912:VAL:HG22	1:B:1065:LEU:HD13	2.01	0.42
1:C:584:ASN:HD22	1:C:1122:LEU:HD22	1.84	0.42
1:D:649:TRP:O	1:D:651:ASP:N	2.52	0.42
1:D:955:ARG:HA	1:D:955:ARG:NH1	2.30	0.42
3:A:1208:Y01:HAE1	3:A:1208:Y01:HAS2	1.83	0.42
1:B:605:ASP:OD1	1:B:605:ASP:N	2.52	0.42
1:B:972:LEU:HD11	1:C:980:GLN:NE2	2.32	0.42
3:C:1205:Y01:HAN1	3:C:1205:Y01:HBB	1.79	0.42
1:D:955:ARG:CG	1:D:956:ASP:H	2.31	0.42
3:B:1205:Y01:HAN2	3:B:1205:Y01:CAC	2.44	0.42
3:A:1206:Y01:HAD2	3:A:1206:Y01:HAS2	1.80	0.42
1:B:796:LEU:C	1:B:796:LEU:CD1	2.86	0.42
1:B:890:LEU:CD1	3:C:1203:Y01:CAU	2.76	0.42
1:B:1015:TYR:CZ	3:B:1205:Y01:CAR	3.01	0.42
3:D:1201:Y01:HAC1	3:D:1201:Y01:CAU	2.36	0.42
3:A:1205:Y01:HAU2	1:D:890:LEU:CD1	2.50	0.41
1:D:1039:LEU:HD23	1:D:1039:LEU:HA	1.91	0.41
1:D:605:ASP:OD1	1:D:605:ASP:N	2.52	0.41
1:A:1072:ARG:HA	1:A:1073:PRO:HD3	1.88	0.41
3:A:1205:Y01:HBA	3:A:1205:Y01:HBB	2.02	0.41
1:B:975:PHE:HE1	1:C:1028:LEU:HD13	1.83	0.41
1:D:787:VAL:HG11	3:D:1205:Y01:HAT2	2.03	0.41
3:D:1201:Y01:HAJ1	3:D:1201:Y01:HAA2	1.73	0.41
3:B:1203:Y01:HAA1	3:B:1203:Y01:HAJ2	1.90	0.41
1:C:605:ASP:N	1:C:605:ASP:OD1	2.52	0.41
1:C:649:TRP:O	1:C:651:ASP:N	2.52	0.41
1:C:972:LEU:HD11	1:D:980:GLN:NE2	2.35	0.41
3:D:1201:Y01:HAS2	3:D:1201:Y01:HAE1	1.84	0.41
1:A:960:PRO:HB2	3:A:1204:Y01:CAI	2.51	0.41
3:A:1209:Y01:HAU2	3:A:1209:Y01:HAC2	2.01	0.41
1:C:973:GLN:NE2	1:C:978:ILE:HG23	2.26	0.41
1:A:900:MET:HE2	3:A:1208:Y01:HAJ1	2.01	0.41
3:A:1205:Y01:HBA	3:A:1205:Y01:CBB	2.51	0.41
1:B:1072:ARG:HA	1:B:1073:PRO:HD3	1.88	0.41
1:D:967:PHE:HD1	3:D:1202:Y01:HAB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:TRP:O	1:B:651:ASP:N	2.52	0.41
3:D:1203:Y01:HAB1	3:D:1203:Y01:HAC1	1.96	0.41
3:D:1204:Y01:HAD2	3:D:1204:Y01:HAS2	1.84	0.41
1:A:887:LEU:HD13	1:A:890:LEU:HD12	2.03	0.41
1:B:887:LEU:HD13	1:B:890:LEU:HD12	2.03	0.41
3:B:1205:Y01:HAS2	3:B:1205:Y01:HAE1	1.90	0.41
1:A:964:ARG:NH1	1:B:984:ASP:OD2	2.39	0.41
1:A:992:ASN:ND2	4:A:1210:NAG:C1	2.80	0.41
3:B:1208:Y01:HAC1	3:B:1208:Y01:HAE2	2.01	0.41
1:C:895:LEU:HD23	1:C:895:LEU:HA	1.92	0.41
1:D:1062:ARG:O	1:D:1066:ILE:HG12	2.21	0.41
3:D:1207:Y01:HAC3	3:D:1207:Y01:CAA	2.50	0.41
1:B:975:PHE:CZ	1:C:1028:LEU:HB3	2.56	0.41
3:A:1206:Y01:HAS1	3:D:1207:Y01:CAE	2.51	0.40
1:B:976:GLY:HA2	1:C:976:GLY:HA3	2.03	0.40
1:B:1161:GLN:CD	1:C:1162:LEU:HD12	2.40	0.40
1:D:620:GLU:O	1:D:624:VAL:HB	2.21	0.40
1:D:973:GLN:HB2	1:D:1027:PHE:HE2	1.86	0.40
3:D:1203:Y01:HAC1	3:D:1203:Y01:HAP1	1.72	0.40
1:A:620:GLU:O	1:A:624:VAL:HB	2.22	0.40
3:D:1203:Y01:HAB1	3:D:1203:Y01:HAC3	1.94	0.40
1:A:967:PHE:CD1	3:A:1204:Y01:CAB	3.05	0.40
1:B:793:PHE:CD1	1:B:793:PHE:O	2.75	0.40
3:C:1205:Y01:HAD2	3:D:1206:Y01:CAD	2.51	0.40
1:A:953:ARG:HA	1:A:954:PRO:HD3	1.90	0.40
1:B:1165:ILE:HG22	1:C:1169:GLU:HG3	2.04	0.40
1:C:887:LEU:HD13	1:C:890:LEU:HD12	2.03	0.40
1:C:973:GLN:HB2	1:C:1027:PHE:HE2	1.86	0.40
3:D:1204:Y01:HAB1	3:D:1204:Y01:HAJ2	1.72	0.40
3:A:1206:Y01:HAD2	3:D:1207:Y01:HAE1	2.04	0.40
3:C:1205:Y01:HAB3	1:D:1023:LEU:HD21	2.02	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	607/977 (62%)	556 (92%)	49 (8%)	2 (0%)	37	67
1	B	607/977 (62%)	556 (92%)	49 (8%)	2 (0%)	37	67
1	C	607/977 (62%)	555 (91%)	50 (8%)	2 (0%)	37	67
1	D	607/977 (62%)	555 (91%)	49 (8%)	3 (0%)	25	57
All	All	2428/3908 (62%)	2222 (92%)	197 (8%)	9 (0%)	32	62

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	701	PRO
1	B	701	PRO
1	C	701	PRO
1	D	701	PRO
1	D	976	GLY
1	A	437	ARG
1	B	437	ARG
1	C	437	ARG
1	D	437	ARG

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	441/655 (67%)	433 (98%)	8 (2%)	54	71
1	B	440/655 (67%)	429 (98%)	11 (2%)	42	62
1	C	440/655 (67%)	432 (98%)	8 (2%)	54	71
1	D	441/655 (67%)	435 (99%)	6 (1%)	62	76
All	All	1762/2620 (67%)	1729 (98%)	33 (2%)	52	70

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	584	ASN
1	A	678	GLN
1	A	797	PHE
1	A	854	GLN
1	A	955	ARG
1	A	1011	CYS
1	A	1162	LEU
1	A	1166	ARG
1	B	678	GLN
1	B	793	PHE
1	B	820	TRP
1	B	853	SER
1	B	955	ARG
1	B	1011	CYS
1	B	1064	ARG
1	B	1067	ARG
1	B	1143	SER
1	B	1162	LEU
1	B	1166	ARG
1	C	584	ASN
1	C	678	GLN
1	C	793	PHE
1	C	955	ARG
1	C	1011	CYS
1	C	1067	ARG
1	C	1162	LEU
1	C	1166	ARG
1	D	584	ASN
1	D	678	GLN
1	D	853	SER
1	D	955	ARG
1	D	1011	CYS
1	D	1166	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	447	HIS
1	A	854	GLN
1	A	973	GLN
1	A	977	GLN
1	B	447	HIS
1	B	980	GLN

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Mol	Chain	Res	Type
1	C	447	HIS
1	C	584	ASN
1	C	973	GLN
1	C	977	GLN
1	C	980	GLN
1	C	992	ASN
1	C	1161	GLN
1	D	447	HIS
1	D	973	GLN
1	D	977	GLN
1	D	980	GLN
1	D	992	ASN
1	D	1161	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](#)

Of 33 ligands modelled in this entry, 5 are monoatomic - leaving 28 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	Y01	C	1202	-	38,38,38	1.91	7 (18%)	57,57,57	1.72	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1209	-	15,15,15	0.43	0	21,21,21	0.64	0
3	Y01	D	1201	-	38,38,38	1.84	6 (15%)	57,57,57	1.61	7 (12%)
3	Y01	A	1204	-	38,38,38	1.90	5 (13%)	57,57,57	1.65	10 (17%)
3	Y01	B	1208	-	38,38,38	1.82	7 (18%)	57,57,57	2.06	14 (24%)
4	NAG	D	1208	-	15,15,15	0.43	0	21,21,21	0.65	0
3	Y01	D	1205	-	38,38,38	1.77	5 (13%)	57,57,57	1.88	16 (28%)
3	Y01	B	1205	-	38,38,38	1.74	5 (13%)	57,57,57	1.74	13 (22%)
4	NAG	A	1210	-	15,15,15	0.62	1 (6%)	21,21,21	1.00	1 (4%)
3	Y01	A	1208	-	38,38,38	1.85	6 (15%)	57,57,57	1.87	14 (24%)
3	Y01	B	1206	-	38,38,38	1.81	5 (13%)	57,57,57	1.79	14 (24%)
3	Y01	C	1201	-	38,38,38	1.82	6 (15%)	57,57,57	1.69	12 (21%)
3	Y01	B	1207	-	38,38,38	1.81	5 (13%)	57,57,57	1.84	15 (26%)
3	Y01	C	1204	-	38,38,38	1.83	6 (15%)	57,57,57	1.88	17 (29%)
3	Y01	A	1209	-	38,38,38	1.86	6 (15%)	57,57,57	1.88	12 (21%)
3	Y01	C	1205	-	38,38,38	1.84	6 (15%)	57,57,57	2.02	15 (26%)
3	Y01	D	1204	-	38,38,38	1.75	5 (13%)	57,57,57	1.77	13 (22%)
3	Y01	A	1207	-	38,38,38	1.81	6 (15%)	57,57,57	1.85	15 (26%)
3	Y01	D	1203	-	38,38,38	1.84	6 (15%)	57,57,57	1.66	11 (19%)
3	Y01	B	1204	-	38,38,38	1.80	7 (18%)	57,57,57	1.89	13 (22%)
3	Y01	A	1206	-	38,38,38	1.84	6 (15%)	57,57,57	1.94	13 (22%)
3	Y01	C	1203	-	38,38,38	1.74	5 (13%)	57,57,57	1.78	13 (22%)
3	Y01	D	1207	-	38,38,38	1.82	6 (15%)	57,57,57	1.91	14 (24%)
3	Y01	A	1205	-	38,38,38	1.73	5 (13%)	57,57,57	1.83	13 (22%)
3	Y01	D	1206	-	38,38,38	1.86	6 (15%)	57,57,57	1.94	12 (21%)
4	NAG	C	1206	-	15,15,15	0.43	0	21,21,21	0.64	0
3	Y01	B	1203	-	38,38,38	1.87	6 (15%)	57,57,57	1.69	10 (17%)
3	Y01	D	1202	-	38,38,38	1.91	6 (15%)	57,57,57	1.71	11 (19%)

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	Y01	C	1202	-	-	9/19/77/77	0/4/4/4
4	NAG	B	1209	-	-	4/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	Y01	D	1201	-	-	7/19/77/77	0/4/4/4
3	Y01	A	1204	-	-	7/19/77/77	0/4/4/4
3	Y01	B	1208	-	-	6/19/77/77	0/4/4/4
4	NAG	D	1208	-	-	4/6/26/26	0/1/1/1
3	Y01	D	1205	-	-	10/19/77/77	0/4/4/4
3	Y01	B	1205	-	-	11/19/77/77	0/4/4/4
4	NAG	A	1210	-	-	1/6/26/26	0/1/1/1
3	Y01	A	1208	-	-	12/19/77/77	0/4/4/4
3	Y01	B	1206	-	-	8/19/77/77	0/4/4/4
3	Y01	C	1201	-	-	5/19/77/77	0/4/4/4
3	Y01	B	1207	-	-	6/19/77/77	0/4/4/4
3	Y01	C	1204	-	-	8/19/77/77	0/4/4/4
3	Y01	A	1209	-	-	11/19/77/77	0/4/4/4
3	Y01	C	1205	-	-	15/19/77/77	0/4/4/4
3	Y01	D	1204	-	-	11/19/77/77	0/4/4/4
3	Y01	A	1207	-	-	10/19/77/77	0/4/4/4
3	Y01	D	1203	-	-	12/19/77/77	0/4/4/4
3	Y01	B	1204	-	-	11/19/77/77	0/4/4/4
3	Y01	A	1206	-	-	9/19/77/77	0/4/4/4
3	Y01	C	1203	-	-	9/19/77/77	0/4/4/4
3	Y01	D	1207	-	-	3/19/77/77	0/4/4/4
3	Y01	A	1205	-	-	9/19/77/77	0/4/4/4
3	Y01	D	1206	-	-	12/19/77/77	0/4/4/4
4	NAG	C	1206	-	-	4/6/26/26	0/1/1/1
3	Y01	B	1203	-	-	5/19/77/77	0/4/4/4
3	Y01	D	1202	-	-	8/19/77/77	0/4/4/4

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1208	Y01	CAV-CAZ	-6.19	1.39	1.51
3	C	1205	Y01	CAV-CAZ	-6.12	1.39	1.51
3	D	1206	Y01	CAV-CAZ	-6.04	1.39	1.51
3	D	1203	Y01	CAV-CAZ	-6.01	1.39	1.51
3	A	1204	Y01	CAV-CAZ	-6.00	1.39	1.51
3	D	1201	Y01	CAV-CAZ	-5.97	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1207	Y01	CAV-CAZ	-5.95	1.39	1.51
3	D	1202	Y01	CAV-CAZ	-5.95	1.39	1.51
3	C	1204	Y01	CAV-CAZ	-5.92	1.39	1.51
3	B	1206	Y01	CAV-CAZ	-5.91	1.39	1.51
3	B	1203	Y01	CAV-CAZ	-5.91	1.39	1.51
3	A	1206	Y01	CAV-CAZ	-5.90	1.39	1.51
3	C	1202	Y01	CAV-CAZ	-5.86	1.39	1.51
3	D	1207	Y01	CAV-CAZ	-5.81	1.40	1.51
3	A	1209	Y01	CAV-CAZ	-5.79	1.40	1.51
3	A	1204	Y01	CBH-CAZ	-5.78	1.41	1.52
3	C	1201	Y01	CAV-CAZ	-5.76	1.40	1.51
3	C	1202	Y01	CBH-CAZ	-5.74	1.41	1.52
3	D	1204	Y01	CAV-CAZ	-5.72	1.40	1.51
3	D	1202	Y01	CBH-CAZ	-5.72	1.42	1.52
3	D	1205	Y01	CAV-CAZ	-5.70	1.40	1.51
3	B	1207	Y01	CAV-CAZ	-5.68	1.40	1.51
3	C	1203	Y01	CAV-CAZ	-5.68	1.40	1.51
3	B	1204	Y01	CAV-CAZ	-5.66	1.40	1.51
3	B	1203	Y01	CBH-CAZ	-5.59	1.42	1.52
3	D	1201	Y01	CBH-CAZ	-5.56	1.42	1.52
3	A	1205	Y01	CAV-CAZ	-5.51	1.40	1.51
3	B	1205	Y01	CAV-CAZ	-5.47	1.40	1.51
3	A	1209	Y01	CBH-CAZ	-5.46	1.42	1.52
3	B	1207	Y01	CBH-CAZ	-5.46	1.42	1.52
3	A	1208	Y01	CBH-CAZ	-5.38	1.42	1.52
3	C	1201	Y01	CBH-CAZ	-5.37	1.42	1.52
3	D	1203	Y01	CBH-CAZ	-5.36	1.42	1.52
3	A	1206	Y01	CBH-CAZ	-5.30	1.42	1.52
3	D	1207	Y01	CBH-CAZ	-5.25	1.42	1.52
3	D	1206	Y01	CBH-CAZ	-5.24	1.42	1.52
3	B	1206	Y01	CBH-CAZ	-5.22	1.42	1.52
3	B	1204	Y01	CBH-CAZ	-5.22	1.42	1.52
3	B	1205	Y01	CBH-CAZ	-5.20	1.43	1.52
3	C	1205	Y01	CBH-CAZ	-5.13	1.43	1.52
3	C	1204	Y01	CBH-CAZ	-5.11	1.43	1.52
3	B	1208	Y01	CAV-CAZ	-5.08	1.41	1.51
3	A	1207	Y01	CBH-CAZ	-5.08	1.43	1.52
3	D	1204	Y01	CBH-CAZ	-5.08	1.43	1.52
3	C	1203	Y01	CBH-CAZ	-5.04	1.43	1.52
3	A	1205	Y01	CBH-CAZ	-5.03	1.43	1.52
3	D	1205	Y01	CBH-CAZ	-4.96	1.43	1.52
3	B	1208	Y01	CBH-CAZ	-4.77	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1204	Y01	CAK-CAI	-4.69	1.40	1.50
3	D	1202	Y01	CAK-CAI	-4.66	1.40	1.50
3	C	1202	Y01	CAK-CAI	-4.62	1.40	1.50
3	D	1203	Y01	CAK-CAI	-4.61	1.40	1.50
3	B	1208	Y01	CAK-CAI	-4.55	1.40	1.50
3	B	1203	Y01	CAK-CAI	-4.50	1.41	1.50
3	D	1205	Y01	CAK-CAI	-4.50	1.41	1.50
3	A	1207	Y01	CAK-CAI	-4.49	1.41	1.50
3	D	1201	Y01	CAK-CAI	-4.46	1.41	1.50
3	C	1204	Y01	CAK-CAI	-4.42	1.41	1.50
3	A	1208	Y01	CAK-CAI	-4.41	1.41	1.50
3	B	1206	Y01	CAK-CAI	-4.37	1.41	1.50
3	D	1207	Y01	CAK-CAI	-4.36	1.41	1.50
3	C	1203	Y01	CAK-CAI	-4.34	1.41	1.50
3	B	1207	Y01	CAK-CAI	-4.32	1.41	1.50
3	C	1205	Y01	CAK-CAI	-4.31	1.41	1.50
3	D	1204	Y01	CAK-CAI	-4.30	1.41	1.50
3	B	1205	Y01	CAK-CAI	-4.29	1.41	1.50
3	D	1206	Y01	CAK-CAI	-4.27	1.41	1.50
3	C	1201	Y01	CAK-CAI	-4.26	1.41	1.50
3	A	1209	Y01	CAK-CAI	-4.20	1.41	1.50
3	A	1205	Y01	CAK-CAI	-4.18	1.41	1.50
3	B	1204	Y01	CAK-CAI	-4.14	1.41	1.50
3	A	1206	Y01	CAK-CAI	-4.13	1.41	1.50
3	A	1205	Y01	CAI-CAZ	3.85	1.40	1.33
3	D	1204	Y01	CAI-CAZ	3.81	1.40	1.33
3	C	1203	Y01	CAI-CAZ	3.81	1.40	1.33
3	B	1205	Y01	CAI-CAZ	3.78	1.40	1.33
3	A	1209	Y01	CAI-CAZ	3.76	1.40	1.33
3	C	1205	Y01	CAI-CAZ	3.75	1.40	1.33
3	B	1204	Y01	CAI-CAZ	3.74	1.40	1.33
3	C	1201	Y01	CAI-CAZ	3.73	1.40	1.33
3	A	1206	Y01	CAI-CAZ	3.70	1.40	1.33
3	B	1206	Y01	CAI-CAZ	3.70	1.40	1.33
3	D	1206	Y01	CAI-CAZ	3.66	1.40	1.33
3	D	1201	Y01	CAI-CAZ	3.65	1.40	1.33
3	A	1208	Y01	CAI-CAZ	3.63	1.40	1.33
3	D	1207	Y01	CAI-CAZ	3.63	1.40	1.33
3	B	1207	Y01	CAI-CAZ	3.62	1.40	1.33
3	C	1204	Y01	CAI-CAZ	3.61	1.40	1.33
3	A	1207	Y01	CAI-CAZ	3.61	1.40	1.33
3	B	1208	Y01	CAI-CAZ	3.60	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1203	Y01	CAI-CAZ	3.59	1.40	1.33
3	D	1203	Y01	CAI-CAZ	3.59	1.40	1.33
3	D	1205	Y01	CAI-CAZ	3.57	1.40	1.33
3	D	1202	Y01	CAI-CAZ	3.45	1.40	1.33
3	C	1202	Y01	CAI-CAZ	3.43	1.40	1.33
3	A	1204	Y01	CAI-CAZ	3.41	1.40	1.33
3	A	1206	Y01	CBI-CBG	-3.25	1.49	1.55
3	C	1204	Y01	CBI-CBG	-3.15	1.49	1.55
3	A	1208	Y01	CBI-CBG	-3.08	1.49	1.55
3	B	1206	Y01	CBI-CBG	-3.01	1.49	1.55
3	A	1204	Y01	CBI-CBG	-2.86	1.49	1.55
3	D	1202	Y01	CBI-CBG	-2.79	1.49	1.55
3	C	1202	Y01	CBI-CBG	-2.77	1.49	1.55
3	A	1209	Y01	CBI-CBG	-2.77	1.49	1.55
3	D	1206	Y01	CBI-CBG	-2.76	1.49	1.55
3	D	1206	Y01	CBI-CBE	-2.73	1.50	1.55
3	B	1208	Y01	CBI-CBE	-2.73	1.50	1.55
3	D	1207	Y01	CBI-CBE	-2.69	1.50	1.55
3	A	1209	Y01	CBI-CBE	-2.67	1.50	1.55
3	B	1203	Y01	CBI-CBG	-2.65	1.50	1.55
3	B	1204	Y01	CBI-CBG	-2.59	1.50	1.55
3	C	1205	Y01	CBI-CBG	-2.59	1.50	1.55
3	D	1201	Y01	CBI-CBG	-2.58	1.50	1.55
3	C	1201	Y01	CBI-CBG	-2.58	1.50	1.55
3	C	1205	Y01	CBD-CBG	-2.52	1.48	1.53
3	B	1207	Y01	CBI-CBE	-2.49	1.50	1.55
3	D	1203	Y01	CBI-CBG	-2.48	1.50	1.55
3	D	1207	Y01	CBI-CBG	-2.47	1.50	1.55
3	B	1203	Y01	CBI-CBE	-2.38	1.50	1.55
3	A	1207	Y01	CBI-CBG	-2.36	1.50	1.55
3	B	1204	Y01	CBI-CBE	-2.34	1.50	1.55
3	B	1208	Y01	CBI-CBG	-2.31	1.50	1.55
3	D	1204	Y01	CBI-CBG	-2.29	1.50	1.55
3	C	1203	Y01	CBI-CBG	-2.25	1.50	1.55
3	D	1201	Y01	CBI-CBE	-2.25	1.50	1.55
3	A	1207	Y01	CBD-CBG	-2.23	1.49	1.53
3	A	1205	Y01	CBI-CBG	-2.21	1.50	1.55
3	C	1204	Y01	CBD-CBG	-2.21	1.49	1.53
3	B	1205	Y01	CBI-CBG	-2.20	1.50	1.55
3	D	1205	Y01	CBI-CBG	-2.18	1.51	1.55
4	A	1210	NAG	O1-C1	-2.15	1.32	1.39
3	A	1206	Y01	CBI-CBE	-2.15	1.51	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1202	Y01	CBI-CBE	-2.13	1.51	1.55
3	C	1201	Y01	CBI-CBE	-2.07	1.51	1.55
3	B	1208	Y01	OAW-CBC	-2.07	1.41	1.46
3	D	1202	Y01	CBD-CBG	-2.06	1.49	1.53
3	C	1202	Y01	CBD-CBG	-2.04	1.49	1.53
3	A	1208	Y01	CBD-CBG	-2.03	1.49	1.53
3	B	1204	Y01	CAU-CBI	-2.03	1.50	1.54
3	D	1203	Y01	CBD-CBG	-2.01	1.49	1.53

All (308) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1204	Y01	CBI-CBE-CBB	-5.97	110.28	119.50
3	C	1205	Y01	CAQ-CBG-CBD	-5.70	110.01	119.10
3	B	1208	Y01	CAV-CAZ-CBH	5.66	123.66	116.42
3	A	1206	Y01	CBI-CBE-CBB	-5.58	110.89	119.50
3	B	1203	Y01	CBI-CBE-CBB	-5.47	111.05	119.50
3	C	1201	Y01	CBI-CBE-CBB	-5.25	111.39	119.50
3	B	1208	Y01	CBC-OAW-CAY	-5.23	105.29	117.80
3	D	1202	Y01	CBI-CBE-CBB	-5.11	111.60	119.50
3	D	1201	Y01	CBI-CBE-CBB	-4.95	111.86	119.50
3	C	1202	Y01	CBI-CBE-CBB	-4.94	111.86	119.50
3	C	1205	Y01	CAD-CBH-CBF	-4.90	106.17	111.66
3	D	1207	Y01	CBI-CBE-CBB	-4.89	111.95	119.50
3	A	1204	Y01	CBI-CBE-CBB	-4.86	111.99	119.50
3	A	1209	Y01	CBI-CBG-CBD	-4.82	107.57	114.41
3	D	1206	Y01	CBI-CBG-CBD	-4.71	107.73	114.41
3	D	1206	Y01	CAQ-CBG-CBD	-4.61	111.74	119.10
3	D	1206	Y01	CBI-CBE-CBB	-4.57	112.44	119.50
3	D	1203	Y01	CBI-CBE-CBB	-4.56	112.45	119.50
3	A	1209	Y01	CBI-CBE-CBB	-4.52	112.52	119.50
3	A	1208	Y01	CBG-CBI-CBE	-4.48	94.95	100.10
3	A	1209	Y01	CAQ-CBG-CBD	-4.47	111.96	119.10
3	C	1205	Y01	CBH-CBF-CBD	-4.40	106.28	112.71
3	A	1206	Y01	CBH-CBF-CBD	-4.34	106.38	112.71
3	D	1206	Y01	CBH-CBF-CBD	-4.27	106.48	112.71
3	D	1206	Y01	CAD-CBH-CBF	-4.26	106.88	111.66
3	B	1208	Y01	CBI-CBE-CBB	-4.25	112.93	119.50
3	B	1204	Y01	CAQ-CBG-CBD	-4.25	112.32	119.10
3	A	1207	Y01	CAD-CBH-CBF	-4.24	106.90	111.66
3	A	1206	Y01	CAD-CBH-CBF	-4.23	106.91	111.66
3	D	1204	Y01	CAQ-CBG-CBD	-4.22	112.38	119.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1208	Y01	CBH-CBF-CBD	-4.20	106.58	112.71
3	C	1205	Y01	CBI-CBG-CBD	-4.18	108.48	114.41
3	C	1203	Y01	CAQ-CBG-CBD	-4.17	112.45	119.10
3	D	1207	Y01	CAD-CBH-CBF	-4.16	106.99	111.66
3	D	1202	Y01	CAQ-CBG-CBD	-4.15	112.47	119.10
3	A	1205	Y01	CAQ-CBG-CBD	-4.13	112.51	119.10
3	B	1207	Y01	CBI-CBE-CBB	-4.12	113.14	119.50
3	C	1204	Y01	CAD-CBH-CBF	-4.12	107.04	111.66
3	A	1206	Y01	CBI-CBG-CBD	-4.11	108.58	114.41
3	A	1209	Y01	CBH-CBF-CBD	-4.09	106.73	112.71
3	C	1204	Y01	CBG-CBI-CBE	-4.08	95.42	100.10
3	C	1201	Y01	CBI-CBG-CBD	-4.06	108.64	114.41
3	C	1203	Y01	CAD-CBH-CBF	-4.06	107.10	111.66
3	A	1205	Y01	CAD-CBH-CBF	-4.05	107.12	111.66
3	A	1207	Y01	CAQ-CBG-CBD	-4.02	112.68	119.10
3	D	1207	Y01	CAQ-CBG-CBD	-4.02	112.69	119.10
3	B	1203	Y01	CBI-CBG-CBD	-4.01	108.72	114.41
3	B	1206	Y01	CBG-CBI-CBE	-3.99	95.52	100.10
3	C	1201	Y01	CAQ-CBG-CBD	-3.99	112.74	119.10
3	B	1204	Y01	CBI-CBG-CBD	-3.98	108.76	114.41
3	D	1204	Y01	CAD-CBH-CBF	-3.98	107.20	111.66
3	D	1201	Y01	CBI-CBG-CBD	-3.94	108.82	114.41
3	C	1205	Y01	CAV-CAZ-CBH	3.94	121.46	116.42
3	A	1205	Y01	CBH-CBF-CBD	-3.93	106.96	112.71
3	D	1207	Y01	CBH-CBF-CBD	-3.90	107.02	112.71
3	A	1208	Y01	CAD-CBH-CBF	-3.89	107.30	111.66
3	B	1203	Y01	CAQ-CBG-CBD	-3.88	112.91	119.10
3	B	1206	Y01	CAD-CBH-CBF	-3.88	107.31	111.66
3	B	1208	Y01	CAQ-CBG-CBD	-3.88	112.91	119.10
3	C	1205	Y01	CBG-CBI-CBE	-3.87	95.65	100.10
3	B	1207	Y01	CAD-CBH-CBF	-3.87	107.32	111.66
3	A	1204	Y01	CBI-CBG-CBD	-3.87	108.92	114.41
3	D	1203	Y01	CAQ-CBG-CBD	-3.86	112.93	119.10
3	C	1202	Y01	CBI-CBG-CBD	-3.85	108.94	114.41
3	A	1208	Y01	CAQ-CBG-CBD	-3.85	112.97	119.10
3	A	1207	Y01	CBG-CBI-CBE	-3.83	95.70	100.10
3	C	1202	Y01	CAQ-CBG-CBD	-3.82	113.01	119.10
3	D	1205	Y01	CBI-CBE-CBB	-3.81	113.62	119.50
3	B	1207	Y01	CBG-CBI-CBE	-3.80	95.74	100.10
3	A	1209	Y01	CAD-CBH-CBF	-3.78	107.42	111.66
3	B	1205	Y01	CAQ-CBG-CBD	-3.78	113.07	119.10
3	D	1207	Y01	CBI-CBG-CBD	-3.77	109.06	114.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1204	Y01	CAQ-CBG-CBD	-3.75	113.12	119.10
3	A	1206	Y01	CAQ-CBG-CBD	-3.74	113.14	119.10
3	D	1205	Y01	CAT-CAR-CBC	-3.74	104.24	110.33
3	D	1202	Y01	CBI-CBG-CBD	-3.72	109.13	114.41
3	A	1205	Y01	CBI-CBG-CBD	-3.72	109.14	114.41
3	A	1204	Y01	CAQ-CBG-CBD	-3.72	113.17	119.10
3	D	1203	Y01	CBI-CBG-CBD	-3.71	109.15	114.41
3	D	1204	Y01	CBI-CBG-CBD	-3.70	109.16	114.41
3	B	1208	Y01	CAV-CAZ-CAI	-3.69	115.57	120.57
3	B	1205	Y01	CBI-CBG-CBD	-3.65	109.24	114.41
3	B	1205	Y01	CAD-CBH-CBF	-3.63	107.59	111.66
4	A	1210	NAG	O1-C1-C2	3.60	116.71	109.22
3	D	1206	Y01	CAV-CAZ-CBH	3.60	121.03	116.42
3	D	1206	Y01	CAT-CAR-CBC	-3.58	104.49	110.33
3	D	1204	Y01	CBI-CBE-CBB	-3.58	113.97	119.50
3	C	1203	Y01	CBI-CBG-CBD	-3.58	109.34	114.41
3	A	1206	Y01	CAT-CAR-CBC	-3.57	104.52	110.33
3	C	1204	Y01	CAV-CAZ-CBH	3.57	120.99	116.42
3	A	1207	Y01	CAV-CAZ-CBH	3.56	120.98	116.42
3	A	1208	Y01	CBC-OAW-CAY	-3.56	109.28	117.80
3	D	1204	Y01	CBH-CBF-CBD	-3.56	107.52	112.71
3	A	1205	Y01	CBI-CBE-CBB	-3.55	114.02	119.50
3	A	1209	Y01	CBF-CBH-CAZ	3.55	114.85	109.65
3	B	1205	Y01	CBI-CBE-CBB	-3.54	114.03	119.50
3	C	1203	Y01	CBH-CBF-CBD	-3.51	107.58	112.71
3	D	1201	Y01	CAQ-CBG-CBD	-3.51	113.50	119.10
3	B	1204	Y01	CAP-CBE-CBI	-3.51	99.72	103.84
3	B	1206	Y01	CBI-CBG-CBD	-3.50	109.44	114.41
3	D	1205	Y01	CAV-CAZ-CBH	3.49	120.89	116.42
3	C	1203	Y01	CAV-CAZ-CBH	3.49	120.89	116.42
3	C	1203	Y01	CBI-CBE-CBB	-3.47	114.14	119.50
3	A	1208	Y01	CBH-CBF-CBD	-3.46	107.65	112.71
3	B	1204	Y01	CAD-CBH-CBF	-3.45	107.78	111.66
3	D	1204	Y01	CAV-CAZ-CBH	3.45	120.84	116.42
3	D	1205	Y01	CBG-CBI-CBE	-3.44	96.15	100.10
3	B	1207	Y01	CAQ-CBG-CBD	-3.43	113.62	119.10
3	A	1205	Y01	CAV-CAZ-CBH	3.41	120.79	116.42
3	D	1205	Y01	CAQ-CBG-CBD	-3.41	113.66	119.10
3	B	1206	Y01	CBH-CBF-CBD	-3.40	107.74	112.71
3	A	1206	Y01	CAV-CAZ-CBH	3.40	120.78	116.42
3	A	1208	Y01	CBI-CBG-CBD	-3.40	109.59	114.41
3	A	1208	Y01	CAV-CAZ-CBH	3.38	120.75	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1206	Y01	CAV-CAZ-CBH	3.35	120.71	116.42
3	C	1204	Y01	CBI-CBE-CBB	-3.35	114.33	119.50
3	B	1206	Y01	CAQ-CBG-CBD	-3.34	113.78	119.10
3	B	1205	Y01	CBH-CBF-CBD	-3.33	107.85	112.71
3	D	1207	Y01	CAV-CAZ-CBH	3.33	120.68	116.42
3	B	1208	Y01	CBI-CBG-CBD	-3.32	109.70	114.41
3	B	1207	Y01	CAV-CAZ-CBH	3.30	120.64	116.42
3	B	1207	Y01	CBH-CBF-CBD	-3.29	107.90	112.71
3	A	1207	Y01	CBI-CBG-CBD	-3.29	109.74	114.41
3	B	1204	Y01	CAC-CBB-CBE	-3.26	107.99	112.88
3	C	1204	Y01	CBH-CBF-CBD	-3.26	107.95	112.71
3	C	1205	Y01	CBF-CBH-CAZ	3.26	114.42	109.65
3	A	1207	Y01	CBH-CBF-CBD	-3.25	107.96	112.71
3	B	1205	Y01	CAV-CAZ-CBH	3.25	120.58	116.42
3	A	1207	Y01	CBI-CBE-CBB	-3.25	114.48	119.50
3	C	1202	Y01	CBC-OAW-CAY	-3.23	110.06	117.80
3	A	1209	Y01	CAV-CAZ-CBH	3.23	120.56	116.42
3	C	1201	Y01	CBC-OAW-CAY	-3.20	110.13	117.80
3	C	1201	Y01	CBF-CBH-CAZ	3.19	114.33	109.65
3	B	1206	Y01	CAP-CBE-CBI	-3.19	100.09	103.84
3	D	1207	Y01	CAT-CAR-CBC	-3.19	105.14	110.33
3	C	1204	Y01	CBI-CBG-CBD	-3.18	109.90	114.41
3	D	1201	Y01	CAS-CAU-CBI	-3.13	107.46	112.74
3	B	1208	Y01	CAT-CAR-CBC	3.13	115.43	110.33
3	D	1207	Y01	CBG-CBI-CBE	-3.13	96.51	100.10
3	D	1202	Y01	CBF-CBH-CAZ	3.12	114.22	109.65
3	A	1208	Y01	CAS-CAU-CBI	-3.12	107.48	112.74
3	B	1203	Y01	CBF-CBH-CAZ	3.10	114.20	109.65
3	D	1205	Y01	CAD-CBH-CBF	-3.10	108.18	111.66
3	B	1204	Y01	CAS-CAU-CBI	-3.10	107.52	112.74
3	B	1208	Y01	CAD-CBH-CBF	-3.08	108.20	111.66
3	A	1205	Y01	CAS-CAU-CBI	-3.07	107.56	112.74
3	B	1208	Y01	CBG-CBI-CBE	-3.06	96.59	100.10
3	B	1205	Y01	CBG-CBI-CBE	-3.05	96.59	100.10
3	C	1205	Y01	CBC-CAV-CAZ	3.03	115.93	111.45
3	D	1205	Y01	CBI-CBG-CBD	-3.03	110.11	114.41
3	D	1202	Y01	CAC-CBB-CBE	-3.03	108.34	112.88
3	C	1202	Y01	CBF-CBH-CAZ	3.03	114.09	109.65
3	B	1204	Y01	CBH-CBF-CBD	-3.03	108.29	112.71
3	D	1202	Y01	CBC-OAW-CAY	-3.00	110.61	117.80
3	B	1206	Y01	CAS-CAU-CBI	-3.00	107.68	112.74
3	D	1203	Y01	CAD-CBH-CBF	-2.99	108.31	111.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1206	Y01	CBF-CBH-CAZ	2.99	114.03	109.65
3	C	1204	Y01	CAS-CAU-CBI	-2.98	107.72	112.74
3	C	1204	Y01	CAT-CAR-CBC	-2.95	105.52	110.33
3	B	1204	Y01	CBF-CBH-CAZ	2.94	113.96	109.65
3	A	1204	Y01	CBF-CBH-CAZ	2.94	113.96	109.65
3	A	1206	Y01	CAS-CAU-CBI	-2.93	107.79	112.74
3	C	1201	Y01	CAS-CAU-CBI	-2.91	107.82	112.74
3	C	1203	Y01	CBG-CBI-CBE	-2.91	96.76	100.10
3	D	1206	Y01	CBF-CBH-CAZ	2.91	113.91	109.65
3	D	1203	Y01	CAS-CAU-CBI	-2.90	107.85	112.74
3	A	1205	Y01	CBC-OAW-CAY	-2.89	110.89	117.80
3	B	1207	Y01	CBI-CBG-CBD	-2.88	110.32	114.41
3	A	1207	Y01	CAS-CAU-CBI	-2.88	107.89	112.74
3	B	1203	Y01	CAS-CAU-CBI	-2.87	107.90	112.74
3	B	1208	Y01	CAS-CAU-CBI	-2.86	107.91	112.74
3	D	1207	Y01	CBF-CBH-CAZ	2.85	113.83	109.65
3	C	1205	Y01	CAS-CAU-CBI	-2.85	107.94	112.74
3	B	1207	Y01	CAS-CAU-CBI	-2.83	107.96	112.74
3	B	1205	Y01	CAS-CAU-CBI	-2.83	107.97	112.74
3	C	1203	Y01	CBC-OAW-CAY	-2.82	111.05	117.80
3	A	1205	Y01	CBG-CBI-CBE	-2.81	96.87	100.10
3	D	1204	Y01	CBG-CBI-CBE	-2.81	96.87	100.10
3	D	1206	Y01	CAS-CAU-CBI	-2.80	108.02	112.74
3	A	1208	Y01	CAP-CBE-CBI	-2.80	100.55	103.84
3	A	1209	Y01	CBC-CAV-CAZ	2.80	115.58	111.45
3	D	1205	Y01	CBH-CBF-CBD	-2.79	108.64	112.71
3	B	1205	Y01	CBF-CBH-CAZ	2.78	113.73	109.65
3	D	1207	Y01	CAC-CBB-CBE	-2.78	108.71	112.88
3	B	1207	Y01	CBF-CBH-CAZ	2.78	113.72	109.65
3	A	1207	Y01	CAT-CAR-CBC	-2.74	105.86	110.33
3	D	1203	Y01	CBC-OAW-CAY	-2.73	111.26	117.80
3	D	1202	Y01	CAS-CAU-CBI	-2.73	108.14	112.74
3	D	1205	Y01	CAS-CAU-CBI	-2.72	108.14	112.74
3	C	1203	Y01	CAS-CAU-CBI	-2.71	108.16	112.74
3	D	1204	Y01	CAS-CAU-CBI	-2.71	108.16	112.74
3	D	1205	Y01	CBD-CAK-CAI	2.71	116.52	112.76
3	D	1204	Y01	CBC-OAW-CAY	-2.70	111.33	117.80
3	B	1203	Y01	CAC-CBB-CBE	-2.70	108.83	112.88
3	D	1207	Y01	CAS-CAU-CBI	-2.69	108.19	112.74
3	A	1207	Y01	CAJ-CAO-CBB	-2.69	107.55	115.08
3	A	1207	Y01	CAV-CAZ-CAI	-2.69	116.92	120.57
3	D	1205	Y01	CBF-CBD-CBG	-2.69	105.58	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1204	Y01	CAV-CAZ-CAI	-2.68	116.93	120.57
3	C	1202	Y01	CAS-CAU-CBI	-2.68	108.22	112.74
3	A	1205	Y01	CBF-CBH-CAZ	2.68	113.57	109.65
3	B	1208	Y01	CBD-CAK-CAI	2.68	116.47	112.76
3	D	1201	Y01	CBF-CBH-CAZ	2.67	113.57	109.65
3	B	1204	Y01	CAV-CAZ-CBH	2.66	119.83	116.42
3	C	1204	Y01	CAJ-CAO-CBB	-2.65	107.65	115.08
3	C	1204	Y01	CAP-CBE-CBI	-2.65	100.72	103.84
3	B	1206	Y01	CAT-CAR-CBC	-2.63	106.05	110.33
3	A	1208	Y01	CBF-CBH-CAZ	2.62	113.49	109.65
3	B	1203	Y01	CBC-OAW-CAY	-2.62	111.52	117.80
3	D	1205	Y01	CAV-CAZ-CAI	-2.62	117.02	120.57
3	D	1205	Y01	CAU-CAS-CBF	-2.61	108.69	113.14
3	A	1209	Y01	CAS-CAU-CBI	-2.60	108.35	112.74
3	D	1204	Y01	CBF-CBH-CAZ	2.60	113.46	109.65
3	A	1205	Y01	CAT-CAR-CBC	-2.59	106.12	110.33
3	B	1207	Y01	CAT-CAR-CBC	-2.57	106.14	110.33
3	C	1202	Y01	CAC-CBB-CBE	-2.55	109.06	112.88
3	C	1203	Y01	CAV-CAZ-CAI	-2.55	117.12	120.57
3	A	1208	Y01	CAV-CAZ-CAI	-2.53	117.13	120.57
3	A	1208	Y01	CAT-CAR-CBC	-2.53	106.20	110.33
3	C	1203	Y01	CBF-CBH-CAZ	2.53	113.35	109.65
3	A	1204	Y01	CAC-CBB-CBE	-2.52	109.10	112.88
3	B	1206	Y01	CBF-CBH-CAZ	2.52	113.34	109.65
3	A	1204	Y01	CAS-CAU-CBI	-2.49	108.53	112.74
3	C	1203	Y01	CAT-CAR-CBC	-2.49	106.27	110.33
3	A	1206	Y01	CAP-CBE-CBI	-2.49	100.91	103.84
3	D	1203	Y01	CBF-CBH-CAZ	2.49	113.29	109.65
3	D	1204	Y01	CAV-CAZ-CAI	-2.48	117.21	120.57
3	C	1202	Y01	CAP-CBE-CBB	-2.47	108.44	112.18
3	C	1205	Y01	CAV-CAZ-CAI	-2.47	117.22	120.57
3	C	1202	Y01	CBF-CBD-CBG	-2.46	105.87	109.09
3	A	1204	Y01	CAP-CBE-CBB	-2.46	108.46	112.18
3	D	1205	Y01	CAT-CBH-CAZ	2.45	112.97	108.74
3	B	1203	Y01	CAD-CBH-CBF	-2.42	108.94	111.66
3	A	1204	Y01	CBF-CBD-CBG	-2.42	105.92	109.09
3	A	1208	Y01	CAJ-CAO-CBB	-2.42	108.31	115.08
3	C	1201	Y01	CAC-CBB-CBE	-2.41	109.27	112.88
3	B	1203	Y01	CAV-CAZ-CBH	2.41	119.50	116.42
3	C	1201	Y01	CAD-CBH-CBF	-2.40	108.96	111.66
3	D	1202	Y01	CAJ-CAO-CBB	-2.40	108.37	115.08
3	D	1203	Y01	CAV-CAZ-CBH	2.40	119.49	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1206	Y01	CAV-CAZ-CAI	-2.39	117.33	120.57
3	D	1204	Y01	CAT-CAR-CBC	-2.38	106.45	110.33
3	B	1204	Y01	CAJ-CAO-CBB	-2.38	108.42	115.08
3	D	1201	Y01	CAC-CBB-CBE	-2.37	109.32	112.88
3	C	1201	Y01	CAQ-CBG-CBI	-2.37	101.05	103.84
3	D	1201	Y01	CAD-CBH-CBF	-2.34	109.03	111.66
3	C	1202	Y01	CAJ-CAO-CBB	-2.34	108.54	115.08
3	A	1209	Y01	CAS-CBF-CBH	-2.33	110.21	113.08
3	A	1206	Y01	CAS-CBF-CBH	-2.32	110.22	113.08
3	A	1206	Y01	CAT-CBH-CAZ	2.32	112.75	108.74
3	C	1205	Y01	CAP-CBE-CBB	-2.31	108.69	112.18
3	A	1207	Y01	CBF-CBH-CAZ	2.30	113.02	109.65
3	C	1204	Y01	CBF-CBH-CAZ	2.30	113.02	109.65
3	B	1207	Y01	CAC-CBB-CBE	-2.29	109.44	112.88
3	C	1205	Y01	CBC-OAW-CAY	-2.28	112.34	117.80
3	C	1201	Y01	CAV-CAZ-CBH	2.28	119.34	116.42
3	C	1205	Y01	CAJ-CAO-CBB	-2.28	108.71	115.08
3	B	1204	Y01	CAT-CAR-CBC	-2.27	106.63	110.33
3	D	1206	Y01	CAS-CBF-CBH	-2.26	110.30	113.08
3	D	1206	Y01	CAT-CBH-CAZ	2.25	112.63	108.74
3	D	1202	Y01	CAP-CBE-CBB	-2.25	108.77	112.18
3	B	1208	Y01	CAU-CAS-CBF	-2.25	109.31	113.14
3	B	1205	Y01	CBC-OAW-CAY	-2.25	112.41	117.80
3	A	1207	Y01	CBC-OAW-CAY	-2.25	112.41	117.80
3	B	1205	Y01	CAT-CAR-CBC	-2.25	106.67	110.33
3	D	1203	Y01	CAV-CAZ-CAI	-2.25	117.52	120.57
3	C	1203	Y01	CAJ-CAO-CBB	-2.23	108.84	115.08
3	A	1204	Y01	CAJ-CAO-CBB	-2.23	108.85	115.08
3	C	1205	Y01	CAK-CBD-CBF	-2.22	107.16	109.72
3	D	1206	Y01	CAV-CAZ-CAI	-2.22	117.56	120.57
3	A	1205	Y01	CAV-CAZ-CAI	-2.21	117.57	120.57
3	B	1206	Y01	CAE-CBI-CBE	2.21	115.69	111.68
3	D	1203	Y01	CBF-CBD-CBG	-2.20	106.22	109.09
3	D	1204	Y01	CAJ-CAO-CBB	-2.19	108.95	115.08
3	B	1207	Y01	CAV-CAZ-CAI	-2.19	117.60	120.57
3	B	1205	Y01	CAV-CAZ-CAI	-2.19	117.60	120.57
3	D	1203	Y01	CAJ-CAO-CBB	-2.19	108.96	115.08
3	B	1207	Y01	CBD-CAK-CAI	2.19	115.79	112.76
3	C	1204	Y01	CBD-CAK-CAI	2.19	115.79	112.76
3	D	1205	Y01	CAK-CBD-CBG	-2.17	107.86	110.93
3	A	1205	Y01	CAS-CBF-CBH	-2.16	110.42	113.08
3	C	1201	Y01	CBH-CBF-CBD	-2.16	109.56	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1207	Y01	CBD-CAK-CAI	2.15	115.74	112.76
3	C	1204	Y01	CAU-CAS-CBF	-2.15	109.49	113.14
3	B	1207	Y01	CAT-CBH-CAZ	2.14	112.42	108.74
3	A	1209	Y01	CAK-CBD-CBF	-2.14	107.25	109.72
3	B	1206	Y01	CAJ-CAO-CBB	-2.12	109.15	115.08
3	B	1208	Y01	CBF-CBH-CAZ	2.12	112.76	109.65
3	B	1204	Y01	CAQ-CBG-CBI	-2.11	101.36	103.84
3	C	1204	Y01	CBC-OAW-CAY	-2.11	112.74	117.80
3	D	1207	Y01	CAV-CAZ-CAI	-2.11	117.72	120.57
3	D	1205	Y01	CAR-CBC-CAV	-2.11	108.05	110.97
3	C	1201	Y01	CAJ-CAO-CBB	-2.11	109.19	115.08
3	D	1202	Y01	CBF-CBD-CBG	-2.11	106.34	109.09
3	D	1207	Y01	CAT-CBH-CAZ	2.10	112.36	108.74
3	B	1206	Y01	CAT-CBH-CAZ	2.07	112.32	108.74
3	B	1203	Y01	CAV-CAZ-CAI	-2.07	117.77	120.57
3	B	1205	Y01	CAS-CBF-CBH	-2.06	110.54	113.08
3	C	1204	Y01	CAT-CBH-CAZ	2.06	112.29	108.74
3	A	1207	Y01	CAU-CAS-CBF	-2.04	109.67	113.14
3	A	1204	Y01	OAF-CAX-CAL	-2.03	116.65	123.09
3	B	1207	Y01	CAU-CAS-CBF	-2.03	109.69	113.14
3	D	1202	Y01	CAU-CAS-CBF	-2.02	109.70	113.14
3	D	1207	Y01	CAS-CBF-CBH	-2.02	110.60	113.08
3	A	1209	Y01	OAF-CAX-CAL	-2.01	116.71	123.09
3	C	1205	Y01	CBF-CBD-CBG	2.01	111.71	109.09
3	A	1208	Y01	CAT-CBH-CAZ	2.01	112.21	108.74
3	A	1206	Y01	CAV-CAZ-CAI	-2.00	117.86	120.57

There are no chirality outliers.

All (227) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1205	Y01	OAG-CAY-OAW-CBC
3	A	1205	Y01	CAM-CAY-OAW-CBC
3	A	1208	Y01	CAO-CBB-CBE-CAP
3	B	1205	Y01	CAM-CAY-OAW-CBC
3	B	1206	Y01	CAO-CBB-CBE-CAP
3	B	1206	Y01	CAC-CBB-CBE-CBI
3	B	1208	Y01	CAM-CAY-OAW-CBC
3	C	1201	Y01	CAM-CAY-OAW-CBC
3	C	1203	Y01	OAG-CAY-OAW-CBC
3	C	1203	Y01	CAM-CAY-OAW-CBC
3	D	1203	Y01	CAO-CBB-CBE-CBI

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Mol	Chain	Res	Type	Atoms
4	B	1209	NAG	C1-C2-N2-C7
4	B	1209	NAG	C3-C2-N2-C7
4	B	1209	NAG	C8-C7-N2-C2
4	B	1209	NAG	O7-C7-N2-C2
4	C	1206	NAG	C1-C2-N2-C7
4	C	1206	NAG	C3-C2-N2-C7
4	C	1206	NAG	C8-C7-N2-C2
4	C	1206	NAG	O7-C7-N2-C2
4	D	1208	NAG	C1-C2-N2-C7
4	D	1208	NAG	C3-C2-N2-C7
4	D	1208	NAG	C8-C7-N2-C2
4	D	1208	NAG	O7-C7-N2-C2
3	A	1204	Y01	CAV-CBC-OAW-CAY
3	A	1209	Y01	CAV-CBC-OAW-CAY
3	B	1204	Y01	CAV-CBC-OAW-CAY
3	B	1207	Y01	CAV-CBC-OAW-CAY
3	D	1201	Y01	CAV-CBC-OAW-CAY
3	A	1208	Y01	CAC-CBB-CBE-CBI
3	B	1204	Y01	CAC-CBB-CBE-CBI
3	A	1208	Y01	CAO-CBB-CBE-CBI
3	B	1208	Y01	OAG-CAY-OAW-CBC
3	C	1201	Y01	OAG-CAY-OAW-CBC
3	D	1205	Y01	CAR-CBC-OAW-CAY
3	B	1204	Y01	CAO-CBB-CBE-CBI
3	A	1204	Y01	CAX-CAL-CAM-CAY
3	B	1205	Y01	OAG-CAY-OAW-CBC
3	B	1203	Y01	CAM-CAY-OAW-CBC
3	D	1206	Y01	CAV-CBC-OAW-CAY
3	A	1209	Y01	CAO-CBB-CBE-CAP
3	D	1203	Y01	CAO-CBB-CBE-CAP
3	B	1203	Y01	OAG-CAY-OAW-CBC
3	B	1206	Y01	CAJ-CAO-CBB-CAC
3	A	1205	Y01	CAO-CBB-CBE-CAP
3	C	1203	Y01	CAO-CBB-CBE-CAP
3	D	1204	Y01	CAO-CBB-CBE-CAP
3	D	1205	Y01	CAO-CBB-CBE-CAP
3	A	1205	Y01	CAO-CBB-CBE-CBI
3	D	1204	Y01	CAO-CBB-CBE-CBI
3	D	1205	Y01	CAO-CBB-CBE-CBI
3	A	1204	Y01	CAJ-CAO-CBB-CBE
3	B	1206	Y01	CAJ-CAO-CBB-CBE
3	C	1202	Y01	CAJ-CAO-CBB-CBE

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Mol	Chain	Res	Type	Atoms
3	C	1205	Y01	CAJ-CAO-CBB-CBE
3	A	1206	Y01	CAM-CAY-OAW-CBC
3	D	1207	Y01	CAV-CBC-OAW-CAY
3	A	1208	Y01	CAC-CBB-CBE-CAP
3	D	1206	Y01	CAO-CBB-CBE-CAP
3	C	1203	Y01	CAO-CBB-CBE-CBI
4	A	1210	NAG	C3-C2-N2-C7
3	B	1203	Y01	CAX-CAL-CAM-CAY
3	B	1204	Y01	CAX-CAL-CAM-CAY
3	A	1206	Y01	CAV-CBC-OAW-CAY
3	A	1209	Y01	CAM-CAY-OAW-CBC
3	D	1204	Y01	CAM-CAY-OAW-CBC
3	D	1206	Y01	CAM-CAY-OAW-CBC
3	A	1208	Y01	CAO-CAJ-CAN-CBA
3	D	1203	Y01	CAC-CBB-CBE-CAP
3	B	1205	Y01	CAO-CBB-CBE-CAP
3	B	1205	Y01	CAO-CBB-CBE-CBI
3	B	1206	Y01	CAO-CBB-CBE-CBI
3	C	1203	Y01	CAX-CAL-CAM-CAY
3	C	1205	Y01	CAJ-CAO-CBB-CAC
3	A	1206	Y01	OAG-CAY-OAW-CBC
3	D	1202	Y01	CAN-CAJ-CAO-CBB
3	A	1207	Y01	CAO-CBB-CBE-CBI
3	A	1204	Y01	CAJ-CAO-CBB-CAC
3	C	1202	Y01	CAJ-CAO-CBB-CAC
3	D	1206	Y01	CAN-CAJ-CAO-CBB
3	A	1209	Y01	OAG-CAY-OAW-CBC
3	D	1204	Y01	OAG-CAY-OAW-CBC
3	D	1206	Y01	OAG-CAY-OAW-CBC
3	B	1205	Y01	CAX-CAL-CAM-CAY
3	B	1208	Y01	CAX-CAL-CAM-CAY
3	D	1204	Y01	CAC-CBB-CBE-CAP
3	D	1205	Y01	CAC-CBB-CBE-CAP
3	A	1207	Y01	CAO-CBB-CBE-CAP
3	C	1202	Y01	CAO-CAJ-CAN-CBA
3	C	1202	Y01	CAN-CAJ-CAO-CBB
3	A	1205	Y01	CAC-CBB-CBE-CAP
3	B	1205	Y01	CAC-CBB-CBE-CAP
3	C	1203	Y01	CAC-CBB-CBE-CAP
3	D	1202	Y01	CAO-CAJ-CAN-CBA
3	D	1203	Y01	CAO-CAJ-CAN-CBA
3	D	1202	Y01	CAX-CAL-CAM-CAY

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Mol	Chain	Res	Type	Atoms
3	A	1208	Y01	CAM-CAY-OAW-CBC
3	C	1204	Y01	CAM-CAY-OAW-CBC
3	C	1205	Y01	CAM-CAY-OAW-CBC
3	B	1206	Y01	CAC-CBB-CBE-CAP
3	C	1204	Y01	OAG-CAY-OAW-CBC
3	C	1205	Y01	OAG-CAY-OAW-CBC
3	A	1208	Y01	OAG-CAY-OAW-CBC
3	A	1207	Y01	CAM-CAY-OAW-CBC
3	C	1202	Y01	CAM-CAY-OAW-CBC
3	D	1202	Y01	CAM-CAY-OAW-CBC
3	D	1205	Y01	CAM-CAY-OAW-CBC
3	A	1209	Y01	CAR-CBC-OAW-CAY
3	A	1207	Y01	CAC-CBB-CBE-CAP
3	C	1204	Y01	CAO-CBB-CBE-CAP
3	C	1204	Y01	CAO-CBB-CBE-CBI
3	A	1208	Y01	CAJ-CAO-CBB-CBE
3	D	1202	Y01	OAG-CAY-OAW-CBC
3	D	1205	Y01	OAG-CAY-OAW-CBC
3	B	1204	Y01	CAC-CBB-CBE-CAP
3	C	1205	Y01	CAO-CBB-CBE-CAP
3	A	1204	Y01	CAN-CAJ-CAO-CBB
3	D	1201	Y01	CAN-CAJ-CAO-CBB
3	A	1209	Y01	CAN-CAJ-CAO-CBB
3	C	1205	Y01	CAO-CBB-CBE-CBI
3	C	1201	Y01	CAJ-CAO-CBB-CBE
3	B	1207	Y01	CAR-CBC-OAW-CAY
3	D	1207	Y01	CAR-CBC-OAW-CAY
3	C	1204	Y01	CAC-CBB-CBE-CAP
3	A	1207	Y01	OAG-CAY-OAW-CBC
3	C	1202	Y01	OAG-CAY-OAW-CBC
3	D	1203	Y01	CAM-CAY-OAW-CBC
3	A	1208	Y01	CAJ-CAO-CBB-CAC
3	C	1205	Y01	CAJ-CAN-CBA-CAA
3	D	1203	Y01	CAJ-CAN-CBA-CAB
3	C	1205	Y01	CAJ-CAN-CBA-CAB
3	D	1203	Y01	CAJ-CAN-CBA-CAA
3	A	1205	Y01	CAO-CAJ-CAN-CBA
3	D	1203	Y01	OAG-CAY-OAW-CBC
3	D	1206	Y01	CAO-CAJ-CAN-CBA
3	C	1204	Y01	CAX-CAL-CAM-CAY
3	C	1205	Y01	CAC-CBB-CBE-CAP
3	A	1206	Y01	CAR-CBC-OAW-CAY

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Mol	Chain	Res	Type	Atoms
3	C	1203	Y01	CAO-CAJ-CAN-CBA
3	D	1204	Y01	CAO-CAJ-CAN-CBA
3	C	1201	Y01	CAJ-CAO-CBB-CAC
3	A	1204	Y01	CAO-CBB-CBE-CAP
3	B	1205	Y01	CAN-CAJ-CAO-CBB
3	A	1206	Y01	CAN-CAJ-CAO-CBB
3	B	1205	Y01	CAR-CBC-OAW-CAY
3	A	1209	Y01	CAC-CBB-CBE-CAP
3	D	1201	Y01	CAO-CBB-CBE-CAP
3	B	1205	Y01	CAV-CBC-OAW-CAY
3	B	1206	Y01	CAM-CAY-OAW-CBC
3	D	1201	Y01	CAR-CBC-OAW-CAY
3	D	1206	Y01	CAR-CBC-OAW-CAY
3	D	1205	Y01	CAV-CBC-OAW-CAY
3	B	1204	Y01	CAO-CBB-CBE-CAP
3	C	1202	Y01	CAO-CBB-CBE-CAP
3	C	1204	Y01	CAV-CBC-OAW-CAY
3	B	1208	Y01	CAO-CBB-CBE-CAP
3	D	1206	Y01	CAC-CBB-CBE-CAP
3	B	1206	Y01	OAG-CAY-OAW-CBC
3	B	1204	Y01	CAJ-CAO-CBB-CBE
3	B	1204	Y01	CAO-CAJ-CAN-CBA
3	B	1207	Y01	CAJ-CAO-CBB-CAC
3	A	1204	Y01	CAR-CBC-OAW-CAY
3	D	1201	Y01	CAX-CAL-CAM-CAY
3	C	1204	Y01	CAR-CBC-OAW-CAY
3	D	1201	Y01	CAO-CAJ-CAN-CBA
3	D	1205	Y01	CAN-CAJ-CAO-CBB
3	D	1206	Y01	CAJ-CAO-CBB-CAC
3	B	1204	Y01	CAN-CAJ-CAO-CBB
3	A	1205	Y01	CAX-CAL-CAM-CAY
3	B	1203	Y01	CAN-CAJ-CAO-CBB
3	B	1203	Y01	CAO-CAJ-CAN-CBA
3	D	1205	Y01	CAO-CAJ-CAN-CBA
3	A	1207	Y01	CAO-CAJ-CAN-CBA
3	D	1204	Y01	CAM-CAL-CAX-OAH
3	D	1204	Y01	CAX-CAL-CAM-CAY
3	C	1202	Y01	CAM-CAL-CAX-OAH
3	C	1202	Y01	CAM-CAL-CAX-OAF
3	D	1206	Y01	CAM-CAL-CAX-OAF
3	A	1205	Y01	CAM-CAL-CAX-OAF
3	A	1209	Y01	CAJ-CAO-CBB-CAC

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Mol	Chain	Res	Type	Atoms
3	A	1207	Y01	CAM-CAL-CAX-OAF
3	B	1207	Y01	CAM-CAL-CAX-OAF
3	A	1207	Y01	CAM-CAL-CAX-OAH
3	C	1205	Y01	CAO-CAJ-CAN-CBA
3	A	1206	Y01	CAC-CBB-CBE-CBI
3	D	1204	Y01	CAM-CAL-CAX-OAF
3	B	1207	Y01	CAM-CAL-CAX-OAH
3	B	1208	Y01	CAM-CAL-CAX-OAF
3	D	1202	Y01	CAM-CAL-CAX-OAH
3	D	1202	Y01	CAL-CAM-CAY-OAW
3	D	1206	Y01	CAM-CAL-CAX-OAH
3	D	1201	Y01	CAL-CAM-CAY-OAW
3	A	1205	Y01	CAM-CAL-CAX-OAH
3	B	1205	Y01	CAM-CAL-CAX-OAH
3	D	1203	Y01	CAC-CBB-CBE-CBI
3	B	1205	Y01	CAM-CAL-CAX-OAF
3	C	1205	Y01	CAM-CAL-CAX-OAF
3	D	1202	Y01	CAM-CAL-CAX-OAF
3	C	1205	Y01	CAN-CAJ-CAO-CBB
3	D	1203	Y01	CAL-CAM-CAY-OAW
3	B	1208	Y01	CAM-CAL-CAX-OAH
3	B	1207	Y01	CAO-CAJ-CAN-CBA
3	A	1209	Y01	CAL-CAM-CAY-OAW
3	A	1207	Y01	CAL-CAM-CAY-OAW
3	C	1205	Y01	CAL-CAM-CAY-OAW
3	B	1204	Y01	CAL-CAM-CAY-OAW
3	A	1206	Y01	CAM-CAL-CAX-OAH
3	A	1209	Y01	CAJ-CAO-CBB-CBE
3	C	1205	Y01	CAM-CAL-CAX-OAH
3	A	1208	Y01	CAL-CAM-CAY-OAW
3	D	1204	Y01	CAL-CAM-CAY-OAW
3	D	1203	Y01	CAN-CAJ-CAO-CBB
3	B	1204	Y01	CAR-CBC-OAW-CAY
3	D	1207	Y01	CAO-CAJ-CAN-CBA
3	D	1205	Y01	CAJ-CAN-CBA-CAB
3	A	1206	Y01	CAM-CAL-CAX-OAF
3	D	1206	Y01	CAL-CAM-CAY-OAW
3	A	1209	Y01	CAL-CAM-CAY-OAG
3	C	1203	Y01	CAM-CAL-CAX-OAH
3	A	1206	Y01	CAL-CAM-CAY-OAW
3	C	1205	Y01	CAL-CAM-CAY-OAG
3	C	1203	Y01	CAL-CAM-CAY-OAW

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Mol	Chain	Res	Type	Atoms
3	D	1204	Y01	CAL-CAM-CAY-OAG
3	C	1201	Y01	CAL-CAM-CAY-OAW
3	A	1207	Y01	CAL-CAM-CAY-OAG
3	D	1203	Y01	CAM-CAL-CAX-OAH
3	A	1208	Y01	CAL-CAM-CAY-OAG
3	A	1208	Y01	CAM-CAL-CAX-OAF

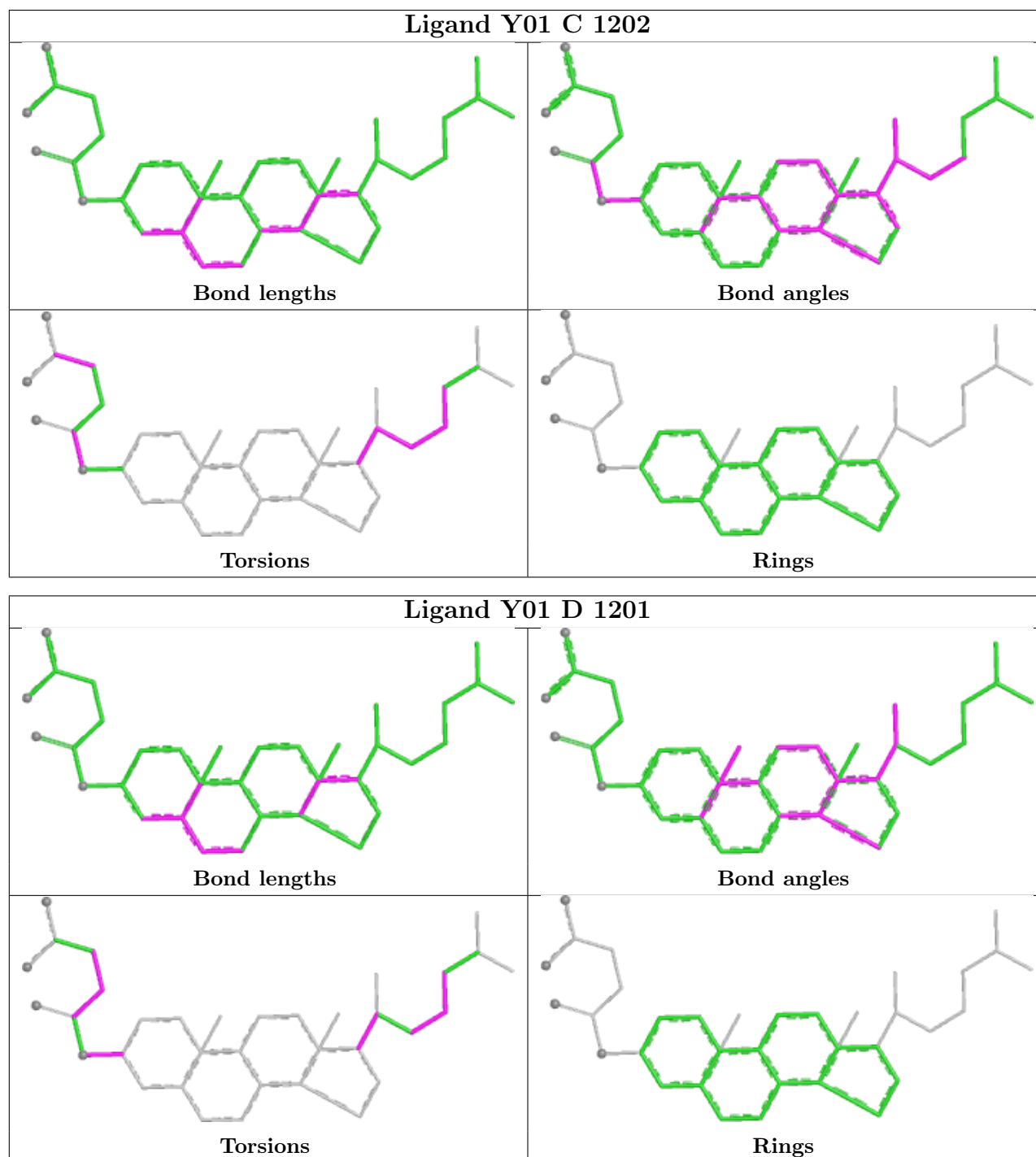
There are no ring outliers.

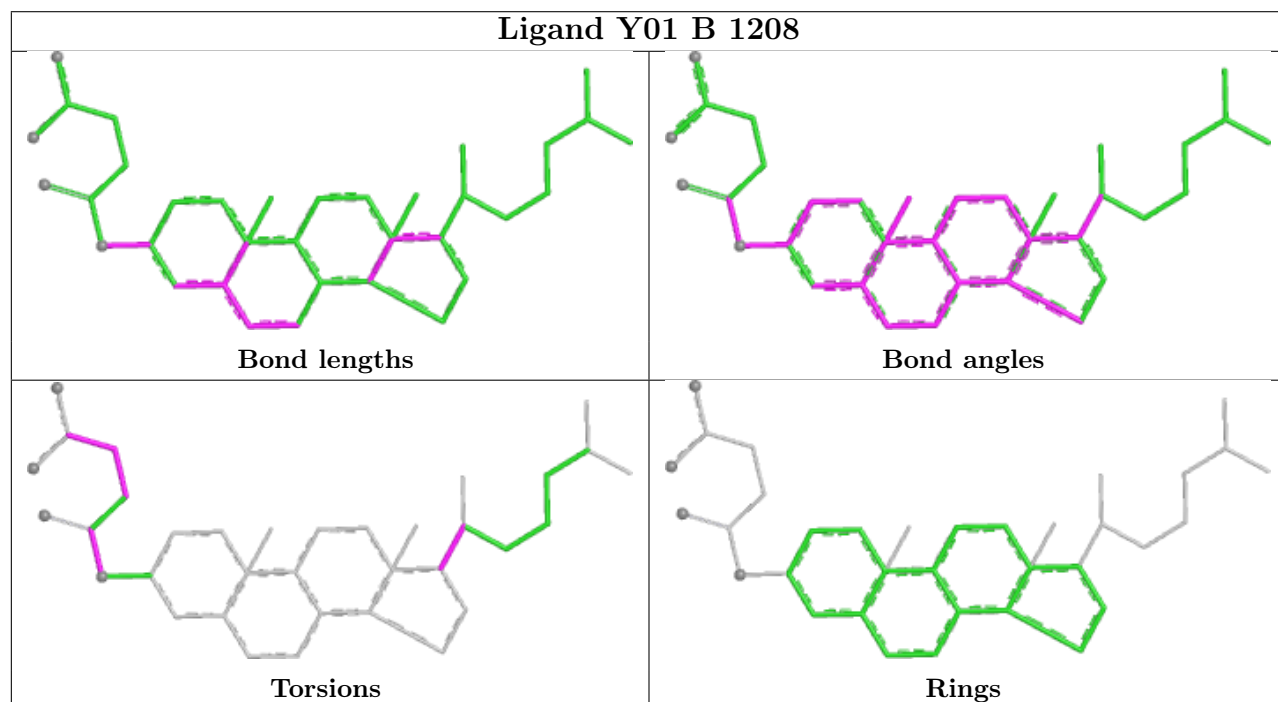
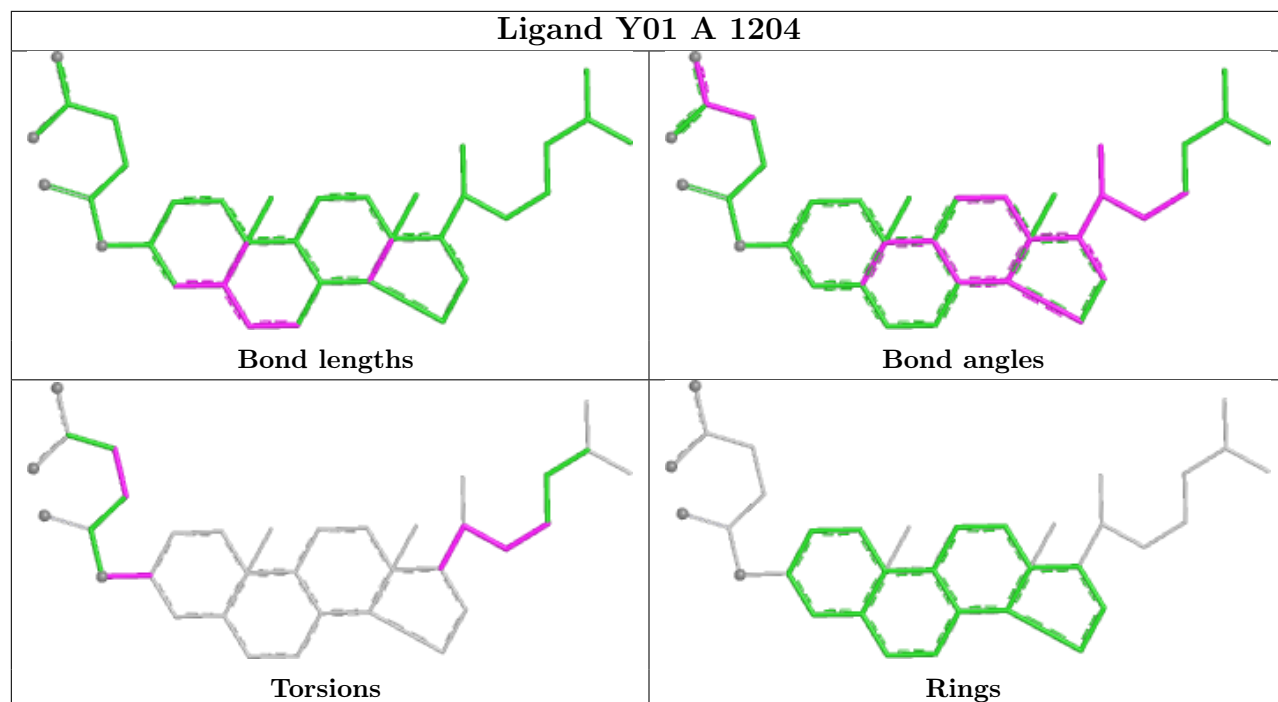
27 monomers are involved in 499 short contacts:

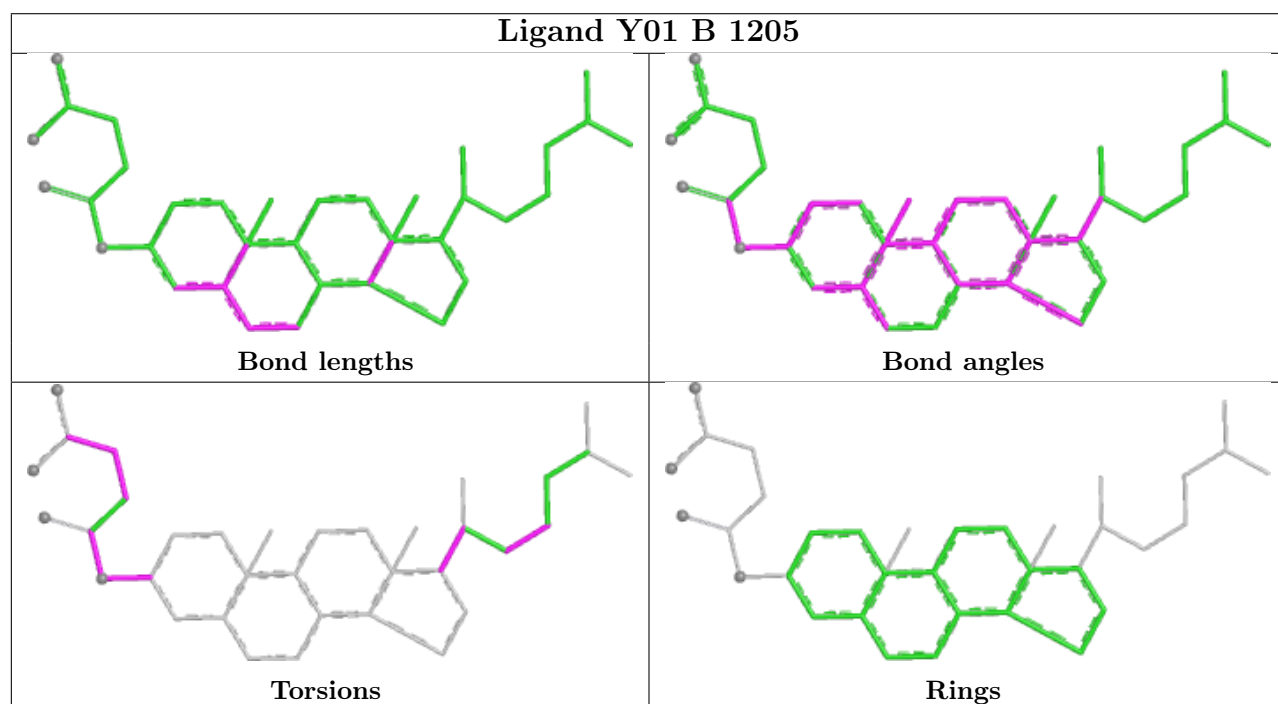
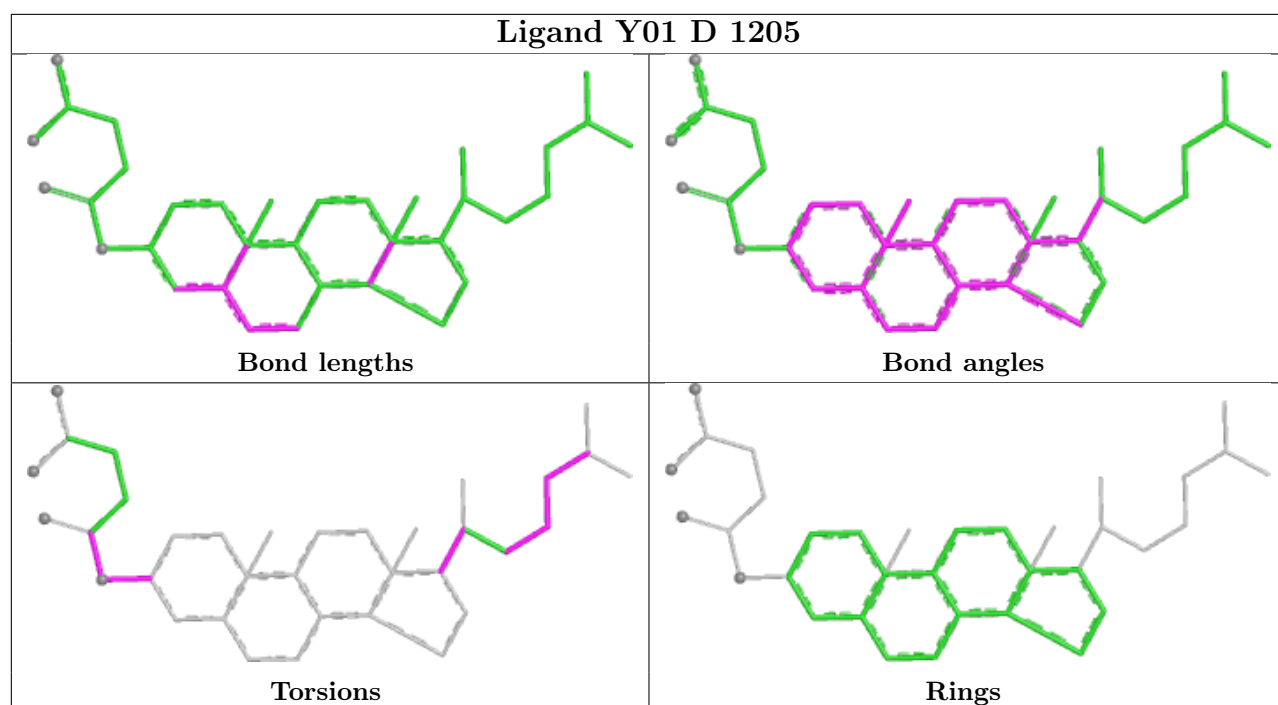
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1202	Y01	8	0
3	D	1201	Y01	13	0
3	A	1204	Y01	11	0
3	B	1208	Y01	13	0
4	D	1208	NAG	4	0
3	D	1205	Y01	32	0
3	B	1205	Y01	29	0
4	A	1210	NAG	5	0
3	A	1208	Y01	32	0
3	B	1206	Y01	10	0
3	C	1201	Y01	13	0
3	B	1207	Y01	21	0
3	C	1204	Y01	13	0
3	A	1209	Y01	25	0
3	C	1205	Y01	50	0
3	D	1204	Y01	23	0
3	A	1207	Y01	12	0
3	D	1203	Y01	17	0
3	B	1204	Y01	20	0
3	A	1206	Y01	32	0
3	C	1203	Y01	23	0
3	D	1207	Y01	42	0
3	A	1205	Y01	34	0
3	D	1206	Y01	20	0
4	C	1206	NAG	3	0
3	B	1203	Y01	7	0
3	D	1202	Y01	5	0

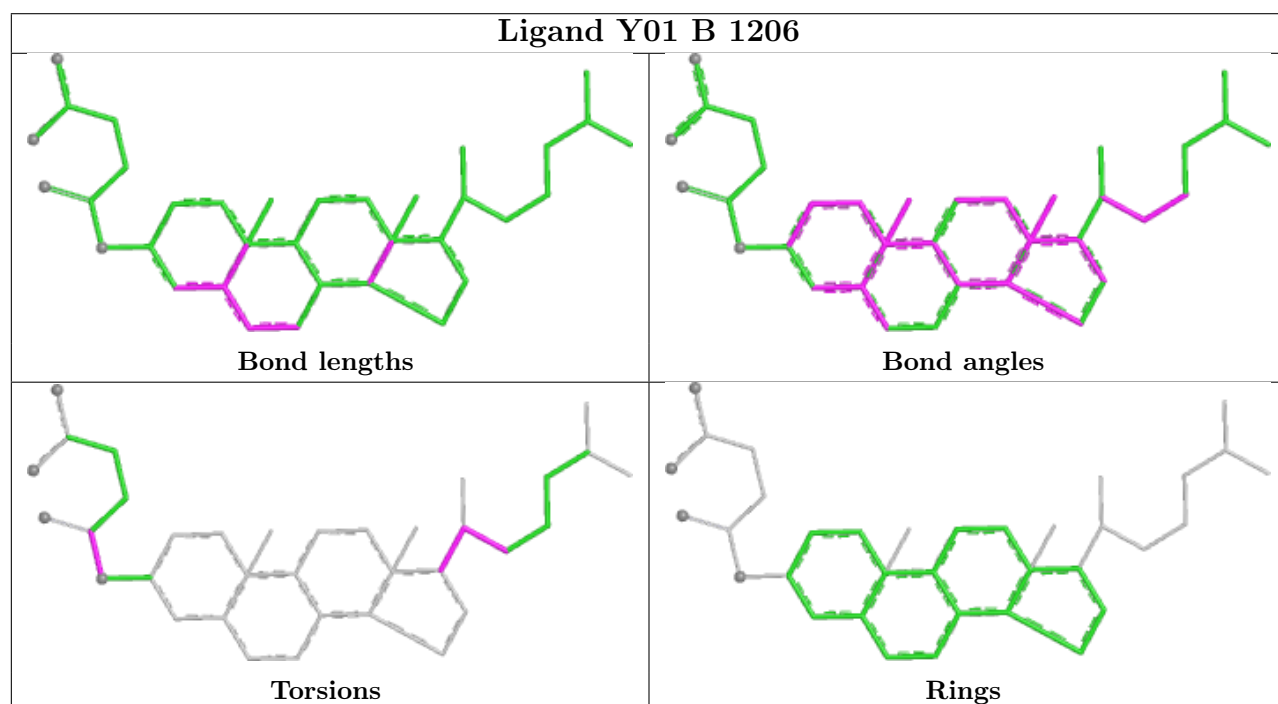
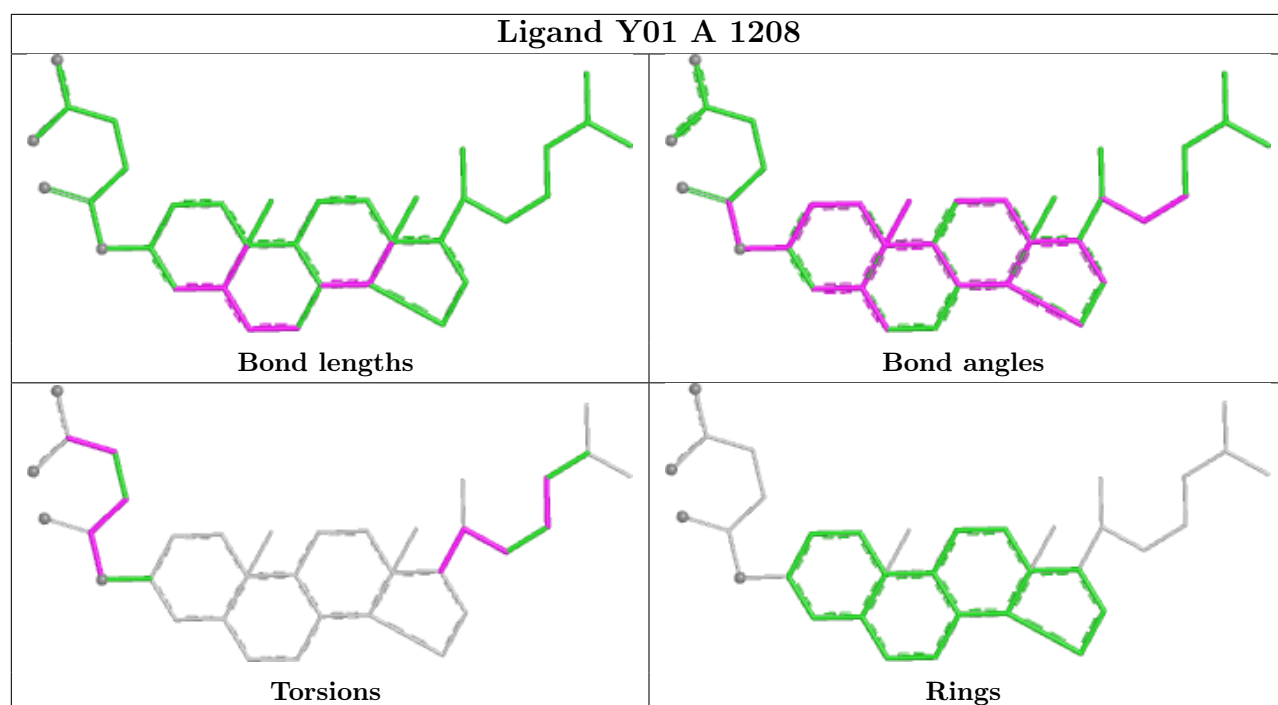
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

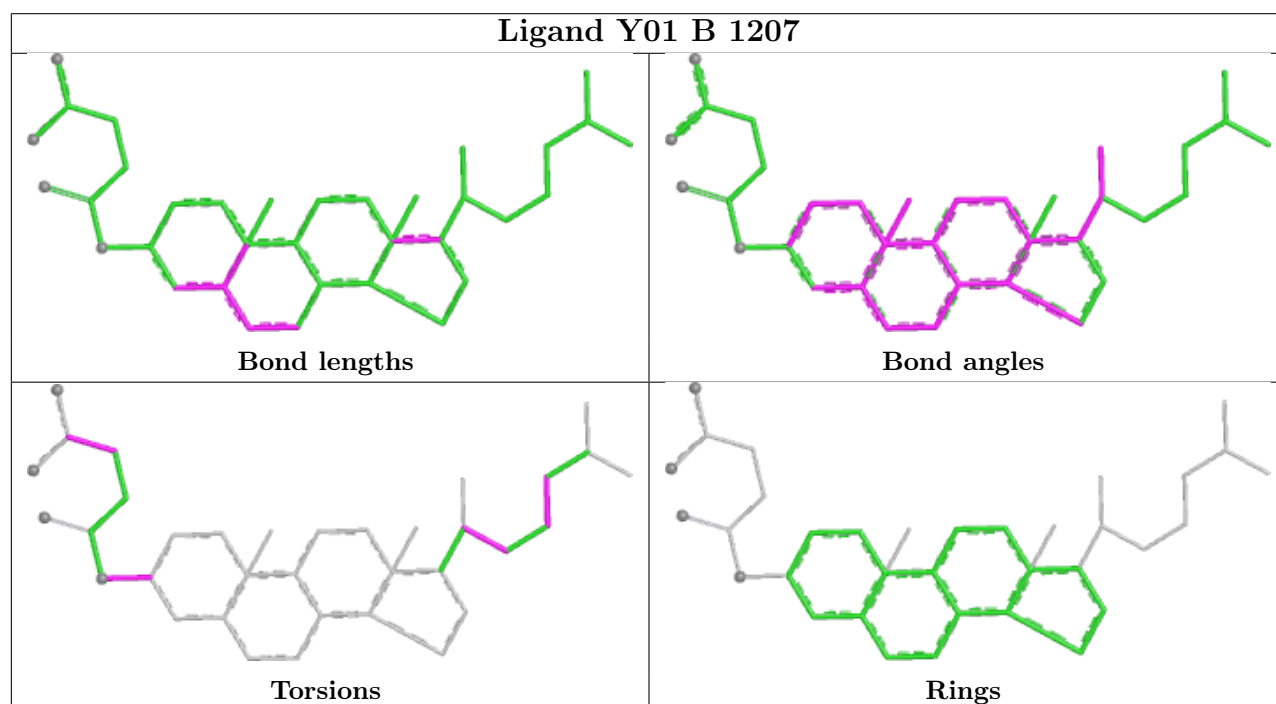
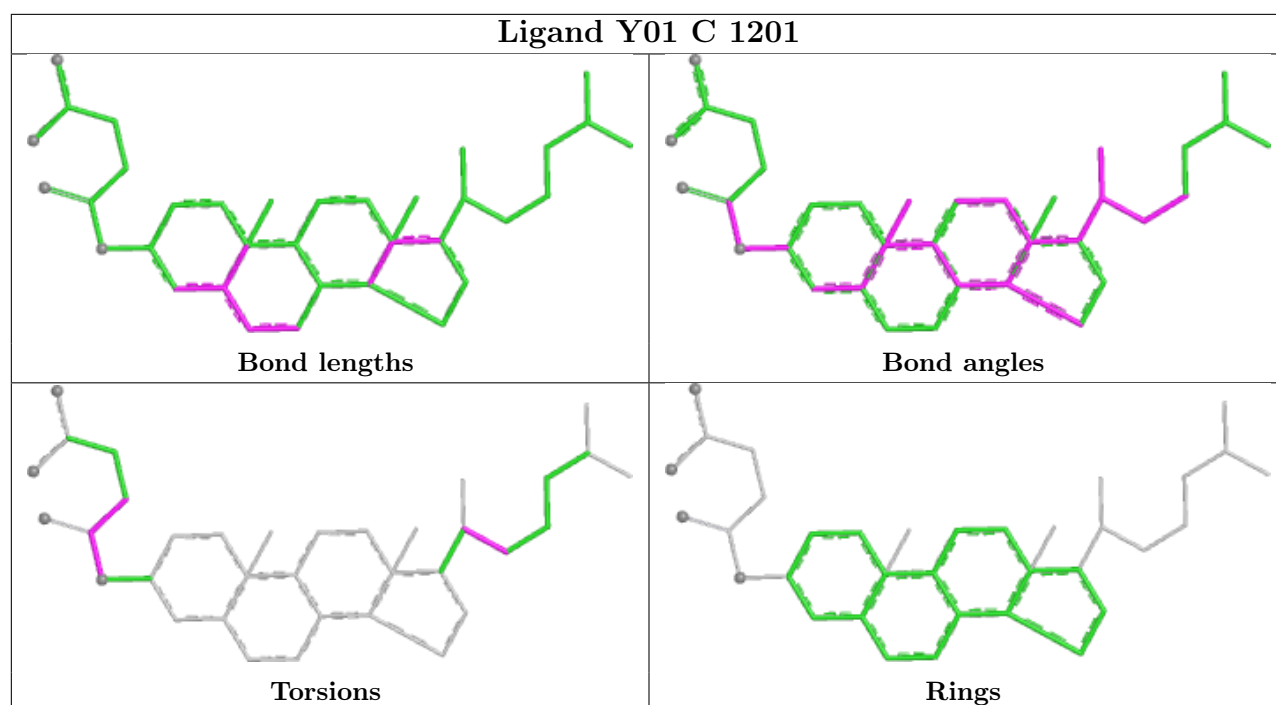
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

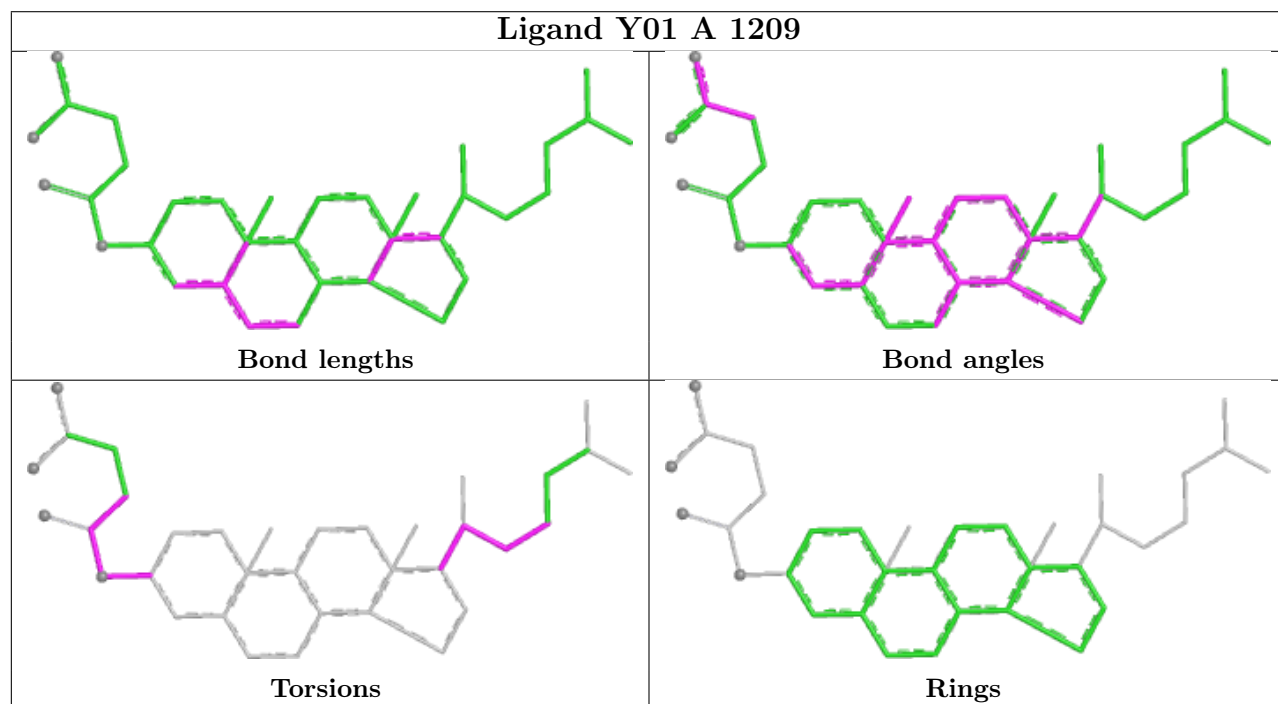
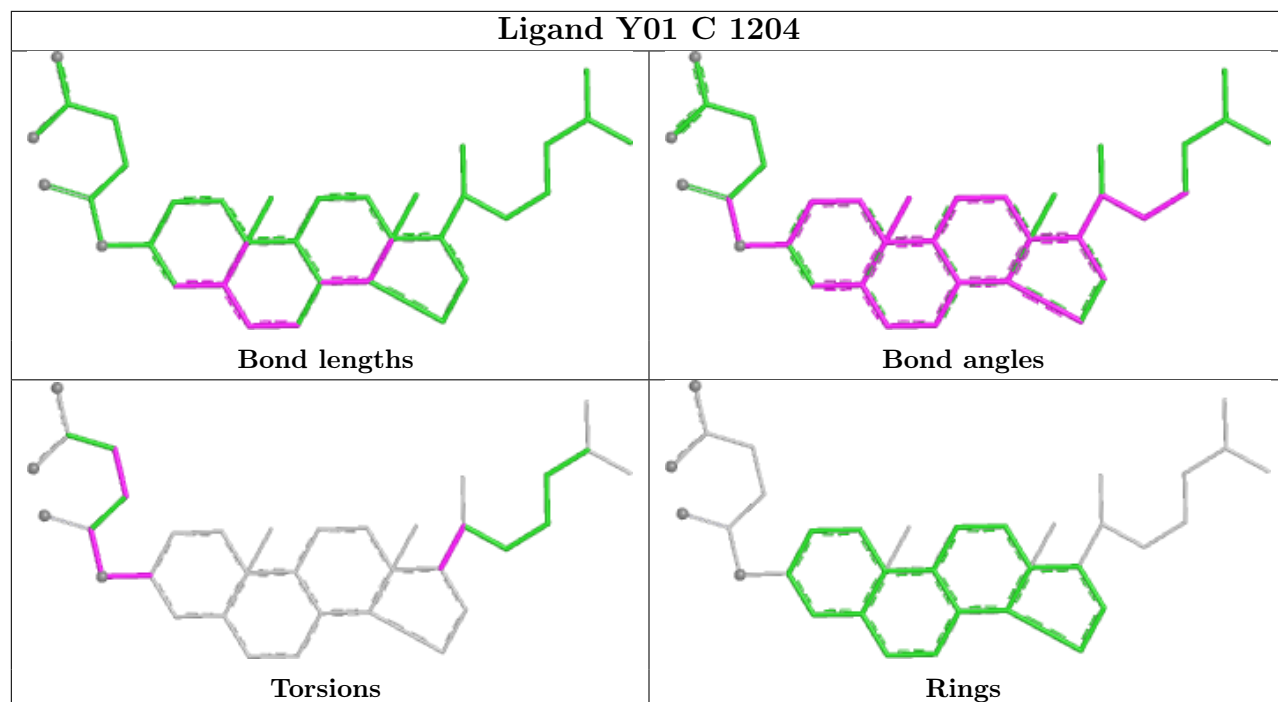


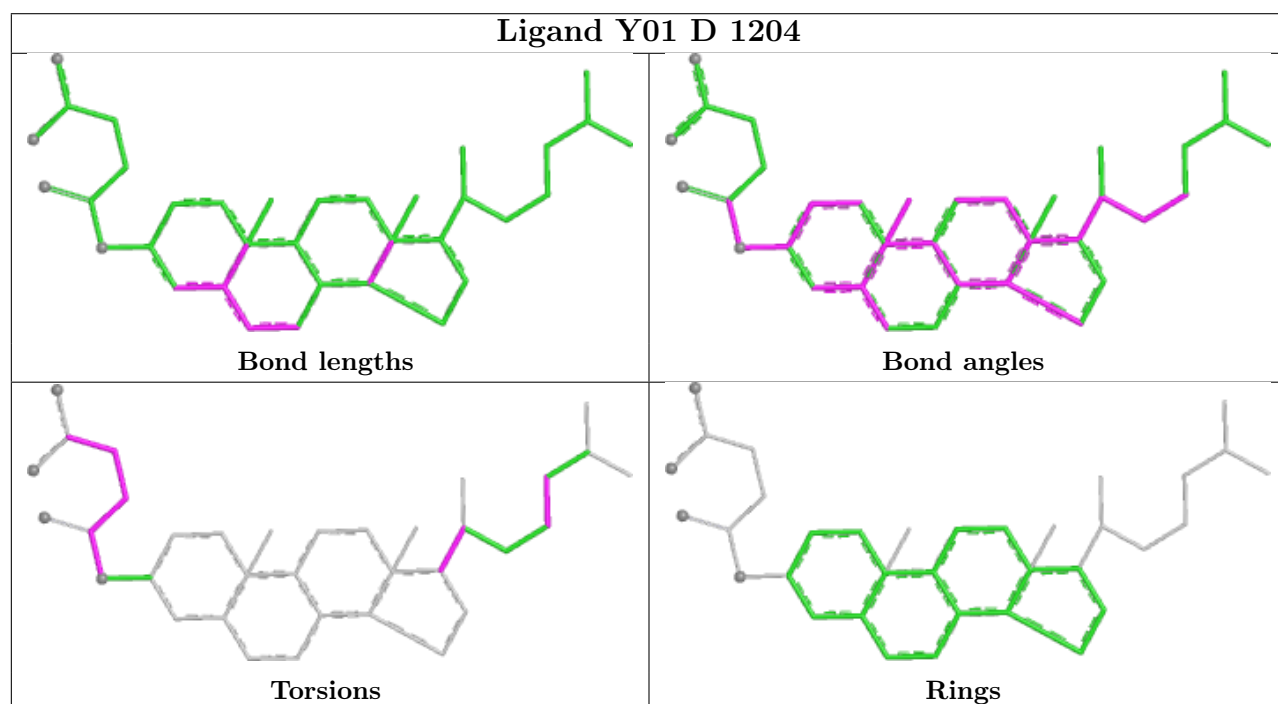
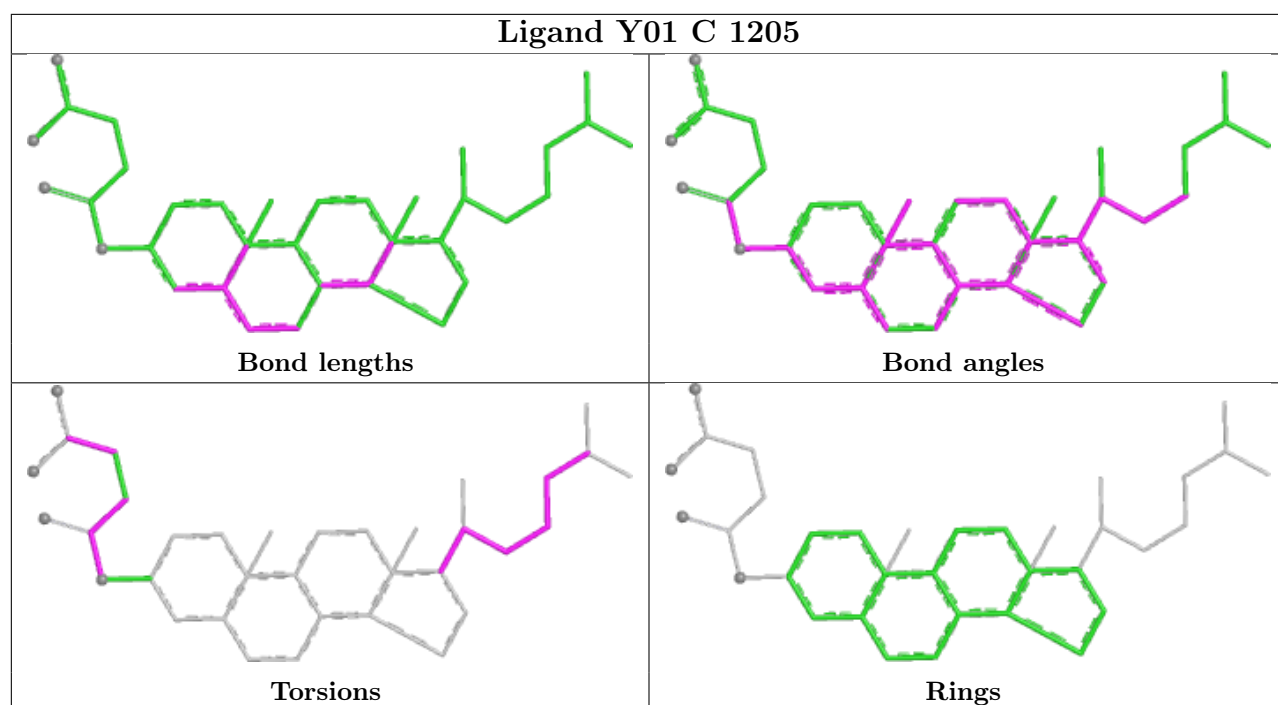


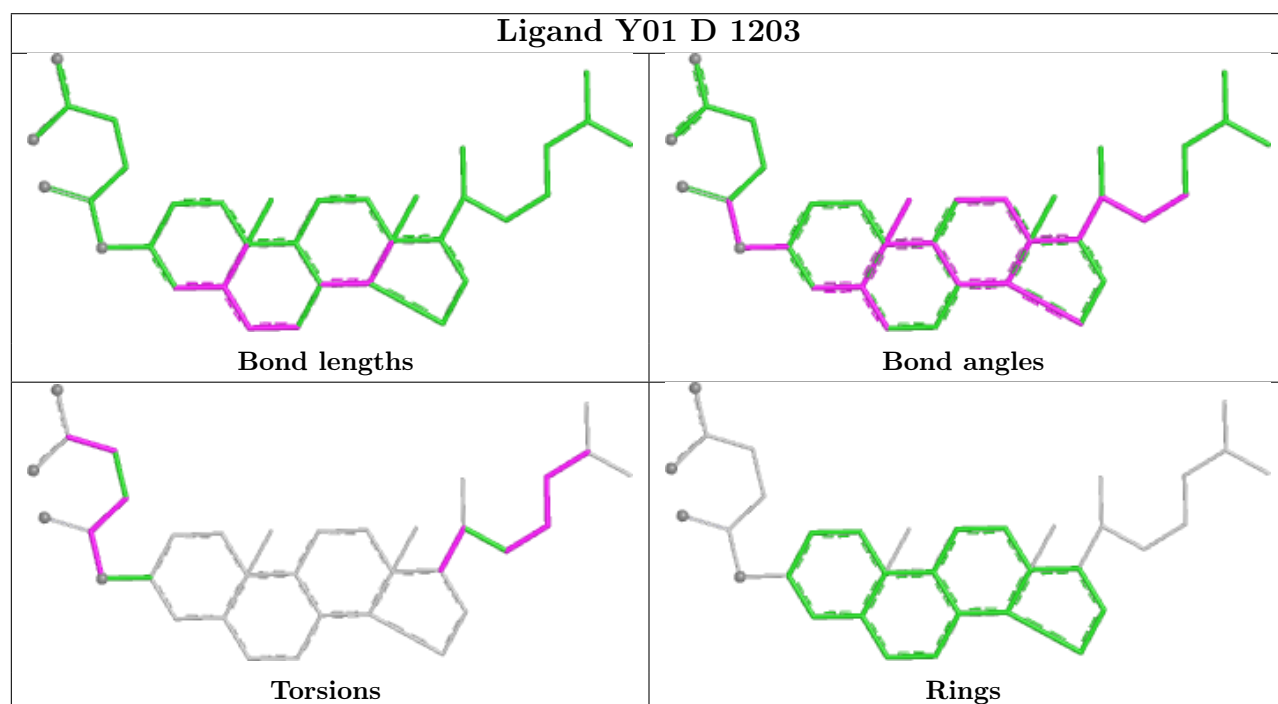
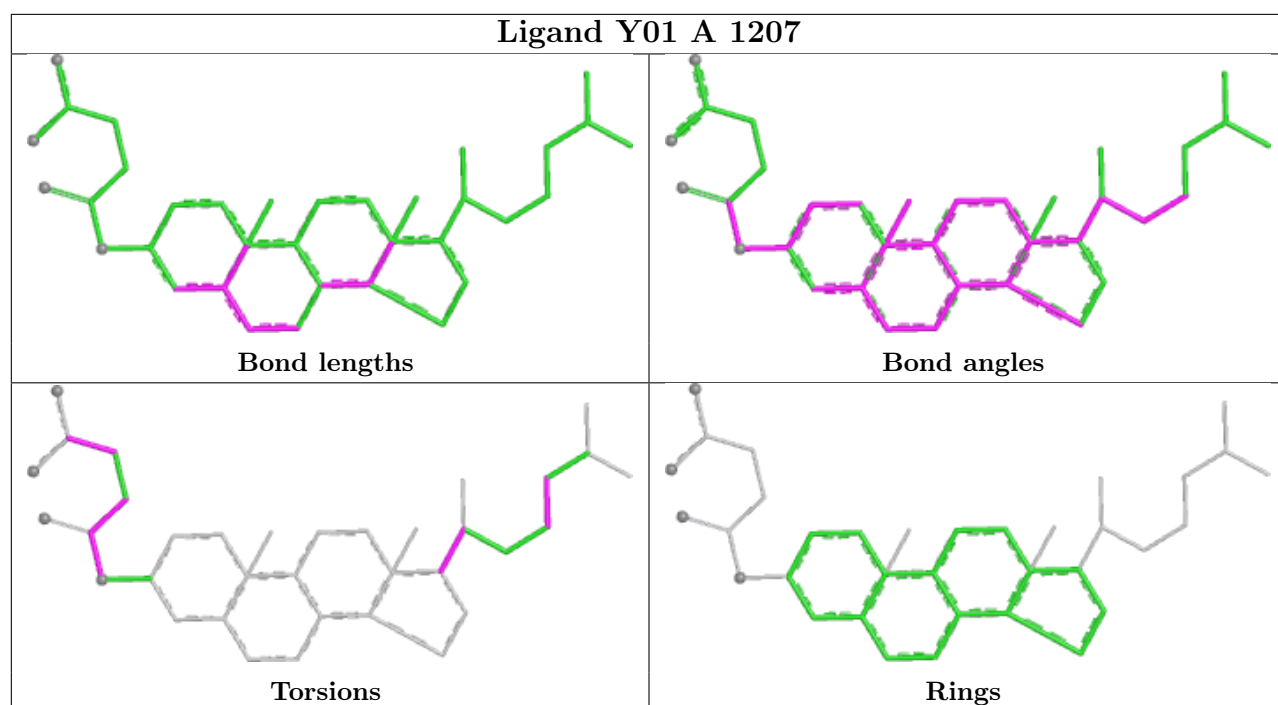


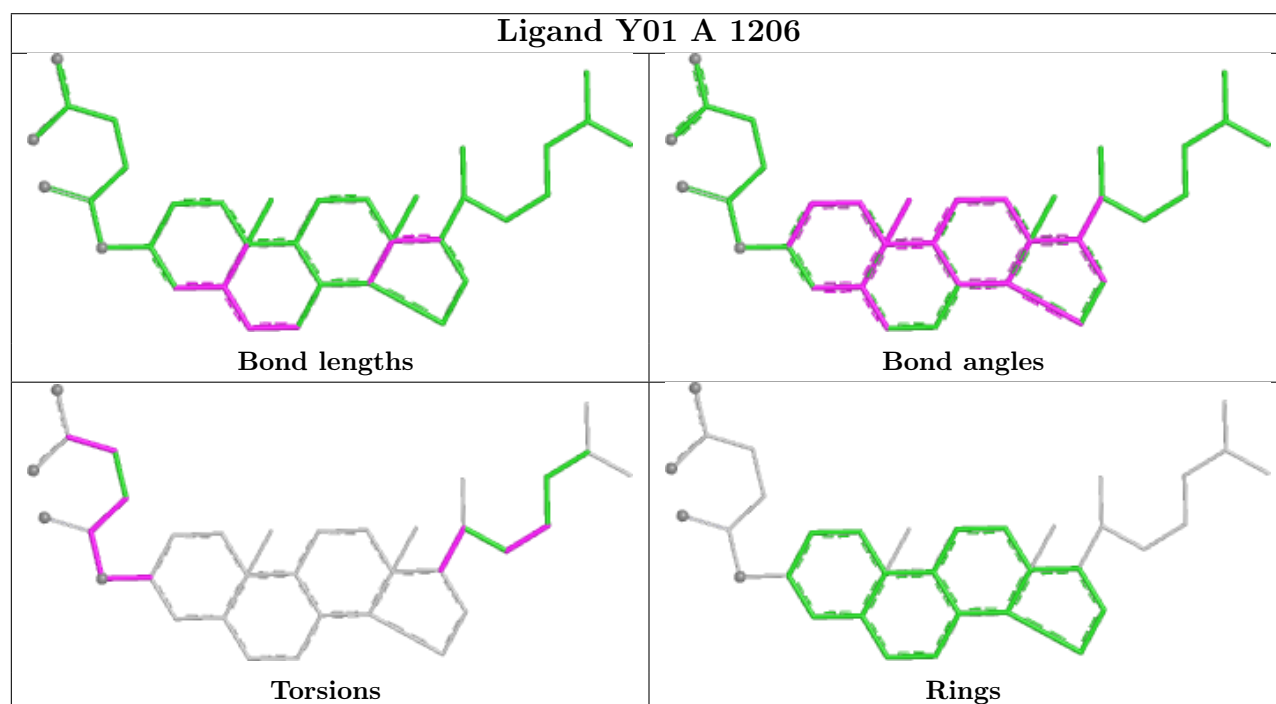
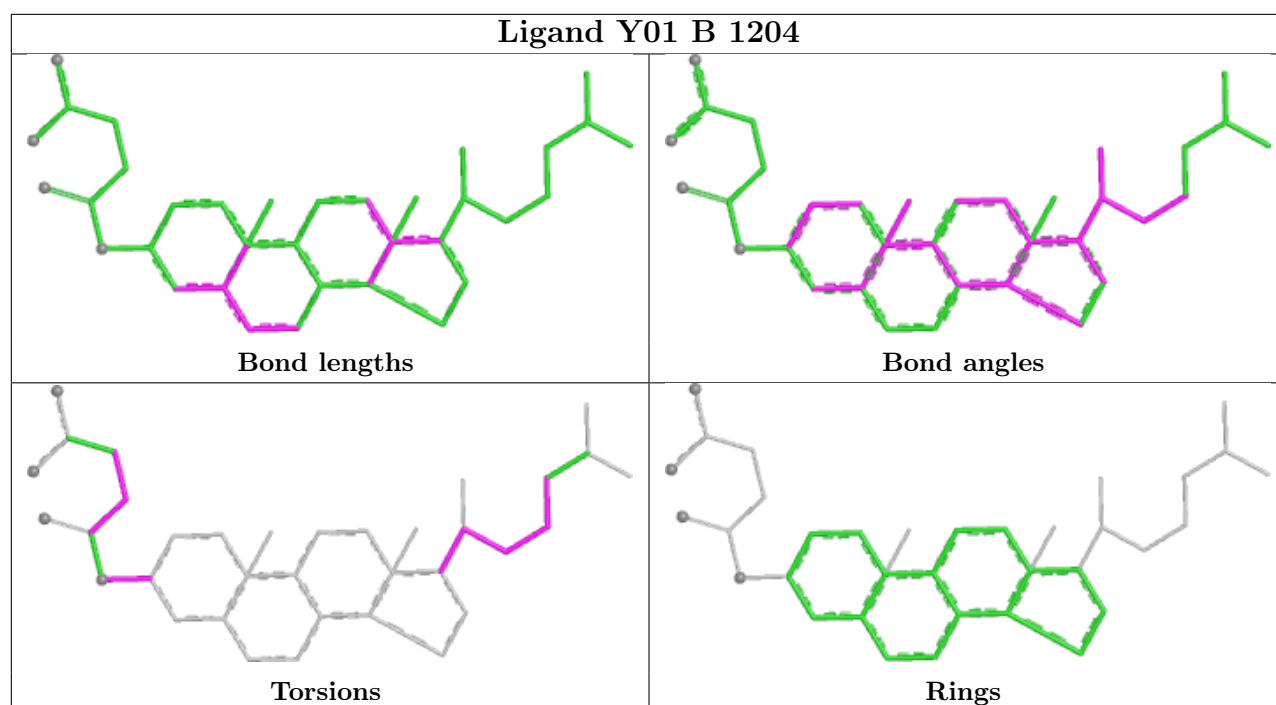


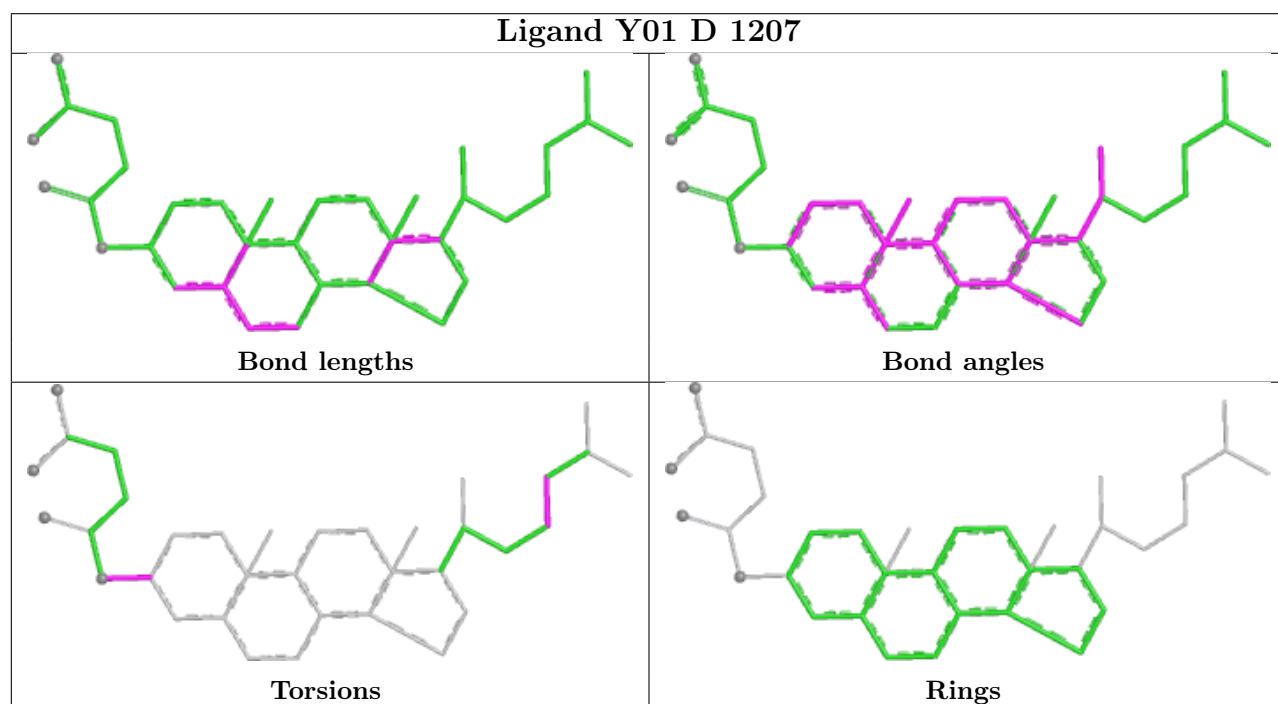
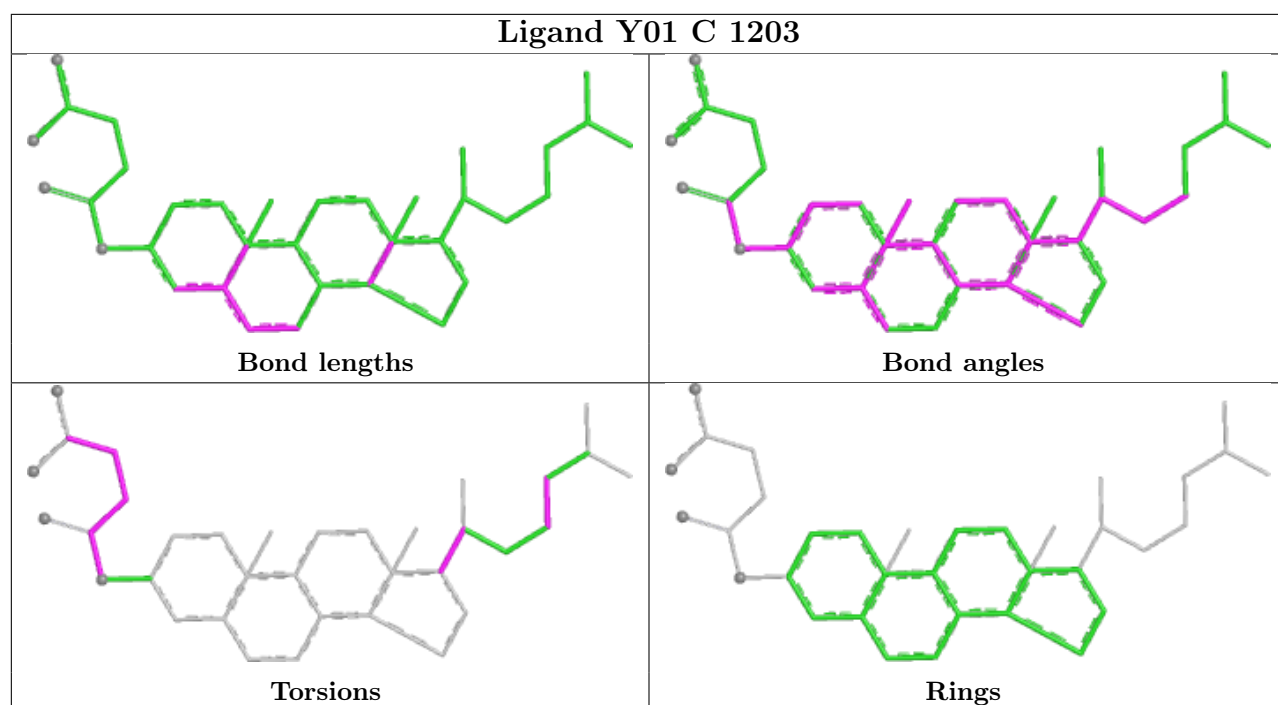


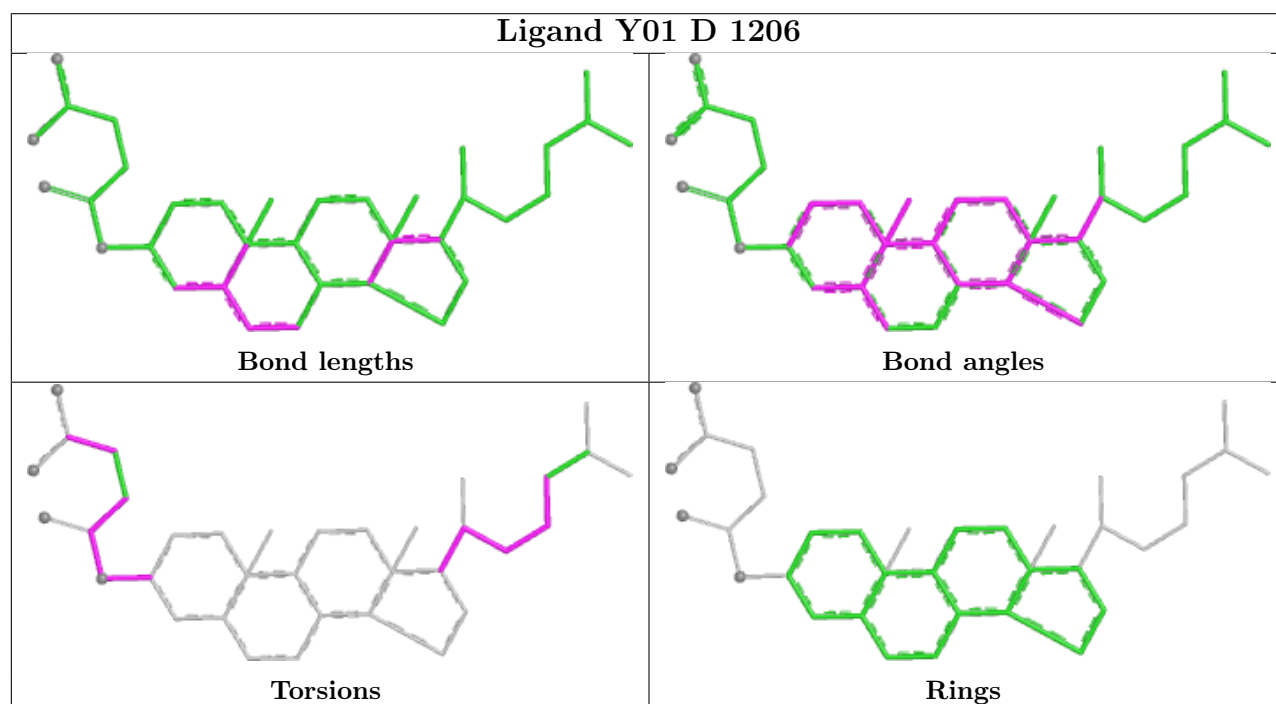
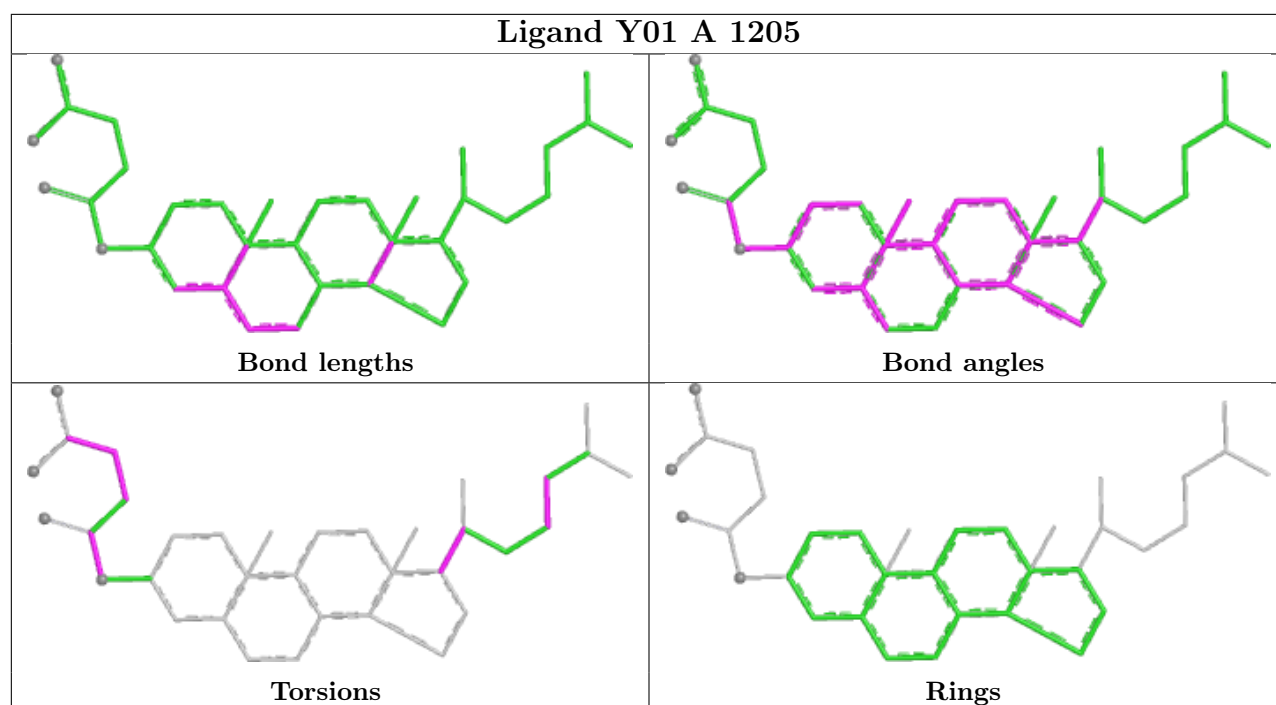


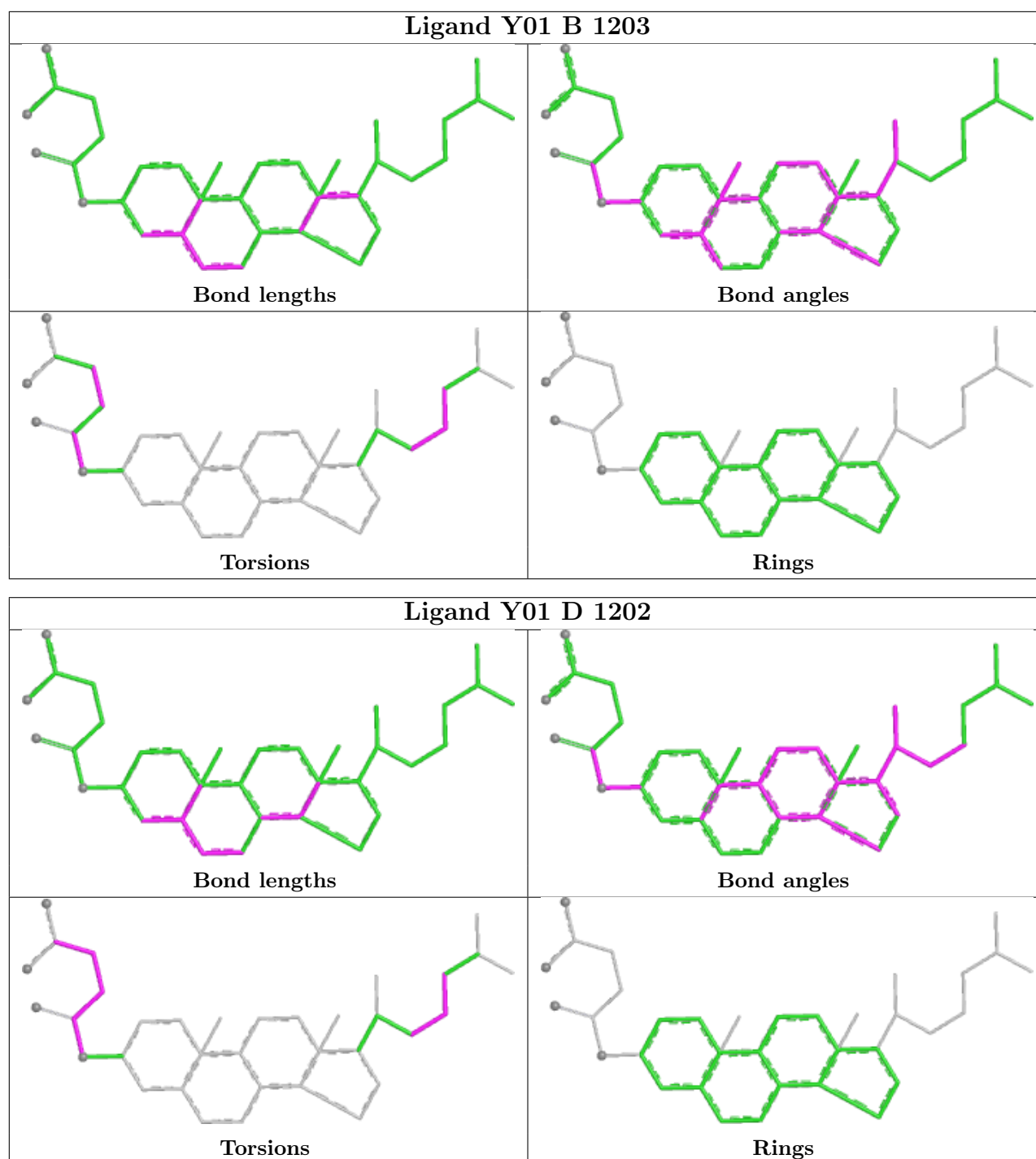












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	7
1	B	7
1	C	7
1	D	7

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	64:UNK	C	73:UNK	N	24.92
1	B	64:UNK	C	73:UNK	N	24.92
1	C	64:UNK	C	73:UNK	N	24.92
1	D	64:UNK	C	73:UNK	N	24.92
1	A	26:UNK	C	31:UNK	N	22.73
1	B	26:UNK	C	31:UNK	N	22.73
1	C	26:UNK	C	31:UNK	N	22.73
1	D	26:UNK	C	31:UNK	N	22.73
1	B	250:UNK	C	260:UNK	N	22.20
1	A	250:UNK	C	260:UNK	N	22.19
1	C	250:UNK	C	260:UNK	N	22.19
1	D	250:UNK	C	260:UNK	N	22.19
1	A	219:UNK	C	227:UNK	N	21.95
1	B	219:UNK	C	227:UNK	N	21.95
1	C	219:UNK	C	227:UNK	N	21.95
1	D	219:UNK	C	227:UNK	N	21.95
1	A	142:UNK	C	196:UNK	N	19.12
1	B	142:UNK	C	196:UNK	N	19.12
1	C	142:UNK	C	196:UNK	N	19.12
1	D	142:UNK	C	196:UNK	N	19.12
1	A	243:UNK	C	245:UNK	N	18.53
1	B	243:UNK	C	245:UNK	N	18.53
1	C	243:UNK	C	245:UNK	N	18.53
1	D	243:UNK	C	245:UNK	N	18.53
1	A	277:UNK	C	395:ASP	N	9.35
1	B	277:UNK	C	395:ASP	N	9.35
1	C	277:UNK	C	395:ASP	N	9.35
1	D	277:UNK	C	395:ASP	N	9.35

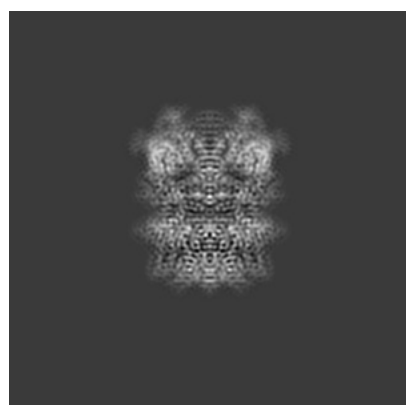
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7299. These allow visual inspection of the internal detail of the map and identification of artifacts.

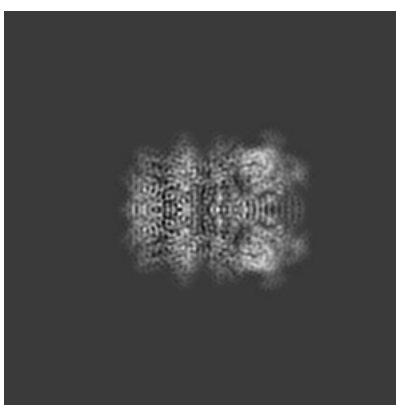
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

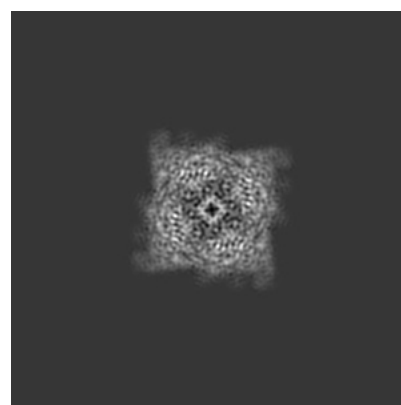
6.1.1 Primary map



X



Y



Z

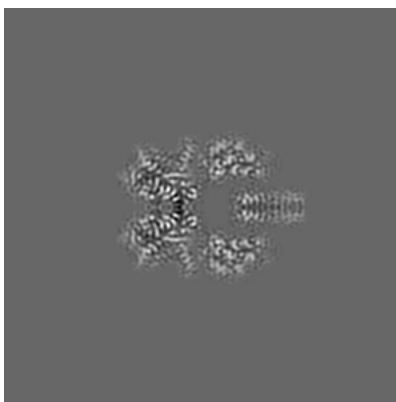
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 128



Y Index: 128



Z Index: 128

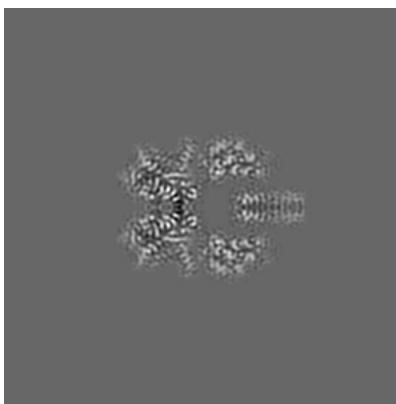
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

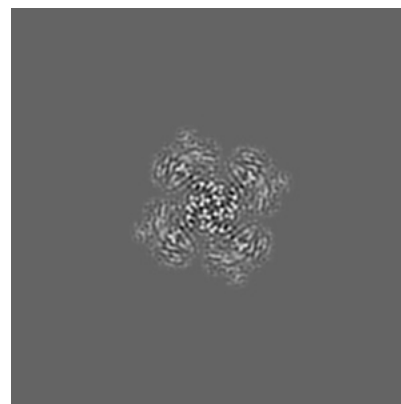
6.3.1 Primary map



X Index: 128



Y Index: 128

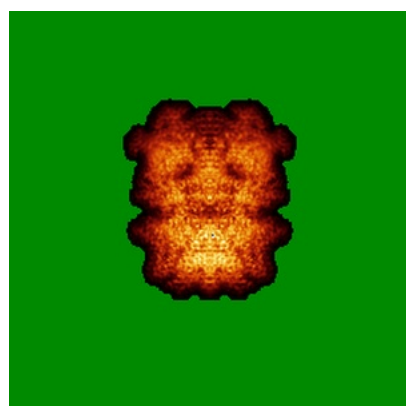


Z Index: 114

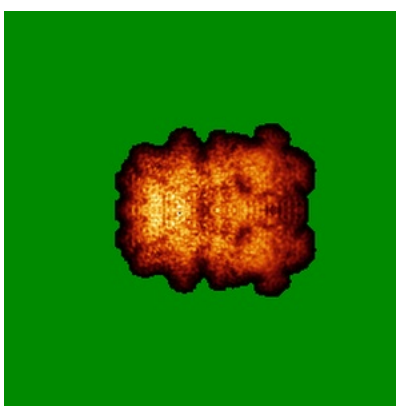
The images above show the largest variance slices of the map in three orthogonal directions.

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

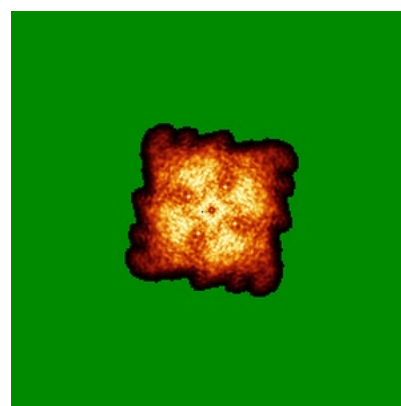
6.4.1 Primary map



X



Y

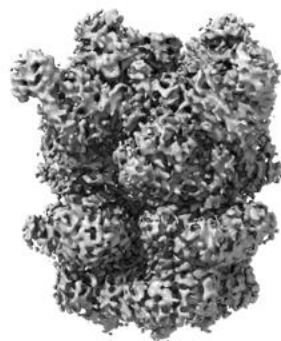


Z

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](#)

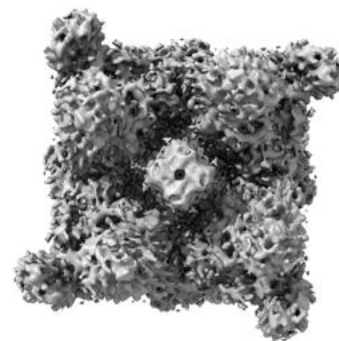
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

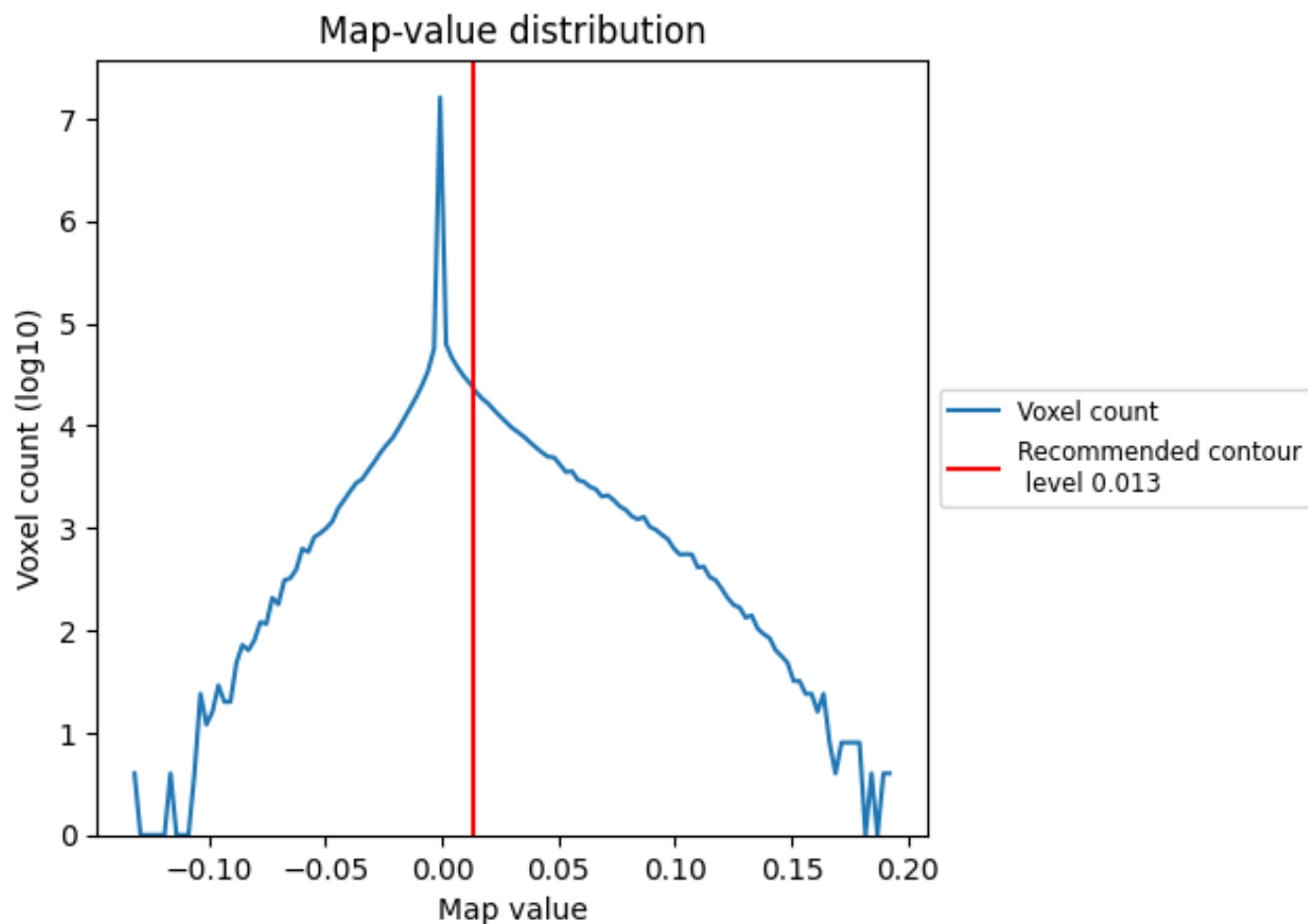
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

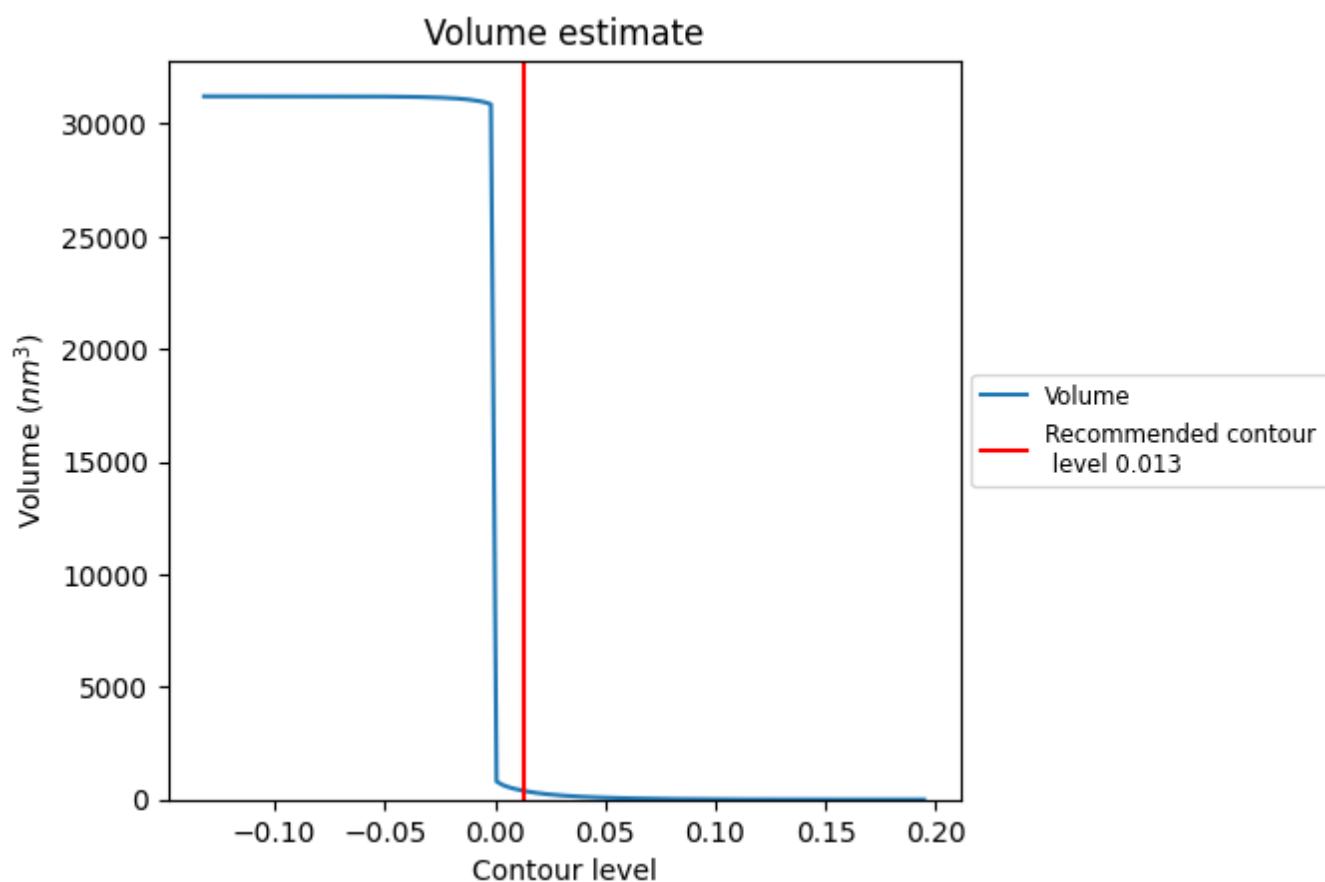
This section contains the results of statistical analysis of the map.

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.

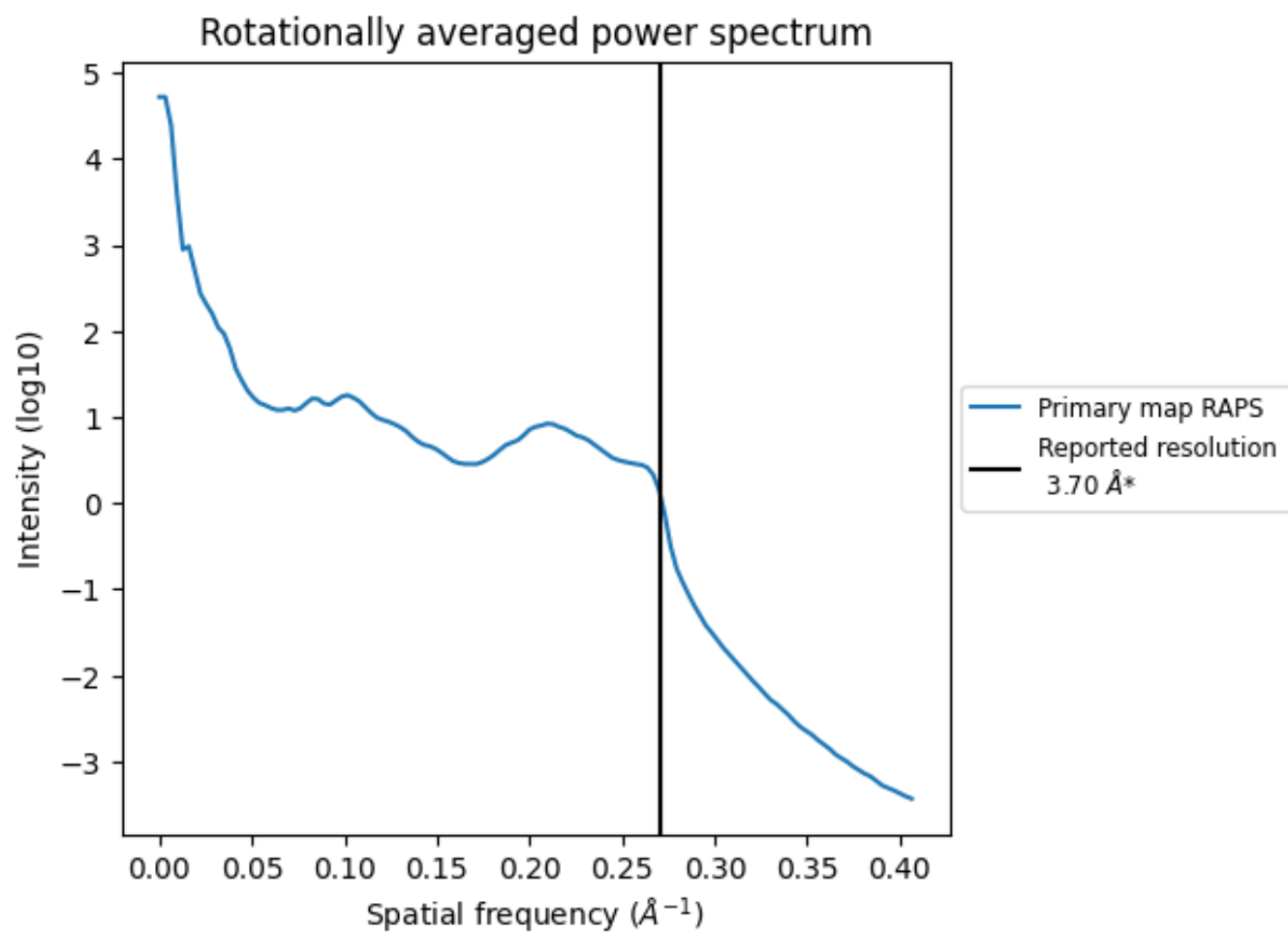
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 388 nm³; this corresponds to an approximate mass of 350 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 ⓘ

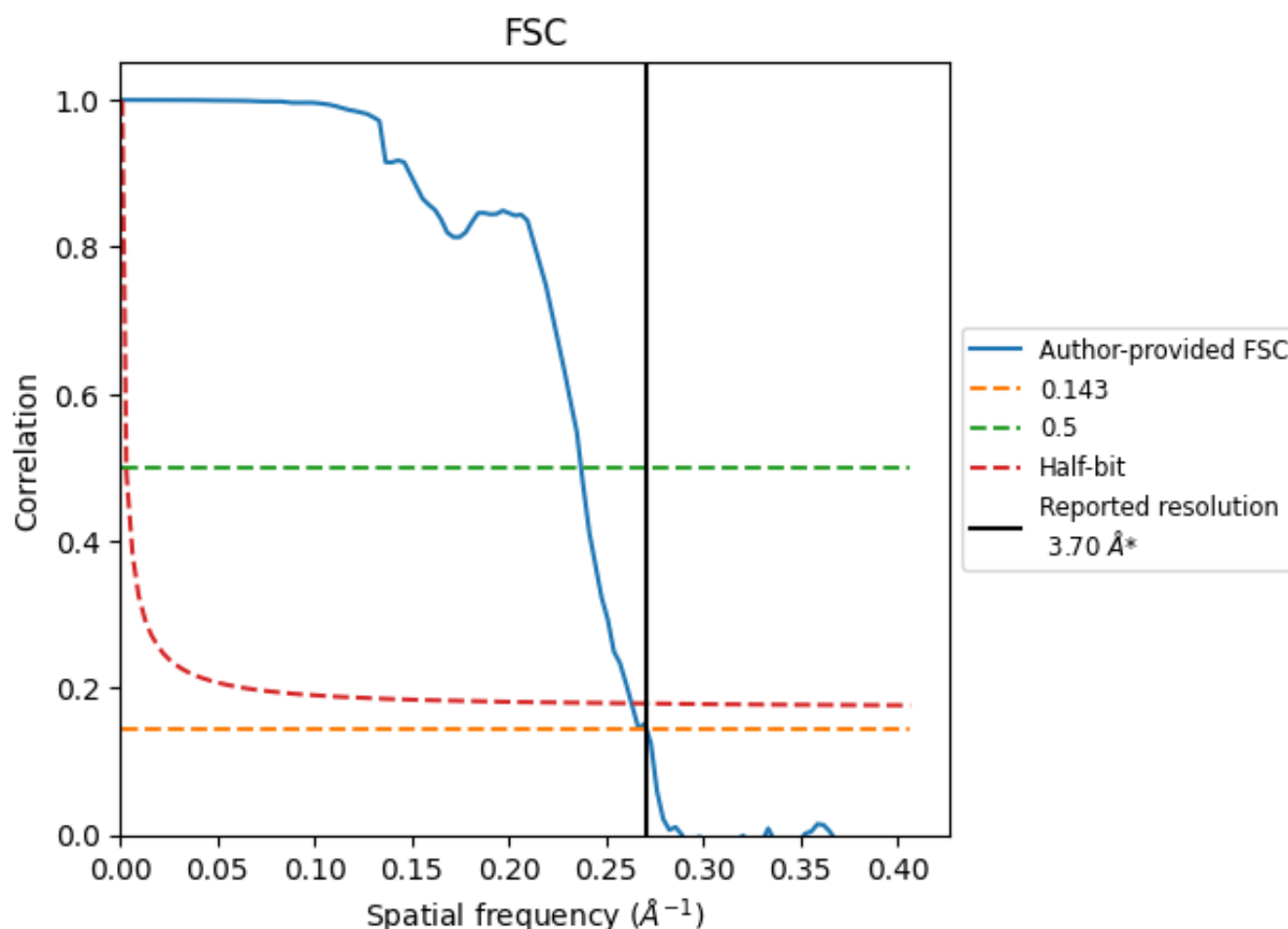


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

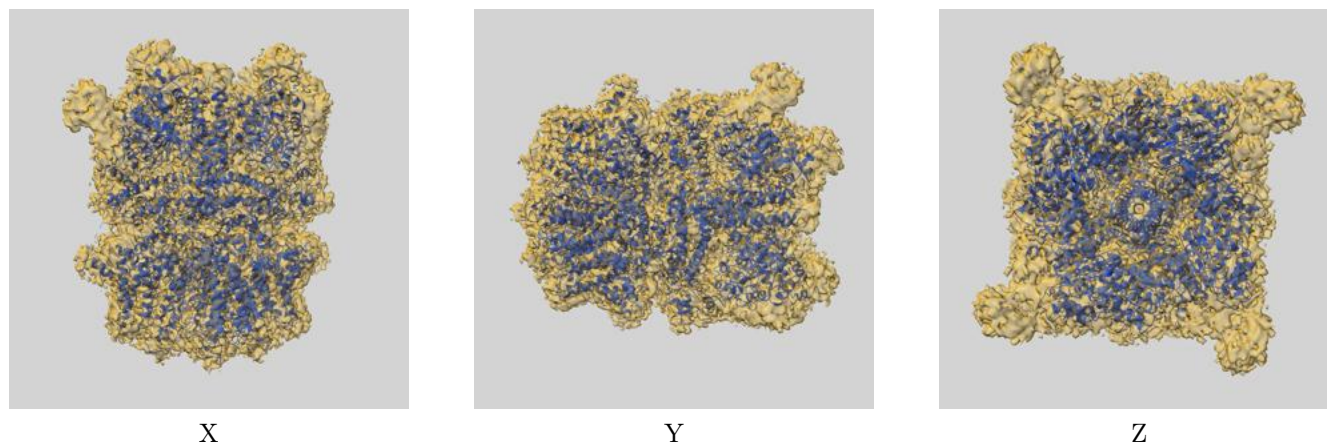
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.69	4.22	3.80
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

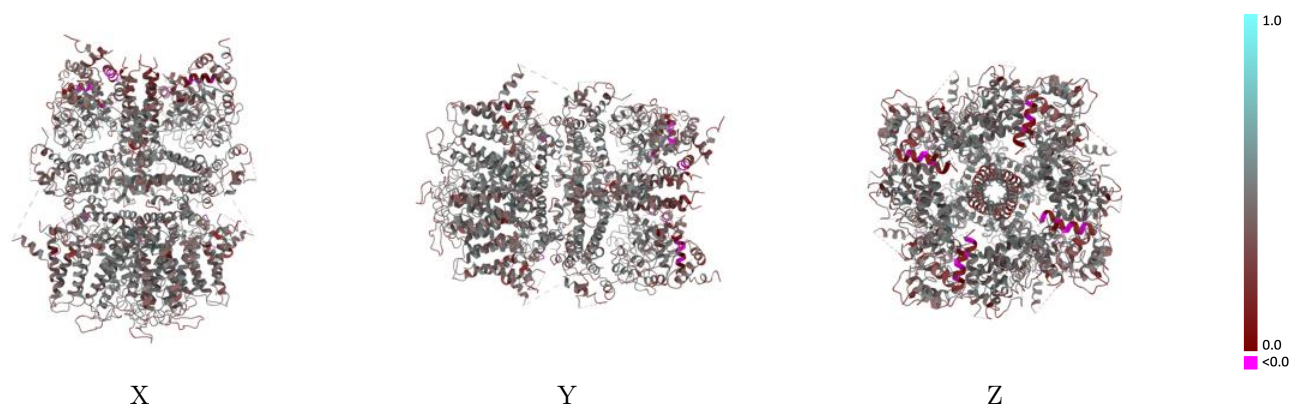
This section contains information regarding the fit between EMDB map EMD-7299 and PDB model 6BWI. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



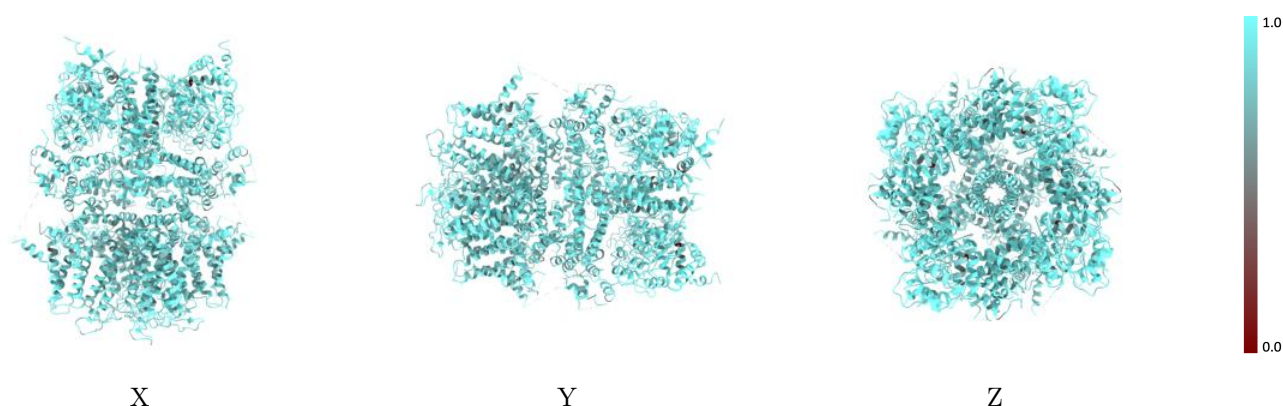
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



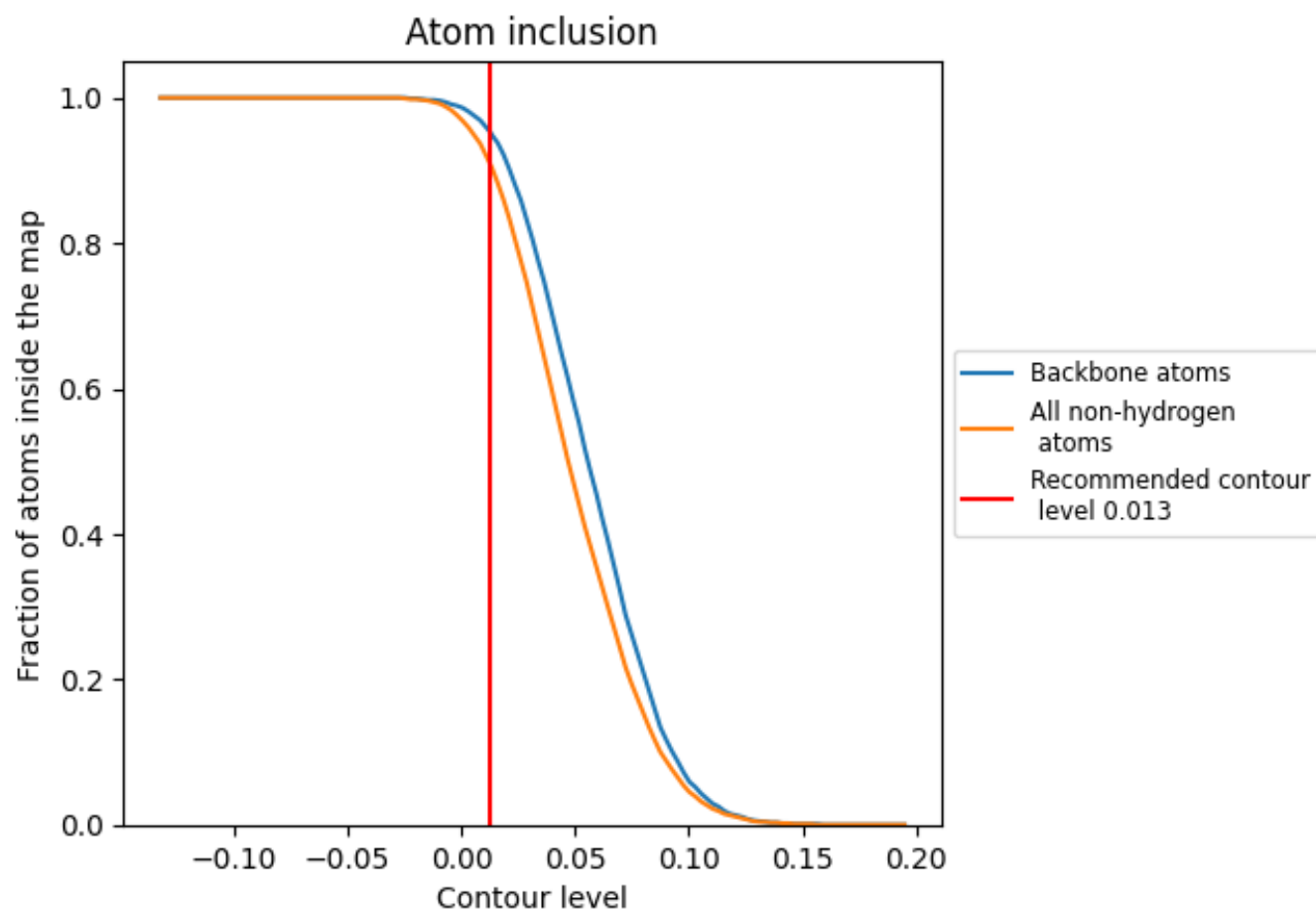
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9070	<div></div> 0.4140
A	<div></div> 0.9080	<div></div> 0.4130
B	<div></div> 0.9080	<div></div> 0.4140
C	<div></div> 0.9070	<div></div> 0.4130
D	<div></div> 0.9080	<div></div> 0.4130

