



Full wwPDB EM Validation Report ⓘ

Aug 10, 2026 – 01:01 PM JST

PDB ID : 9WET / pdb_00009wet
EMDB ID : EMD-65915
Title : Cryo-EM structure of AtABCC2 in ATP-bound, outward-facing state
Authors : Dong, J.; Yang, T.-L.; Lin, H.-Y.; Yang, G.-F.
Deposited on : 2025-08-20
Resolution : 2.85 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

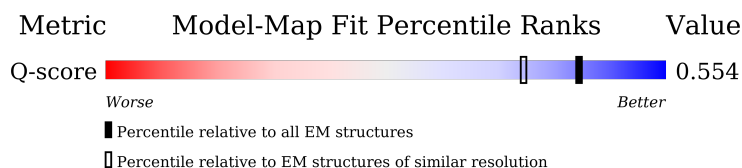
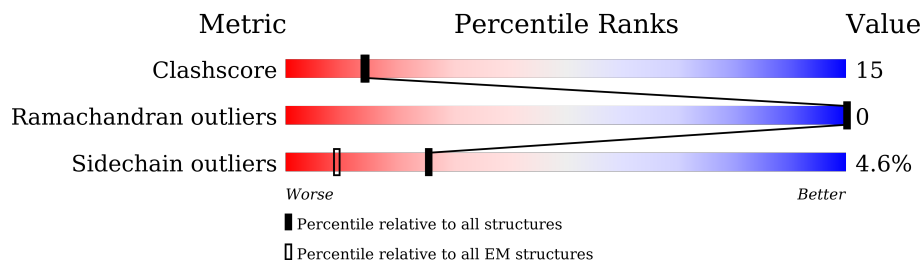
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11965 (2.35 - 3.35)

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	1623	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CLR	A	1705	-	-	X	-
4	CLR	A	1706	-	-	X	-
4	CLR	A	1707	-	-	X	-
4	CLR	A	1708	-	-	X	-
4	CLR	A	1709	-	-	X	-
4	CLR	A	1710	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11442 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.

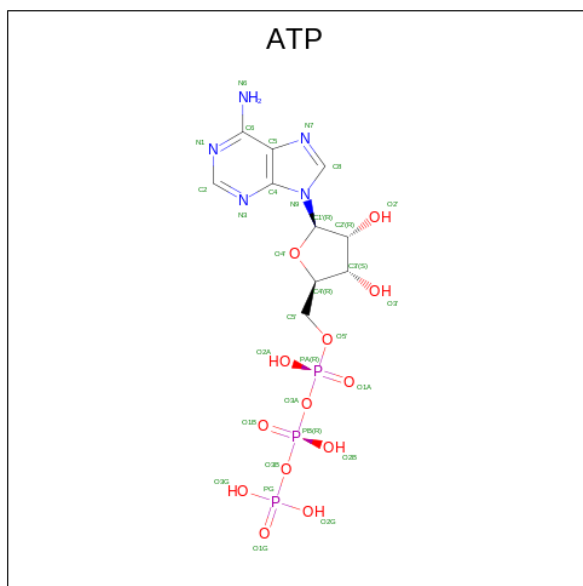
- Molecule 1 is a protein called ABC transporter C family member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1417	11210	7248	1893	2016	53	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1404	GLN	GLU	conflict	UNP Q42093

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

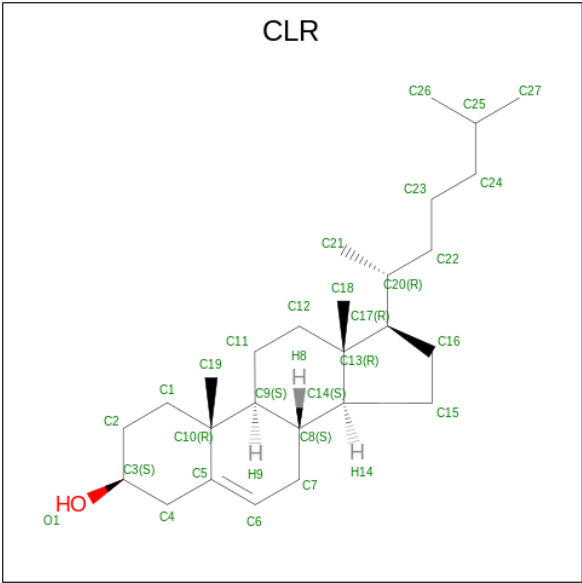


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	31	10	5	13	3	0
2	A	1	31	10	5	13	3	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Mg	0
			2	2	

- Molecule 4 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).

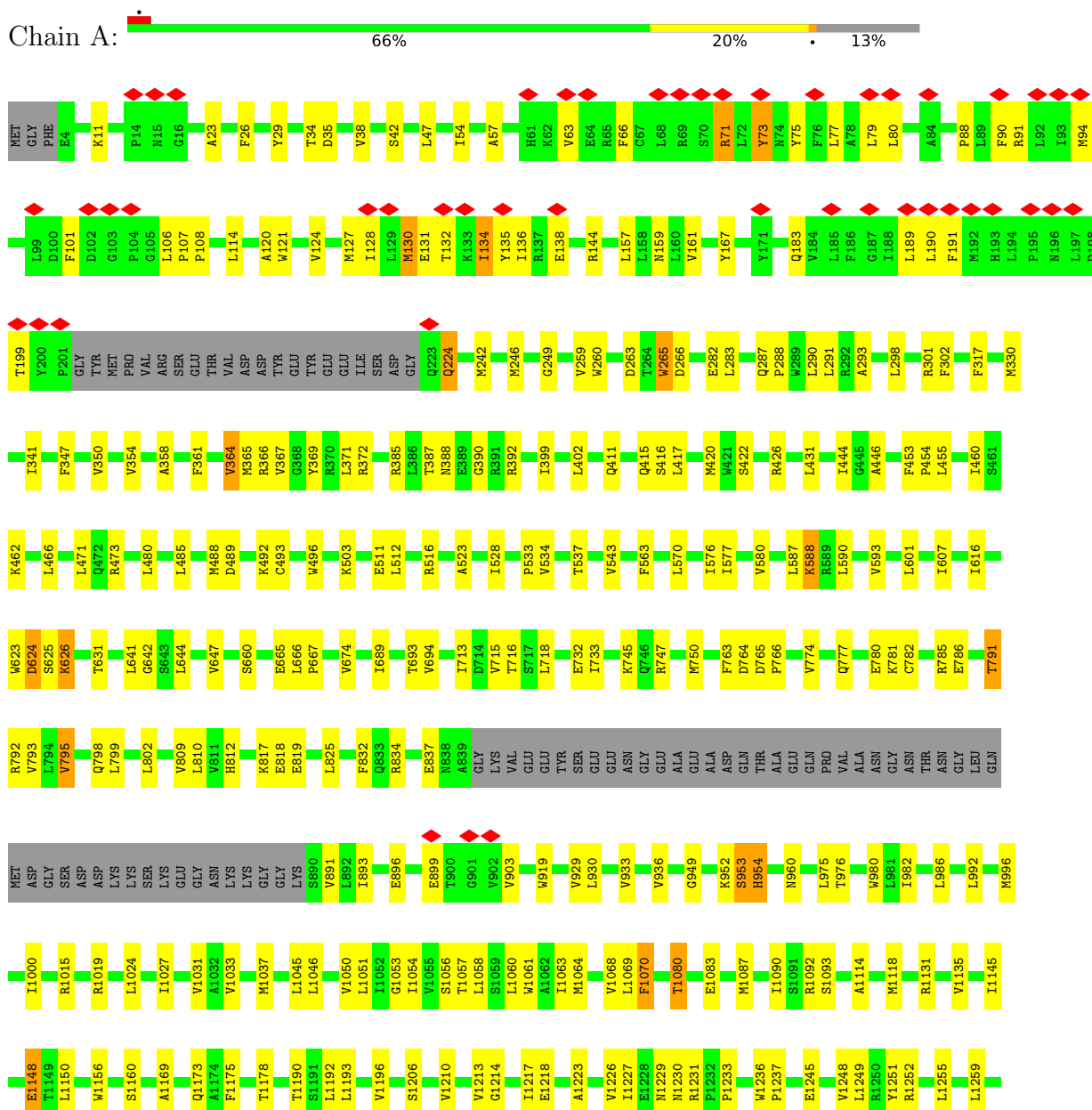


Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			28	27	1	
4	A	1	Total	C	O	0
			28	27	1	
4	A	1	Total	C	O	0
			28	27	1	
4	A	1	Total	C	O	0
			28	27	1	
4	A	1	Total	C	O	0
			28	27	1	
4	A	1	Total	C	O	0
			28	27	1	

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: ABC transporter C family member 2



LEU	V1262	L1387
ALA		
SER	T1269	S1397
LEU		K1398
GLU		
GLU	V1272	I1399
HIS	G1273	L1400
TRP		V1401
ASN	I1274	ALA
ILE	V1275	ALA
ASN	G1276	SER
ILE	R1277	ARG
SER	T1278	GLU
ARG		GLN
GLU		PHE
GLY	L1285	GLY
TRP		TRP
LEU		ALA
LEU	M1430	LEU
SER	L1431	ALA
SER	I1432	ALA
SER	I1433	ALA
LEU		SER
TYR	V1293	LEU
ARG		THR
NET	K1297	ARG
VAL	G1298	SER
GLU	R1299	VAL
GLY		HIS
GLY		ASN
LEU	I1302	ASN
ALA		LEU
VAL	V1307	ALA
NET		GLN
SER		LEU
SER	L1312	SER
ARG	M1313	LEU
LEU		GLU
ILE		ILE
ALA	K1317	LEU
ARG	V1318	GLU
ASN		ASP
ASN		ASP
ARG		ASP
ARG	I1321	ASP
NET		SER
NET	L1328	NET
GLN		GLN
GLN	T1332	ILE
PRO		LEU
ASP		LYS
TYR		ASP
TYR	F1335	ARG
ASN		THR
ASN	N1336	ASN
PHE	L1337	ASN
GLU	D1338	ASP
GLY	P1339	ALA
ASN		VAL
ASN	H1343	VAL
THR		THR
PHE	L1352	THR
ASP	E1353	LEU
TRP	R1354	ARG
ASP		ASP
ASN		VAL
VAL	K1358	LEU
GLU		GLU
GLU	I1361	GLY
NET		LYS
		HIS
	G1376	ASP
	E1377	GLN
		LYS
		GLU
		ILE
	R1384	ALA
		TRP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	180748	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.10	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.919	Depositor
Minimum map value	-1.678	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	290.63998, 290.63998, 290.63998	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.692, 0.692, 0.692	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: ATP, CLR, MG

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	0.18	0/11457	0.35	1/15557 (0.0%)

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	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	949	GLY	N-CA-C	-5.09	107.47	113.99

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1487	ARG	Sidechain

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	11210	0	11398	197	0
2	A	62	0	22	2	0
3	A	2	0	0	0	0
4	A	168	0	204	163	0
All	All	11442	0	11624	357	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 15.

All (357) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1709:CLR:C16	4:A:1709:CLR:C17	1.74	1.65
4:A:1705:CLR:C16	4:A:1705:CLR:C17	1.74	1.64
4:A:1707:CLR:C16	4:A:1707:CLR:C17	1.74	1.64
4:A:1708:CLR:C5	4:A:1708:CLR:C4	1.76	1.64
4:A:1710:CLR:C17	4:A:1710:CLR:C16	1.74	1.63
4:A:1705:CLR:C4	4:A:1705:CLR:C5	1.76	1.61
4:A:1706:CLR:C5	4:A:1706:CLR:C4	1.76	1.58
4:A:1710:CLR:C5	4:A:1710:CLR:C4	1.76	1.58
4:A:1707:CLR:C4	4:A:1707:CLR:C5	1.76	1.56
4:A:1709:CLR:C5	4:A:1709:CLR:C4	1.76	1.56
4:A:1707:CLR:C13	4:A:1707:CLR:C14	1.85	1.54
4:A:1710:CLR:C14	4:A:1710:CLR:C13	1.85	1.53
4:A:1705:CLR:C13	4:A:1705:CLR:C14	1.85	1.52
4:A:1709:CLR:C13	4:A:1709:CLR:C14	1.85	1.49
4:A:1707:CLR:C11	4:A:1707:CLR:C9	1.91	1.48
4:A:1709:CLR:C11	4:A:1709:CLR:C9	1.91	1.48
4:A:1705:CLR:C11	4:A:1705:CLR:C9	1.91	1.46
4:A:1706:CLR:C9	4:A:1706:CLR:C11	1.91	1.46
4:A:1710:CLR:C9	4:A:1710:CLR:C11	1.91	1.45
4:A:1708:CLR:C11	4:A:1708:CLR:C9	1.91	1.45
4:A:1710:CLR:C3	4:A:1710:CLR:O1	1.70	1.40
4:A:1709:CLR:C3	4:A:1709:CLR:O1	1.70	1.40
4:A:1705:CLR:C3	4:A:1705:CLR:O1	1.70	1.39
4:A:1708:CLR:O1	4:A:1708:CLR:C3	1.70	1.38
4:A:1706:CLR:C3	4:A:1706:CLR:O1	1.70	1.36
4:A:1707:CLR:C3	4:A:1707:CLR:O1	1.70	1.36
4:A:1708:CLR:C13	4:A:1708:CLR:C14	1.85	1.34
2:A:1702:ATP:O4'	2:A:1702:ATP:C1'	1.64	1.23
4:A:1706:CLR:C14	4:A:1706:CLR:C13	1.85	1.22
2:A:1701:ATP:O4'	2:A:1701:ATP:C1'	1.64	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1709:CLR:H162	4:A:1709:CLR:H221	1.41	1.02
4:A:1710:CLR:H162	4:A:1710:CLR:H221	1.42	1.02
4:A:1707:CLR:H221	4:A:1707:CLR:H162	1.43	1.01
4:A:1709:CLR:C4	4:A:1709:CLR:C6	2.41	0.98
4:A:1706:CLR:C4	4:A:1706:CLR:C6	2.42	0.97
4:A:1705:CLR:C4	4:A:1705:CLR:C6	2.41	0.97
4:A:1708:CLR:C4	4:A:1708:CLR:C6	2.42	0.97
4:A:1707:CLR:C4	4:A:1707:CLR:C6	2.43	0.96
4:A:1709:CLR:C16	4:A:1709:CLR:C13	2.43	0.96
4:A:1710:CLR:C4	4:A:1710:CLR:C6	2.43	0.95
4:A:1707:CLR:C16	4:A:1707:CLR:C13	2.44	0.95
4:A:1705:CLR:H221	4:A:1705:CLR:H162	1.49	0.94
4:A:1710:CLR:C16	4:A:1710:CLR:C13	2.43	0.94
4:A:1705:CLR:C16	4:A:1705:CLR:C13	2.43	0.92
1:A:358:ALA:HB2	1:A:1145:ILE:HD11	1.51	0.92
4:A:1709:CLR:C13	4:A:1709:CLR:C15	2.53	0.86
4:A:1705:CLR:C13	4:A:1705:CLR:C15	2.53	0.86
4:A:1710:CLR:C13	4:A:1710:CLR:C15	2.53	0.86
4:A:1705:CLR:C16	4:A:1705:CLR:H221	2.07	0.85
4:A:1709:CLR:C16	4:A:1709:CLR:H221	2.07	0.85
4:A:1707:CLR:C13	4:A:1707:CLR:C15	2.54	0.84
4:A:1710:CLR:C11	4:A:1710:CLR:C19	2.55	0.84
4:A:1705:CLR:C17	4:A:1705:CLR:C14	2.53	0.83
4:A:1708:CLR:C11	4:A:1708:CLR:C19	2.57	0.83
4:A:1710:CLR:C17	4:A:1710:CLR:C14	2.52	0.82
4:A:1710:CLR:C16	4:A:1710:CLR:H221	2.09	0.81
4:A:1710:CLR:C13	4:A:1710:CLR:C8	2.55	0.81
4:A:1707:CLR:C13	4:A:1707:CLR:C8	2.57	0.81
4:A:1705:CLR:C13	4:A:1705:CLR:C8	2.57	0.81
4:A:1707:CLR:C11	4:A:1707:CLR:H193	2.11	0.81
4:A:1709:CLR:C13	4:A:1709:CLR:C8	2.58	0.80
1:A:416:SER:HB3	1:A:576:ILE:HG13	1.63	0.80
4:A:1707:CLR:C17	4:A:1707:CLR:C14	2.53	0.79
4:A:1708:CLR:C13	4:A:1708:CLR:C8	2.57	0.79
4:A:1707:CLR:C16	4:A:1707:CLR:H221	2.13	0.78
4:A:1709:CLR:C17	4:A:1709:CLR:C14	2.53	0.78
4:A:1706:CLR:C13	4:A:1706:CLR:C8	2.59	0.76
4:A:1709:CLR:C11	4:A:1709:CLR:H193	2.15	0.76
4:A:1707:CLR:C11	4:A:1707:CLR:C19	2.63	0.76
4:A:1705:CLR:C11	4:A:1705:CLR:H193	2.15	0.76
4:A:1706:CLR:C11	4:A:1706:CLR:H193	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1705:CLR:C14	4:A:1705:CLR:C12	2.63	0.75
4:A:1709:CLR:C14	4:A:1709:CLR:C12	2.63	0.74
4:A:1710:CLR:C14	4:A:1710:CLR:C12	2.63	0.74
1:A:246:MET:HA	1:A:1080:THR:HG21	1.69	0.74
4:A:1707:CLR:C14	4:A:1707:CLR:C12	2.63	0.74
4:A:1708:CLR:C14	4:A:1708:CLR:C12	2.63	0.74
4:A:1708:CLR:C11	4:A:1708:CLR:H193	2.18	0.74
1:A:144:ARG:HH12	1:A:191:PHE:HA	1.54	0.72
4:A:1705:CLR:C11	4:A:1705:CLR:C10	2.64	0.72
4:A:1706:CLR:C9	4:A:1706:CLR:C12	2.65	0.72
4:A:1706:CLR:C14	4:A:1706:CLR:C12	2.64	0.72
4:A:1709:CLR:C11	4:A:1709:CLR:C10	2.64	0.72
1:A:624:ASP:HB2	1:A:626:LYS:HG3	1.72	0.71
4:A:1706:CLR:C11	4:A:1706:CLR:C19	2.69	0.70
4:A:1705:CLR:C11	4:A:1705:CLR:C19	2.69	0.70
4:A:1709:CLR:C11	4:A:1709:CLR:C19	2.69	0.70
4:A:1705:CLR:C9	4:A:1705:CLR:C12	2.66	0.70
1:A:1069:LEU:HB3	1:A:1150:LEU:HD21	1.74	0.69
4:A:1710:CLR:C9	4:A:1710:CLR:C12	2.66	0.69
4:A:1706:CLR:C11	4:A:1706:CLR:C10	2.64	0.69
1:A:1328:LEU:HD21	1:A:1387:LEU:HD12	1.75	0.69
4:A:1707:CLR:C11	4:A:1707:CLR:C10	2.67	0.68
4:A:1710:CLR:C11	4:A:1710:CLR:C8	2.70	0.68
4:A:1705:CLR:C17	4:A:1705:CLR:C15	2.73	0.67
4:A:1708:CLR:O1	4:A:1708:CLR:C2	2.39	0.67
1:A:473:ARG:HB3	1:A:511:GLU:HB2	1.77	0.67
4:A:1709:CLR:C9	4:A:1709:CLR:C12	2.66	0.66
4:A:1709:CLR:C17	4:A:1709:CLR:C15	2.73	0.66
4:A:1709:CLR:C16	4:A:1709:CLR:C22	2.74	0.66
4:A:1708:CLR:C11	4:A:1708:CLR:C8	2.71	0.66
4:A:1707:CLR:C9	4:A:1707:CLR:C12	2.67	0.65
4:A:1708:CLR:C9	4:A:1708:CLR:C12	2.66	0.65
4:A:1705:CLR:C16	4:A:1705:CLR:C20	2.71	0.65
1:A:282:GLU:HG3	1:A:293:ALA:HB2	1.79	0.65
4:A:1710:CLR:C11	4:A:1710:CLR:H193	2.26	0.65
4:A:1707:CLR:C17	4:A:1707:CLR:C15	2.73	0.64
4:A:1710:CLR:C16	4:A:1710:CLR:C22	2.74	0.64
4:A:1710:CLR:O1	4:A:1710:CLR:C2	2.39	0.64
4:A:1705:CLR:C16	4:A:1705:CLR:C22	2.75	0.64
4:A:1707:CLR:C16	4:A:1707:CLR:C22	2.76	0.64
4:A:1705:CLR:C11	4:A:1705:CLR:C8	2.74	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1707:CLR:O1	4:A:1707:CLR:C2	2.39	0.63
4:A:1709:CLR:C16	4:A:1709:CLR:C20	2.70	0.63
1:A:1060:LEU:O	1:A:1064:MET:HG2	1.98	0.63
1:A:444:ILE:HD11	1:A:543:VAL:HG21	1.81	0.63
1:A:462:LYS:O	1:A:466:LEU:HD22	1.99	0.63
1:A:1031:VAL:HG22	1:A:1206:SER:HB3	1.79	0.63
4:A:1709:CLR:C11	4:A:1709:CLR:C8	2.73	0.62
4:A:1710:CLR:C16	4:A:1710:CLR:C20	2.71	0.62
4:A:1710:CLR:C17	4:A:1710:CLR:C15	2.73	0.62
4:A:1707:CLR:C16	4:A:1707:CLR:C20	2.71	0.62
1:A:106:LEU:HD12	1:A:107:PRO:HD2	1.80	0.62
4:A:1706:CLR:C4	4:A:1706:CLR:O1	2.43	0.61
4:A:1705:CLR:H162	4:A:1705:CLR:C22	2.28	0.61
1:A:71:ARG:HH21	1:A:132:THR:HG21	1.65	0.61
4:A:1707:CLR:C11	4:A:1707:CLR:C8	2.75	0.61
4:A:1709:CLR:O1	4:A:1709:CLR:C2	2.39	0.61
1:A:128:ILE:HA	1:A:131:GLU:HG2	1.83	0.61
1:A:1083:GLU:O	1:A:1087:MET:HG3	2.00	0.61
4:A:1706:CLR:O1	4:A:1706:CLR:C2	2.39	0.61
1:A:1033:VAL:O	1:A:1037:MET:HG3	2.02	0.60
1:A:763:PHE:HB3	1:A:766:PRO:HG3	1.83	0.60
1:A:1070:PHE:HD2	1:A:1150:LEU:HD23	1.66	0.60
1:A:1276:GLY:HA2	1:A:1474:MET:HE1	1.83	0.60
1:A:764:ASP:HA	1:A:795:VAL:HG13	1.84	0.59
4:A:1708:CLR:C14	4:A:1708:CLR:C18	2.79	0.59
4:A:1710:CLR:C4	4:A:1710:CLR:O1	2.44	0.59
1:A:301:ARG:HB2	1:A:367:VAL:HG23	1.84	0.59
1:A:616:ILE:HG12	1:A:674:VAL:HG22	1.84	0.59
1:A:1045:LEU:HG	1:A:1192:LEU:HB3	1.85	0.59
1:A:1430:MET:HE3	1:A:1432:ILE:HD11	1.85	0.59
1:A:130:MET:HB2	1:A:134:ILE:HB	1.85	0.58
1:A:694:VAL:HG22	1:A:733:ILE:HD11	1.85	0.58
1:A:1313:MET:O	1:A:1317:LYS:HG2	2.04	0.58
4:A:1706:CLR:C11	4:A:1706:CLR:C8	2.75	0.58
4:A:1707:CLR:C4	4:A:1707:CLR:O1	2.43	0.58
1:A:810:LEU:HD22	1:A:818:GLU:HG3	1.85	0.57
1:A:224:GLN:HG2	1:A:260:TRP:HB3	1.85	0.57
4:A:1705:CLR:C4	4:A:1705:CLR:O1	2.44	0.57
4:A:1705:CLR:O1	4:A:1705:CLR:C2	2.39	0.57
4:A:1710:CLR:C14	4:A:1710:CLR:C18	2.79	0.57
1:A:121:TRP:NE1	1:A:183:GLN:HE21	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1249:LEU:HD11	1:A:1293:VAL:HG13	1.87	0.56
4:A:1709:CLR:C14	4:A:1709:CLR:C18	2.80	0.56
1:A:1227:ILE:HG22	1:A:1230:ASN:H	1.70	0.56
1:A:1337:LEU:HD11	1:A:1387:LEU:HD22	1.88	0.56
4:A:1708:CLR:C6	4:A:1708:CLR:H41	2.35	0.56
4:A:1706:CLR:C14	4:A:1706:CLR:C18	2.81	0.55
4:A:1707:CLR:C3	4:A:1707:CLR:H1	2.13	0.55
4:A:1707:CLR:C6	4:A:1707:CLR:H41	2.36	0.55
1:A:523:ALA:HB2	1:A:982:ILE:HG13	1.88	0.55
1:A:455:LEU:HD11	1:A:528:ILE:HD13	1.88	0.54
1:A:1045:LEU:HD12	1:A:1196:VAL:HG21	1.88	0.54
1:A:1056:SER:O	1:A:1057:THR:HG22	2.08	0.54
1:A:387:THR:HG23	1:A:390:GLY:H	1.72	0.54
1:A:642:GLY:H	1:A:791:THR:HB	1.73	0.54
1:A:493:CYS:HB3	1:A:1321:ILE:HG21	1.89	0.54
1:A:1289:LEU:HD11	1:A:1302:ILE:HD11	1.90	0.54
1:A:302:PHE:HZ	1:A:417:LEU:HB3	1.72	0.54
1:A:936:VAL:HG13	1:A:1051:LEU:HD12	1.91	0.53
1:A:1249:LEU:HD13	1:A:1288:ALA:HB2	1.91	0.53
4:A:1709:CLR:C4	4:A:1709:CLR:O1	2.43	0.53
4:A:1705:CLR:C14	4:A:1705:CLR:C18	2.80	0.53
1:A:66:PHE:HB2	1:A:135:TYR:HD1	1.74	0.52
1:A:607:ILE:HD13	1:A:641:LEU:HD11	1.91	0.52
1:A:347:PHE:HB2	1:A:1156:TRP:HB2	1.91	0.52
1:A:1402:LEU:HD12	1:A:1432:ILE:HG12	1.91	0.52
1:A:1402:LEU:HB2	1:A:1432:ILE:HA	1.92	0.52
4:A:1707:CLR:C14	4:A:1707:CLR:C18	2.80	0.52
4:A:1709:CLR:C3	4:A:1709:CLR:H1	2.13	0.52
1:A:1045:LEU:HD11	1:A:1193:LEU:HD23	1.92	0.52
4:A:1708:CLR:C4	4:A:1708:CLR:O1	2.43	0.52
1:A:1464:LEU:HD21	1:A:1475:VAL:HG21	1.90	0.52
1:A:372:ARG:HH22	1:A:1092:ARG:HD2	1.74	0.52
1:A:930:LEU:HA	1:A:933:VAL:HG22	1.90	0.52
1:A:644:LEU:HB2	1:A:792:ARG:NH2	2.25	0.52
1:A:263:ASP:HB3	1:A:265:TRP:CE3	2.44	0.52
1:A:812:HIS:HB3	1:A:817:LYS:HG3	1.92	0.51
1:A:516:ARG:HG3	1:A:986:LEU:HD13	1.91	0.51
1:A:1272:VAL:HG22	1:A:1445:LYS:HB2	1.93	0.51
1:A:26:PHE:HB3	1:A:29:TYR:HB2	1.92	0.51
1:A:689:ILE:HG13	1:A:745:LYS:HG2	1.92	0.51
1:A:460:ILE:HD11	1:A:577:ILE:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1226:VAL:HG13	1:A:1231:ARG:HE	1.75	0.51
1:A:747:ARG:HH12	1:A:1278:THR:HB	1.75	0.50
1:A:660:SER:HB3	1:A:665:GLU:HB2	1.93	0.50
1:A:834:ARG:O	1:A:837:GLU:HG3	2.10	0.50
1:A:11:LYS:HD2	1:A:107:PRO:HB3	1.94	0.50
1:A:716:THR:O	1:A:747:ARG:HD2	2.11	0.49
1:A:34:THR:O	1:A:38:VAL:HB	2.13	0.49
1:A:1050:VAL:HG11	4:A:1708:CLR:H182	1.95	0.49
1:A:1114:ALA:O	1:A:1118:MET:HG2	2.11	0.49
1:A:350:VAL:O	1:A:354:VAL:HG23	2.12	0.49
1:A:1332:THR:HG23	1:A:1335:PHE:H	1.78	0.49
1:A:488:MET:HE3	1:A:492:LYS:HE2	1.93	0.49
1:A:1070:PHE:CD2	1:A:1150:LEU:HD23	2.48	0.49
1:A:399:ILE:HA	1:A:402:LEU:HD12	1.94	0.49
1:A:372:ARG:HB2	1:A:411:GLN:HB2	1.94	0.49
1:A:929:VAL:O	1:A:933:VAL:HG13	2.12	0.48
4:A:1705:CLR:C6	4:A:1705:CLR:H41	2.38	0.48
1:A:124:VAL:O	1:A:128:ILE:HG13	2.13	0.48
4:A:1710:CLR:C3	4:A:1710:CLR:H1	2.13	0.48
1:A:1252:ARG:NH1	1:A:1255:LEU:HD11	2.28	0.48
1:A:1131:ARG:O	1:A:1135:VAL:HG23	2.14	0.48
1:A:1338:ASP:OD2	1:A:1343:HIS:HB2	2.13	0.48
1:A:1015:ARG:HB2	1:A:1093:SER:HB3	1.94	0.48
1:A:1417:ILE:HA	1:A:1420:THR:HG22	1.95	0.48
1:A:799:LEU:HD22	1:A:802:LEU:HD11	1.95	0.48
4:A:1708:CLR:H41	4:A:1708:CLR:H6	1.94	0.48
1:A:782:CYS:HA	1:A:786:GLU:HB3	1.95	0.47
4:A:1706:CLR:C4	4:A:1706:CLR:H6	2.41	0.47
1:A:121:TRP:HE1	1:A:183:GLN:HE21	1.61	0.47
1:A:249:GLY:HA3	1:A:1080:THR:HG22	1.96	0.47
1:A:1274:ILE:HB	1:A:1433:ILE:HG12	1.95	0.47
1:A:88:PRO:HA	1:A:114:LEU:HD12	1.97	0.47
1:A:63:VAL:HG21	1:A:138:GLU:HB2	1.97	0.47
1:A:480:LEU:HD11	1:A:503:LYS:HD3	1.97	0.47
1:A:361:PHE:O	1:A:365:MET:HG3	2.15	0.47
1:A:485:LEU:HA	1:A:488:MET:HG2	1.96	0.47
1:A:1245:GLU:HB2	1:A:1299:ARG:HG2	1.97	0.46
1:A:341:ILE:HD11	4:A:1705:CLR:H161	1.98	0.46
4:A:1707:CLR:H183	4:A:1707:CLR:H20	1.63	0.46
4:A:1709:CLR:C14	4:A:1709:CLR:C11	2.85	0.46
1:A:1214:GLY:O	1:A:1218:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:PHE:HE1	1:A:167:TYR:HB2	1.81	0.46
1:A:1213:VAL:O	1:A:1217:ILE:HG13	2.16	0.46
1:A:1328:LEU:HD22	1:A:1384:ARG:HG2	1.96	0.46
1:A:1482:ASN:O	1:A:1483:ALA:C	2.59	0.46
4:A:1708:CLR:C3	4:A:1708:CLR:H1	2.13	0.46
1:A:66:PHE:HB2	1:A:135:TYR:CD1	2.51	0.46
4:A:1706:CLR:C3	4:A:1706:CLR:H1	2.13	0.46
4:A:1706:CLR:C6	4:A:1706:CLR:H41	2.39	0.46
1:A:647:VAL:HB	1:A:795:VAL:HB	1.98	0.46
1:A:77:LEU:HD13	1:A:80:LEU:HD12	1.98	0.46
1:A:1251:TYR:HA	1:A:1293:VAL:HG21	1.97	0.45
4:A:1705:CLR:H183	4:A:1705:CLR:H20	1.64	0.45
1:A:1054:ILE:HG13	4:A:1710:CLR:H151	1.97	0.45
1:A:260:TRP:CH2	1:A:1135:VAL:HG22	2.52	0.45
1:A:644:LEU:HB2	1:A:792:ARG:HH21	1.79	0.45
1:A:392:ARG:NH2	1:A:623:TRP:O	2.49	0.45
1:A:588:LYS:HA	1:A:588:LYS:HD3	1.78	0.45
1:A:996:MET:HE1	1:A:1024:LEU:HG	1.99	0.45
1:A:290:LEU:HD23	1:A:587:LEU:HD12	1.99	0.45
1:A:330:MET:HE1	1:A:1175:PHE:HB2	1.99	0.45
1:A:1046:LEU:HD12	4:A:1708:CLR:H263	1.97	0.45
1:A:354:VAL:CG2	1:A:1148:GLU:HB3	2.46	0.45
1:A:431:LEU:HD22	1:A:446:ALA:HB2	1.98	0.45
1:A:1060:LEU:HA	1:A:1063:ILE:HG12	1.99	0.45
1:A:1262:VAL:HG11	1:A:1285:LEU:HD21	1.98	0.45
1:A:1448:VAL:HG11	1:A:1470:SER:HB3	1.99	0.45
1:A:127:MET:HE3	1:A:127:MET:C	2.42	0.45
1:A:750:MET:HB3	1:A:750:MET:HE2	1.72	0.45
1:A:1259:LEU:HD22	1:A:1262:VAL:HG21	1.98	0.45
4:A:1707:CLR:C13	4:A:1707:CLR:C9	2.85	0.45
4:A:1707:CLR:H41	4:A:1707:CLR:H6	1.99	0.45
4:A:1708:CLR:H232	4:A:1708:CLR:H211	1.71	0.45
1:A:623:TRP:HA	1:A:666:LEU:HD21	1.99	0.44
1:A:1269:THR:O	1:A:1269:THR:HG22	2.16	0.44
4:A:1710:CLR:H6	4:A:1710:CLR:H41	1.99	0.44
1:A:266:ASP:OD1	1:A:369:TYR:HE1	2.00	0.44
1:A:364:VAL:CG1	1:A:415:GLN:HA	2.47	0.44
1:A:420:MET:HE2	1:A:580:VAL:HG21	1.99	0.44
1:A:834:ARG:HH11	1:A:837:GLU:HG2	1.81	0.44
1:A:992:LEU:HD13	1:A:1027:ILE:HD13	1.99	0.44
4:A:1705:CLR:H211	4:A:1705:CLR:H232	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1710:CLR:C11	4:A:1710:CLR:H191	2.42	0.44
4:A:1710:CLR:C6	4:A:1710:CLR:H41	2.38	0.44
1:A:263:ASP:HB3	1:A:265:TRP:CZ3	2.53	0.44
1:A:364:VAL:HG13	1:A:415:GLN:HA	2.00	0.44
1:A:291:LEU:HD13	1:A:587:LEU:HD21	1.98	0.44
1:A:496:TRP:CE2	1:A:1339:PRO:HG3	2.53	0.44
1:A:47:LEU:HB2	1:A:120:ALA:HA	2.00	0.44
1:A:747:ARG:HH12	1:A:1278:THR:CB	2.30	0.44
1:A:159:ASN:ND2	1:A:1057:THR:HG21	2.32	0.44
1:A:825:LEU:HB3	1:A:832:PHE:CD2	2.52	0.44
1:A:976:THR:HG23	1:A:980:TRP:HD1	1.83	0.44
1:A:1236:TRP:HB3	1:A:1237:PRO:HD3	2.00	0.44
4:A:1708:CLR:H183	4:A:1708:CLR:H20	1.62	0.44
1:A:713:ILE:HG23	1:A:718:LEU:HB3	2.00	0.44
1:A:953:SER:HB3	1:A:954:HIS:CE1	2.53	0.44
4:A:1705:CLR:C3	4:A:1705:CLR:H1	2.13	0.44
4:A:1706:CLR:H232	4:A:1706:CLR:H211	1.77	0.44
4:A:1707:CLR:C14	4:A:1707:CLR:C11	2.86	0.44
1:A:42:SER:HB2	1:A:1061:TRP:HE1	1.83	0.43
1:A:57:ALA:HA	1:A:136:ILE:HG21	2.00	0.43
1:A:157:LEU:O	1:A:161:VAL:HG22	2.18	0.43
1:A:480:LEU:HD21	1:A:503:LYS:HB3	2.01	0.43
1:A:354:VAL:HG21	1:A:1148:GLU:HB3	2.00	0.43
1:A:1233:PRO:HD2	1:A:1236:TRP:HB2	2.00	0.43
1:A:777:GLN:O	1:A:781:LYS:HB2	2.18	0.43
1:A:1027:ILE:HD11	1:A:1210:VAL:HA	2.00	0.43
1:A:809:VAL:HG22	1:A:819:GLU:HG2	2.01	0.43
4:A:1709:CLR:H183	4:A:1709:CLR:H20	1.63	0.43
1:A:91:ARG:NH1	1:A:114:LEU:HD11	2.33	0.43
1:A:471:LEU:HD23	1:A:471:LEU:HA	1.84	0.42
1:A:715:VAL:HG23	1:A:716:THR:HG23	2.01	0.42
1:A:1027:ILE:HG12	1:A:1210:VAL:HG22	2.01	0.42
1:A:1031:VAL:HA	1:A:1206:SER:HB3	2.01	0.42
4:A:1706:CLR:H183	4:A:1706:CLR:H20	1.84	0.42
1:A:23:ALA:HB1	1:A:1169:ALA:HB2	2.02	0.42
1:A:283:LEU:HD23	1:A:288:PRO:HB3	2.02	0.42
1:A:366:ARG:HA	1:A:369:TYR:CE2	2.55	0.42
1:A:1353:GLU:HB2	1:A:1358:LYS:HD2	2.01	0.42
1:A:1354:ARG:CZ	1:A:1354:ARG:HB2	2.50	0.42
1:A:90:PHE:O	1:A:94:MET:HG2	2.20	0.42
1:A:259:VAL:HG13	1:A:1135:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:THR:HG22	1:A:563:PHE:CG	2.55	0.42
1:A:1053:GLY:HA3	1:A:1060:LEU:HD22	2.00	0.42
1:A:1056:SER:C	1:A:1058:LEU:H	2.28	0.42
1:A:512:LEU:HD23	1:A:512:LEU:HA	1.86	0.42
1:A:693:THR:HA	1:A:732:GLU:HA	2.02	0.42
1:A:1387:LEU:HD23	1:A:1387:LEU:HA	1.86	0.42
4:A:1710:CLR:H183	4:A:1710:CLR:H20	1.66	0.42
1:A:1328:LEU:HB2	1:A:1376:GLY:HA3	2.02	0.41
1:A:291:LEU:HB2	1:A:587:LEU:HD21	2.03	0.41
1:A:385:ARG:HG2	1:A:601:LEU:HD12	2.01	0.41
1:A:1223:ALA:HB3	1:A:1312:LEU:HG	2.02	0.41
1:A:35:ASP:OD2	1:A:35:ASP:C	2.63	0.41
1:A:388:ASN:HD21	1:A:667:PRO:HD3	1.85	0.41
1:A:533:PRO:O	1:A:537:THR:HG23	2.20	0.41
1:A:1160:SER:HB3	4:A:1706:CLR:H213	2.03	0.41
1:A:1262:VAL:HG13	1:A:1454:VAL:HG23	2.01	0.41
4:A:1706:CLR:H272	4:A:1706:CLR:H231	1.86	0.41
1:A:453:PHE:HB2	1:A:454:PRO:HD3	2.03	0.41
1:A:533:PRO:HG3	1:A:570:LEU:HD22	2.01	0.41
1:A:1352:LEU:HD13	1:A:1361:ILE:HG13	2.02	0.41
1:A:623:TRP:CD1	1:A:631:THR:HG21	2.55	0.41
1:A:666:LEU:HD23	1:A:666:LEU:HA	1.85	0.41
1:A:402:LEU:HD11	1:A:593:VAL:HG21	2.03	0.41
1:A:747:ARG:NH1	1:A:774:VAL:HG11	2.36	0.41
1:A:780:GLU:O	1:A:785:ARG:HG3	2.21	0.41
1:A:1248:VAL:HB	1:A:1297:LYS:HB2	2.02	0.41
4:A:1709:CLR:C6	4:A:1709:CLR:H41	2.42	0.41
1:A:73:TYR:C	1:A:75:TYR:H	2.29	0.40
1:A:107:PRO:HA	1:A:108:PRO:HD3	1.97	0.40
1:A:242:MET:HE3	1:A:242:MET:HB3	1.78	0.40
1:A:317:PHE:HZ	1:A:426:ARG:O	2.04	0.40
1:A:1400:LEU:O	1:A:1430:MET:HA	2.21	0.40
1:A:1321:ILE:HG13	1:A:1401:VAL:HG12	2.04	0.40
4:A:1705:CLR:C4	4:A:1705:CLR:H6	2.44	0.40
4:A:1708:CLR:H162	4:A:1708:CLR:H221	1.69	0.40
1:A:896:GLU:HB2	1:A:1090:ILE:HD12	2.03	0.40
1:A:1229:ASN:OD1	1:A:1229:ASN:C	2.64	0.40
1:A:1398:LYS:HE2	1:A:1398:LYS:HB2	1.82	0.40
1:A:136:ILE:HD12	1:A:138:GLU:HB3	2.03	0.40
4:A:1705:CLR:C11	4:A:1705:CLR:C1	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1411/1623 (87%)	1368 (97%)	43 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1226/1399 (88%)	1169 (95%)	57 (5%)	24	48

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ILE
1	A	71	ARG
1	A	73	TYR
1	A	79	LEU
1	A	130	MET
1	A	134	ILE
1	A	189	LEU
1	A	190	LEU
1	A	199	THR
1	A	224	GLN
1	A	265	TRP
1	A	287	GLN
1	A	298	LEU

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Mol	Chain	Res	Type
1	A	364	VAL
1	A	371	LEU
1	A	422	SER
1	A	489	ASP
1	A	534	VAL
1	A	588	LYS
1	A	590	LEU
1	A	624	ASP
1	A	625	SER
1	A	626	LYS
1	A	765	ASP
1	A	791	THR
1	A	793	VAL
1	A	795	VAL
1	A	798	GLN
1	A	891	VAL
1	A	893	ILE
1	A	899	GLU
1	A	903	VAL
1	A	919	TRP
1	A	952	LYS
1	A	953	SER
1	A	954	HIS
1	A	960	ASN
1	A	975	LEU
1	A	1000	ILE
1	A	1019	ARG
1	A	1068	VAL
1	A	1070	PHE
1	A	1080	THR
1	A	1148	GLU
1	A	1173	GLN
1	A	1178	THR
1	A	1190	THR
1	A	1307	VAL
1	A	1318	VAL
1	A	1377	GLU
1	A	1397	SER
1	A	1400	LEU
1	A	1401	VAL
1	A	1449	LEU
1	A	1459	SER

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Mol	Chain	Res	Type
1	A	1463	LEU
1	A	1490	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	183	GLN
1	A	324	ASN
1	A	412	GLN
1	A	472	GLN
1	A	505	GLN
1	A	636	ASN
1	A	954	HIS
1	A	977	ASN
1	A	993	HIS
1	A	1036	ASN
1	A	1041	GLN
1	A	1104	ASN
1	A	1462	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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
4	CLR	A	1706	-	31,31,31	11.81	20 (64%)	48,48,48	3.36	15 (31%)
4	CLR	A	1708	-	31,31,31	11.80	20 (64%)	48,48,48	3.33	18 (37%)
4	CLR	A	1709	-	31,31,31	11.83	21 (67%)	48,48,48	3.29	14 (29%)
4	CLR	A	1710	-	31,31,31	11.80	20 (64%)	48,48,48	3.30	15 (31%)
2	ATP	A	1701	3	29,33,33	2.99	8 (27%)	44,52,52	1.97	12 (27%)
4	CLR	A	1705	-	31,31,31	11.81	20 (64%)	48,48,48	3.34	14 (29%)
2	ATP	A	1702	3	29,33,33	2.99	8 (27%)	44,52,52	2.03	12 (27%)
4	CLR	A	1707	-	31,31,31	11.80	20 (64%)	48,48,48	3.33	15 (31%)

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
4	CLR	A	1706	-	-	6/10/68/68	0/4/4/4
4	CLR	A	1708	-	-	8/10/68/68	0/4/4/4
4	CLR	A	1709	-	-	10/10/68/68	0/4/4/4
4	CLR	A	1710	-	-	6/10/68/68	0/4/4/4
2	ATP	A	1701	3	-	1/22/38/38	0/3/3/3
4	CLR	A	1705	-	-	8/10/68/68	0/4/4/4
2	ATP	A	1702	3	-	2/22/38/38	0/3/3/3
4	CLR	A	1707	-	-	7/10/68/68	0/4/4/4

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1709	CLR	C7-C8	-31.33	1.00	1.53
4	A	1710	CLR	C7-C8	-31.19	1.00	1.53
4	A	1705	CLR	C7-C8	-31.14	1.00	1.53
4	A	1706	CLR	C7-C8	-31.07	1.00	1.53
4	A	1707	CLR	C7-C8	-31.05	1.00	1.53
4	A	1708	CLR	C7-C8	-31.04	1.00	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1708	CLR	C10-C5	-23.26	1.06	1.52
4	A	1710	CLR	C10-C5	-23.26	1.06	1.52
4	A	1707	CLR	C10-C5	-22.97	1.07	1.52
4	A	1706	CLR	C10-C5	-22.94	1.07	1.52
4	A	1709	CLR	C10-C5	-22.91	1.07	1.52
4	A	1705	CLR	C10-C5	-22.90	1.07	1.52
4	A	1708	CLR	C11-C9	22.75	1.91	1.53
4	A	1710	CLR	C11-C9	22.68	1.91	1.53
4	A	1707	CLR	C11-C9	22.65	1.91	1.53
4	A	1709	CLR	C11-C9	22.42	1.91	1.53
4	A	1705	CLR	C11-C9	22.40	1.91	1.53
4	A	1706	CLR	C11-C9	22.37	1.91	1.53
4	A	1705	CLR	C10-C9	-19.25	1.23	1.56
4	A	1709	CLR	C10-C9	-19.23	1.23	1.56
4	A	1706	CLR	C10-C9	-19.17	1.23	1.56
4	A	1707	CLR	C10-C9	-18.87	1.24	1.56
4	A	1708	CLR	C10-C9	-18.50	1.25	1.56
4	A	1710	CLR	C10-C9	-18.44	1.25	1.56
4	A	1708	CLR	C8-C14	-16.49	1.22	1.53
4	A	1710	CLR	C8-C14	-16.38	1.22	1.53
4	A	1706	CLR	C8-C14	-16.34	1.22	1.53
4	A	1707	CLR	C8-C14	-16.32	1.22	1.53
4	A	1705	CLR	C8-C14	-16.31	1.22	1.53
4	A	1709	CLR	C8-C14	-16.31	1.22	1.53
4	A	1709	CLR	C13-C14	16.11	1.85	1.55
4	A	1707	CLR	C13-C14	16.10	1.85	1.55
4	A	1706	CLR	C13-C14	16.09	1.85	1.55
4	A	1705	CLR	C13-C14	16.08	1.85	1.55
4	A	1708	CLR	C13-C14	16.04	1.85	1.55
4	A	1710	CLR	C13-C14	16.03	1.85	1.55
4	A	1705	CLR	C12-C11	-14.06	1.23	1.53
4	A	1706	CLR	C12-C11	-14.05	1.23	1.53
4	A	1707	CLR	C12-C11	-14.00	1.23	1.53
4	A	1709	CLR	C12-C11	-13.98	1.23	1.53
4	A	1708	CLR	C12-C11	-13.91	1.23	1.53
4	A	1710	CLR	C12-C11	-13.90	1.23	1.53
4	A	1706	CLR	C4-C3	-13.27	1.28	1.52
4	A	1710	CLR	C4-C3	-13.25	1.28	1.52
4	A	1708	CLR	C4-C3	-13.25	1.29	1.52
4	A	1709	CLR	C4-C3	-13.23	1.29	1.52
4	A	1705	CLR	C4-C3	-13.22	1.29	1.52
4	A	1707	CLR	C4-C3	-13.19	1.29	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1709	CLR	C7-C6	-12.23	1.23	1.50
4	A	1708	CLR	C7-C6	-12.18	1.24	1.50
4	A	1706	CLR	C7-C6	-12.10	1.24	1.50
4	A	1710	CLR	C7-C6	-12.10	1.24	1.50
4	A	1705	CLR	C7-C6	-12.09	1.24	1.50
4	A	1707	CLR	C7-C6	-12.08	1.24	1.50
4	A	1707	CLR	C2-C3	-11.96	1.23	1.51
4	A	1705	CLR	C2-C3	-11.94	1.23	1.51
4	A	1708	CLR	C2-C3	-11.91	1.23	1.51
4	A	1710	CLR	C2-C3	-11.90	1.23	1.51
4	A	1706	CLR	C2-C3	-11.89	1.23	1.51
4	A	1709	CLR	C2-C3	-11.89	1.23	1.51
4	A	1706	CLR	C12-C13	-11.76	1.33	1.54
4	A	1707	CLR	C12-C13	-11.72	1.33	1.54
4	A	1705	CLR	C12-C13	-11.72	1.33	1.54
4	A	1709	CLR	C12-C13	-11.64	1.33	1.54
4	A	1710	CLR	C12-C13	-11.57	1.33	1.54
4	A	1708	CLR	C12-C13	-11.55	1.33	1.54
4	A	1707	CLR	C4-C5	11.55	1.76	1.51
4	A	1710	CLR	C4-C5	11.52	1.76	1.51
4	A	1706	CLR	C4-C5	11.49	1.76	1.51
4	A	1708	CLR	C4-C5	11.49	1.76	1.51
4	A	1705	CLR	C4-C5	11.45	1.76	1.51
4	A	1709	CLR	C4-C5	11.44	1.76	1.51
4	A	1706	CLR	C13-C17	-9.91	1.36	1.55
4	A	1705	CLR	C13-C17	-9.79	1.36	1.55
4	A	1710	CLR	C16-C17	9.72	1.74	1.54
4	A	1710	CLR	C13-C17	-9.71	1.36	1.55
4	A	1708	CLR	C13-C17	-9.71	1.36	1.55
4	A	1709	CLR	C13-C17	-9.70	1.36	1.55
4	A	1707	CLR	C13-C17	-9.69	1.36	1.55
4	A	1707	CLR	C16-C17	9.68	1.74	1.54
4	A	1709	CLR	C16-C17	9.68	1.74	1.54
4	A	1705	CLR	C16-C17	9.67	1.74	1.54
4	A	1708	CLR	C16-C17	9.65	1.74	1.54
4	A	1706	CLR	C16-C17	9.64	1.74	1.54
2	A	1702	ATP	O4'-C1'	9.30	1.64	1.42
2	A	1701	ATP	O4'-C1'	9.28	1.64	1.42
4	A	1708	CLR	O1-C3	8.98	1.70	1.43
4	A	1710	CLR	O1-C3	8.98	1.70	1.43
4	A	1705	CLR	O1-C3	8.96	1.70	1.43
4	A	1709	CLR	O1-C3	8.96	1.70	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1706	CLR	O1-C3	8.94	1.70	1.43
4	A	1707	CLR	O1-C3	8.94	1.70	1.43
4	A	1708	CLR	C15-C14	-8.27	1.37	1.54
4	A	1710	CLR	C15-C14	-8.12	1.37	1.54
4	A	1709	CLR	C15-C14	-8.09	1.37	1.54
4	A	1707	CLR	C15-C14	-8.06	1.37	1.54
4	A	1705	CLR	C15-C14	-8.02	1.37	1.54
4	A	1707	CLR	C1-C10	-7.99	1.39	1.54
4	A	1706	CLR	C1-C10	-7.96	1.39	1.54
4	A	1708	CLR	C1-C10	-7.93	1.39	1.54
4	A	1706	CLR	C15-C14	-7.92	1.37	1.54
4	A	1709	CLR	C1-C10	-7.83	1.39	1.54
4	A	1710	CLR	C1-C10	-7.81	1.39	1.54
4	A	1705	CLR	C1-C10	-7.78	1.39	1.54
2	A	1702	ATP	C2'-C1'	-7.35	1.30	1.53
2	A	1701	ATP	C2'-C1'	-7.32	1.30	1.53
2	A	1701	ATP	O4'-C4'	-6.72	1.30	1.45
2	A	1702	ATP	O4'-C4'	-6.72	1.30	1.45
4	A	1709	CLR	C8-C9	-6.66	1.40	1.53
4	A	1705	CLR	C8-C9	-6.57	1.41	1.53
4	A	1706	CLR	C8-C9	-6.48	1.41	1.53
4	A	1707	CLR	C8-C9	-6.39	1.41	1.53
4	A	1710	CLR	C8-C9	-6.34	1.41	1.53
4	A	1708	CLR	C8-C9	-6.33	1.41	1.53
4	A	1705	CLR	C16-C15	6.32	1.71	1.54
4	A	1706	CLR	C16-C15	6.28	1.71	1.54
4	A	1709	CLR	C16-C15	6.28	1.71	1.54
4	A	1710	CLR	C16-C15	6.27	1.71	1.54
4	A	1707	CLR	C16-C15	6.26	1.71	1.54
4	A	1708	CLR	C16-C15	6.18	1.70	1.54
4	A	1709	CLR	C6-C5	4.18	1.42	1.33
4	A	1705	CLR	C6-C5	4.16	1.42	1.33
4	A	1706	CLR	C6-C5	4.12	1.42	1.33
2	A	1702	ATP	O3'-C3'	-4.06	1.33	1.43
2	A	1701	ATP	O3'-C3'	-4.05	1.33	1.43
4	A	1707	CLR	C6-C5	4.03	1.41	1.33
4	A	1710	CLR	C6-C5	3.93	1.41	1.33
4	A	1708	CLR	C6-C5	3.82	1.41	1.33
2	A	1701	ATP	C6-N6	3.77	1.43	1.34
2	A	1702	ATP	C6-N6	3.75	1.43	1.34
2	A	1702	ATP	O2'-C2'	3.49	1.51	1.43
2	A	1701	ATP	O2'-C2'	3.49	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1702	ATP	C8-N9	-2.77	1.32	1.37
2	A	1701	ATP	C8-N9	-2.77	1.32	1.37
2	A	1701	ATP	C5'-C4'	2.10	1.58	1.51
2	A	1702	ATP	C5'-C4'	2.09	1.58	1.51
4	A	1709	CLR	C23-C22	2.03	1.60	1.52

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1709	CLR	C4-C5-C6	-15.61	98.11	120.61
4	A	1705	CLR	C4-C5-C6	-15.54	98.22	120.61
4	A	1706	CLR	C4-C5-C6	-15.37	98.46	120.61
4	A	1708	CLR	C4-C5-C6	-14.92	99.11	120.61
4	A	1707	CLR	C4-C5-C6	-14.83	99.23	120.61
4	A	1710	CLR	C4-C5-C6	-14.82	99.25	120.61
4	A	1706	CLR	C19-C10-C9	-6.93	103.42	111.68
4	A	1705	CLR	C19-C10-C9	-6.91	103.44	111.68
4	A	1709	CLR	C19-C10-C9	-6.84	103.53	111.68
4	A	1707	CLR	C19-C10-C9	-6.76	103.62	111.68
4	A	1710	CLR	C10-C5-C6	-6.27	113.31	122.90
4	A	1705	CLR	C19-C10-C1	-6.07	99.84	109.43
4	A	1709	CLR	C19-C10-C1	-6.04	99.88	109.43
4	A	1706	CLR	C19-C10-C1	-5.99	99.96	109.43
4	A	1708	CLR	C10-C5-C6	-5.98	113.76	122.90
4	A	1707	CLR	C12-C13-C17	-5.88	107.77	116.57
4	A	1705	CLR	C12-C13-C17	-5.87	107.79	116.57
4	A	1710	CLR	C7-C6-C5	-5.84	114.28	125.06
4	A	1708	CLR	C12-C13-C17	-5.79	107.90	116.57
4	A	1708	CLR	C19-C10-C9	-5.76	104.82	111.68
2	A	1701	ATP	C5-C4-N3	-5.72	119.28	126.75
2	A	1702	ATP	C5-C4-N3	-5.70	119.31	126.75
4	A	1708	CLR	C7-C6-C5	-5.70	114.55	125.06
4	A	1709	CLR	C12-C13-C17	-5.59	108.21	116.57
4	A	1710	CLR	C12-C13-C17	-5.56	108.25	116.57
4	A	1706	CLR	C12-C13-C17	-5.51	108.32	116.57
4	A	1707	CLR	C19-C10-C5	-5.47	99.50	108.34
4	A	1710	CLR	C19-C10-C9	-5.42	105.22	111.68
4	A	1707	CLR	C7-C6-C5	-5.40	115.09	125.06
4	A	1705	CLR	C1-C10-C5	5.19	118.26	108.75
4	A	1706	CLR	C1-C10-C9	5.16	115.93	108.73
4	A	1707	CLR	C1-C10-C5	5.13	118.14	108.75
4	A	1707	CLR	C19-C10-C1	-5.09	101.38	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1705	CLR	C19-C10-C5	-5.01	100.24	108.34
4	A	1706	CLR	C1-C10-C5	4.97	117.86	108.75
4	A	1709	CLR	C19-C10-C5	-4.97	100.30	108.34
4	A	1710	CLR	C19-C10-C1	-4.96	101.60	109.43
4	A	1708	CLR	C19-C10-C5	-4.95	100.33	108.34
4	A	1707	CLR	C1-C10-C9	4.88	115.55	108.73
4	A	1706	CLR	C19-C10-C5	-4.86	100.47	108.34
4	A	1709	CLR	C1-C10-C9	4.85	115.51	108.73
4	A	1710	CLR	C1-C10-C9	4.77	115.38	108.73
4	A	1708	CLR	C1-C10-C5	4.75	117.45	108.75
4	A	1706	CLR	C7-C6-C5	-4.74	116.31	125.06
4	A	1707	CLR	C10-C5-C6	-4.71	115.70	122.90
4	A	1705	CLR	C1-C10-C9	4.69	115.28	108.73
4	A	1708	CLR	C1-C10-C9	4.66	115.24	108.73
4	A	1709	CLR	C1-C10-C5	4.66	117.28	108.75
4	A	1710	CLR	C1-C10-C5	4.62	117.21	108.75
4	A	1708	CLR	C19-C10-C1	-4.58	102.20	109.43
4	A	1710	CLR	C19-C10-C5	-4.44	101.16	108.34
2	A	1702	ATP	N3-C2-N1	-4.43	121.67	128.60
2	A	1701	ATP	N3-C2-N1	-4.39	121.74	128.60
2	A	1702	ATP	N3-C4-N9	4.35	134.25	127.08
2	A	1701	ATP	N3-C4-N9	4.28	134.13	127.08
4	A	1705	CLR	C7-C6-C5	-4.16	117.40	125.06
4	A	1709	CLR	C9-C10-C5	4.13	116.12	109.65
4	A	1706	CLR	C10-C5-C6	-4.11	116.61	122.90
4	A	1709	CLR	C7-C6-C5	-4.09	117.52	125.06
4	A	1705	CLR	C13-C17-C20	-3.92	113.35	119.49
4	A	1707	CLR	C13-C17-C20	-3.87	113.43	119.49
4	A	1705	CLR	C9-C10-C5	3.74	115.51	109.65
2	A	1702	ATP	C2-N3-C4	3.70	120.50	111.75
2	A	1701	ATP	C2-N3-C4	3.69	120.46	111.75
4	A	1710	CLR	C13-C17-C20	-3.68	113.72	119.49
2	A	1702	ATP	N9-C8-N7	-3.66	108.91	113.91
4	A	1709	CLR	C13-C17-C20	-3.65	113.76	119.49
2	A	1701	ATP	N9-C8-N7	-3.59	109.00	113.91
4	A	1708	CLR	C13-C17-C20	-3.47	114.06	119.49
4	A	1705	CLR	C10-C5-C6	-3.47	117.60	122.90
4	A	1706	CLR	C9-C10-C5	3.43	115.04	109.65
2	A	1701	ATP	C5-N7-C8	3.43	108.38	103.51
2	A	1702	ATP	C5-N7-C8	3.39	108.32	103.51
4	A	1710	CLR	C11-C9-C10	3.29	117.41	113.08
4	A	1707	CLR	C9-C10-C5	3.23	114.71	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1702	ATP	C3'-C2'-C1'	3.17	107.44	101.43
2	A	1702	ATP	C4-N9-C8	3.10	109.09	105.73
4	A	1706	CLR	C13-C17-C20	-3.05	114.71	119.49
2	A	1701	ATP	C3'-C2'-C1'	3.01	107.15	101.43
4	A	1710	CLR	C11-C9-C8	-3.00	107.44	111.75
2	A	1702	ATP	PB-O3B-PG	-2.98	122.59	132.83
2	A	1701	ATP	C4-N9-C8	2.97	108.95	105.73
2	A	1701	ATP	C4-C5-N7	-2.90	107.09	110.62
4	A	1706	CLR	C8-C7-C6	2.90	116.90	112.73
4	A	1709	CLR	C10-C5-C6	-2.88	118.50	122.90
4	A	1705	CLR	C8-C7-C6	2.79	116.75	112.73
2	A	1702	ATP	C4-C5-N7	-2.78	107.23	110.62
4	A	1708	CLR	C17-C13-C14	2.69	103.26	100.07
4	A	1708	CLR	C11-C9-C10	2.68	116.61	113.08
4	A	1706	CLR	C12-C13-C14	2.68	111.43	107.27
4	A	1706	CLR	C14-C8-C9	2.65	112.64	109.09
4	A	1708	CLR	C9-C10-C5	2.63	113.78	109.65
4	A	1707	CLR	C14-C8-C9	2.62	112.60	109.09
4	A	1706	CLR	C21-C20-C17	-2.58	108.97	112.92
4	A	1708	CLR	C8-C7-C6	2.50	116.33	112.73
4	A	1710	CLR	C13-C14-C8	-2.46	110.73	114.38
4	A	1707	CLR	C8-C7-C6	2.46	116.27	112.73
4	A	1707	CLR	C17-C13-C14	2.43	102.95	100.07
4	A	1710	CLR	C9-C10-C5	2.42	113.45	109.65
4	A	1708	CLR	C11-C9-C8	-2.41	108.28	111.75
2	A	1702	ATP	PA-O3A-PB	-2.32	124.85	132.83
4	A	1710	CLR	C12-C13-C14	2.28	110.81	107.27
4	A	1705	CLR	C17-C13-C14	2.23	102.72	100.07
2	A	1701	ATP	PA-O3A-PB	-2.23	125.18	132.83
4	A	1707	CLR	C3-C4-C5	2.18	115.73	112.03
2	A	1701	ATP	PB-O3B-PG	-2.16	125.42	132.83
4	A	1705	CLR	C12-C13-C14	2.15	110.60	107.27
4	A	1708	CLR	C16-C15-C14	-2.13	100.91	105.13
4	A	1708	CLR	C12-C13-C14	2.12	110.56	107.27
2	A	1701	ATP	C2'-C3'-C4'	2.11	106.74	102.64
2	A	1702	ATP	C2'-C3'-C4'	2.08	106.68	102.64
4	A	1709	CLR	C8-C7-C6	2.07	115.71	112.73
4	A	1709	CLR	C17-C13-C14	2.07	102.52	100.07
4	A	1708	CLR	C3-C4-C5	2.06	115.53	112.03
4	A	1709	CLR	C12-C13-C14	2.01	110.38	107.27

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1705	CLR	C13-C17-C20-C21
4	A	1706	CLR	C13-C17-C20-C22
4	A	1706	CLR	C16-C17-C20-C22
4	A	1707	CLR	C13-C17-C20-C21
4	A	1708	CLR	C13-C17-C20-C21
4	A	1709	CLR	C13-C17-C20-C21
4	A	1710	CLR	C13-C17-C20-C21
4	A	1705	CLR	C16-C17-C20-C21
4	A	1706	CLR	C16-C17-C20-C21
4	A	1707	CLR	C16-C17-C20-C21
4	A	1710	CLR	C16-C17-C20-C21
4	A	1706	CLR	C13-C17-C20-C21
4	A	1707	CLR	C16-C17-C20-C22
4	A	1705	CLR	C13-C17-C20-C22
4	A	1707	CLR	C13-C17-C20-C22
4	A	1709	CLR	C13-C17-C20-C22
4	A	1710	CLR	C13-C17-C20-C22
4	A	1705	CLR	C21-C20-C22-C23
4	A	1709	CLR	C21-C20-C22-C23
4	A	1708	CLR	C16-C17-C20-C21
4	A	1709	CLR	C16-C17-C20-C21
4	A	1705	CLR	C16-C17-C20-C22
4	A	1710	CLR	C16-C17-C20-C22
4	A	1708	CLR	C13-C17-C20-C22
4	A	1708	CLR	C16-C17-C20-C22
4	A	1709	CLR	C16-C17-C20-C22
4	A	1710	CLR	C21-C20-C22-C23
4	A	1705	CLR	C17-C20-C22-C23
4	A	1707	CLR	C21-C20-C22-C23
4	A	1708	CLR	C21-C20-C22-C23
4	A	1707	CLR	C17-C20-C22-C23
4	A	1710	CLR	C17-C20-C22-C23
4	A	1705	CLR	C20-C22-C23-C24
4	A	1706	CLR	C20-C22-C23-C24
4	A	1708	CLR	C20-C22-C23-C24
4	A	1709	CLR	C22-C23-C24-C25
4	A	1709	CLR	C17-C20-C22-C23
4	A	1707	CLR	C22-C23-C24-C25
4	A	1706	CLR	C22-C23-C24-C25
4	A	1709	CLR	C20-C22-C23-C24
4	A	1708	CLR	C23-C24-C25-C27
4	A	1708	CLR	C23-C24-C25-C26

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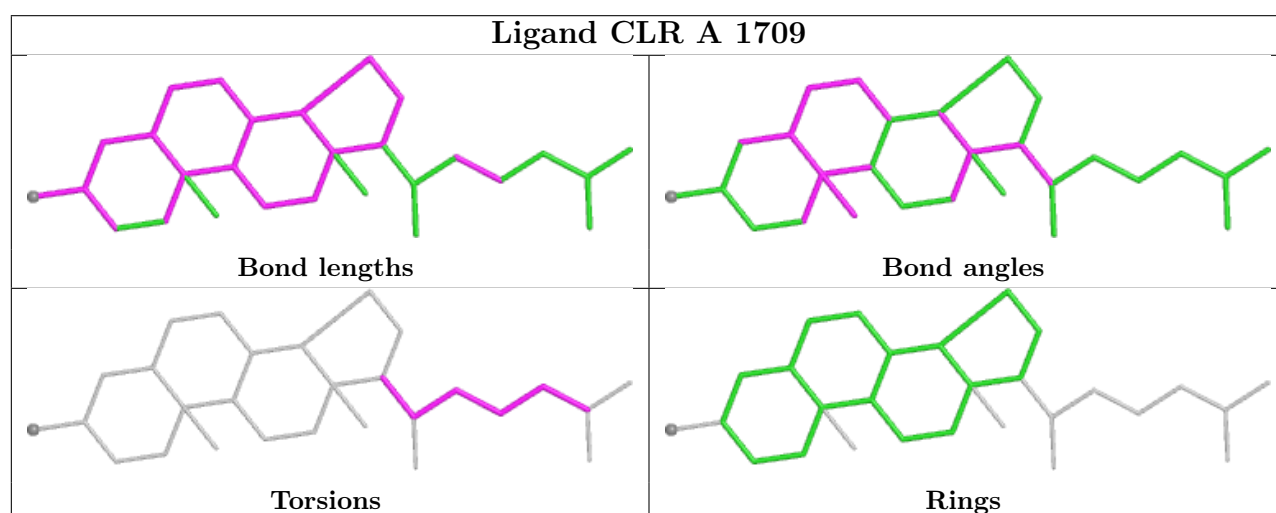
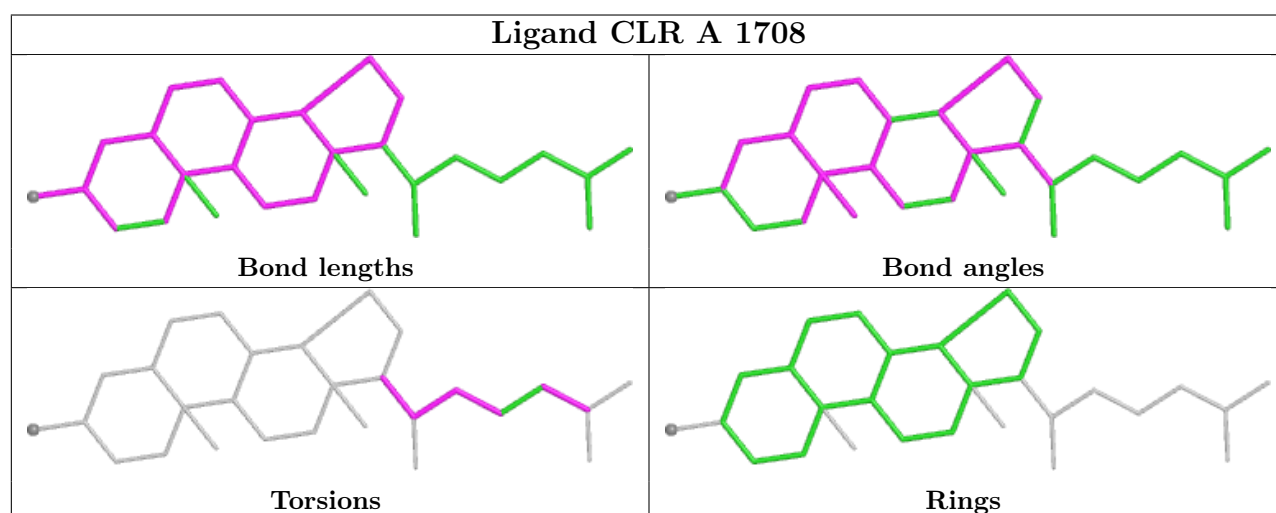
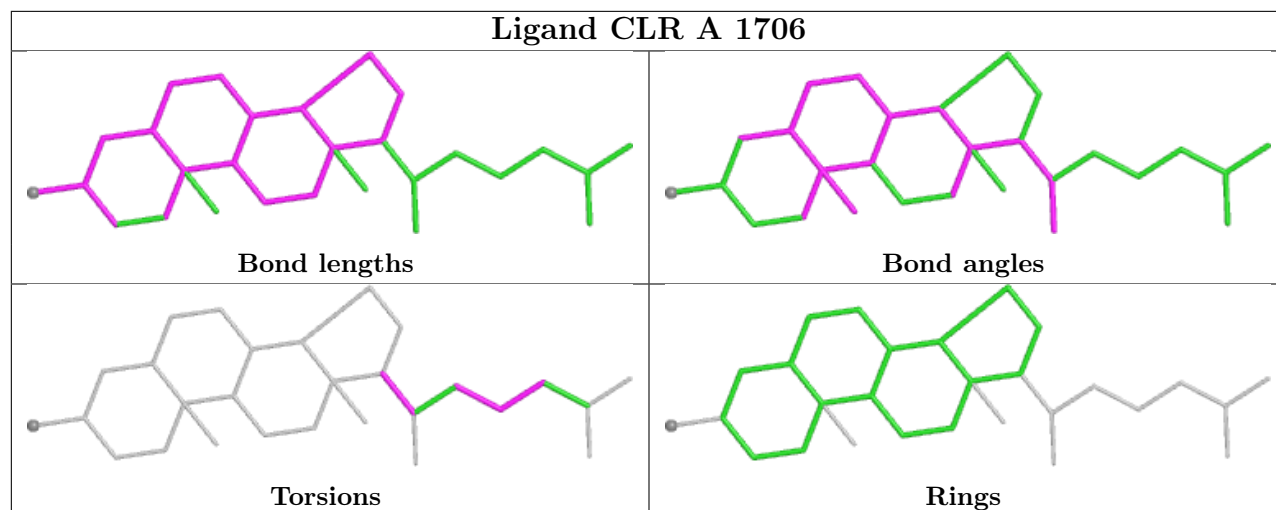
Mol	Chain	Res	Type	Atoms
4	A	1705	CLR	C22-C23-C24-C25
2	A	1702	ATP	C5'-O5'-PA-O3A
4	A	1709	CLR	C23-C24-C25-C27
4	A	1709	CLR	C23-C24-C25-C26
2	A	1701	ATP	PA-O3A-PB-O2B
2	A	1702	ATP	C5'-O5'-PA-O2A

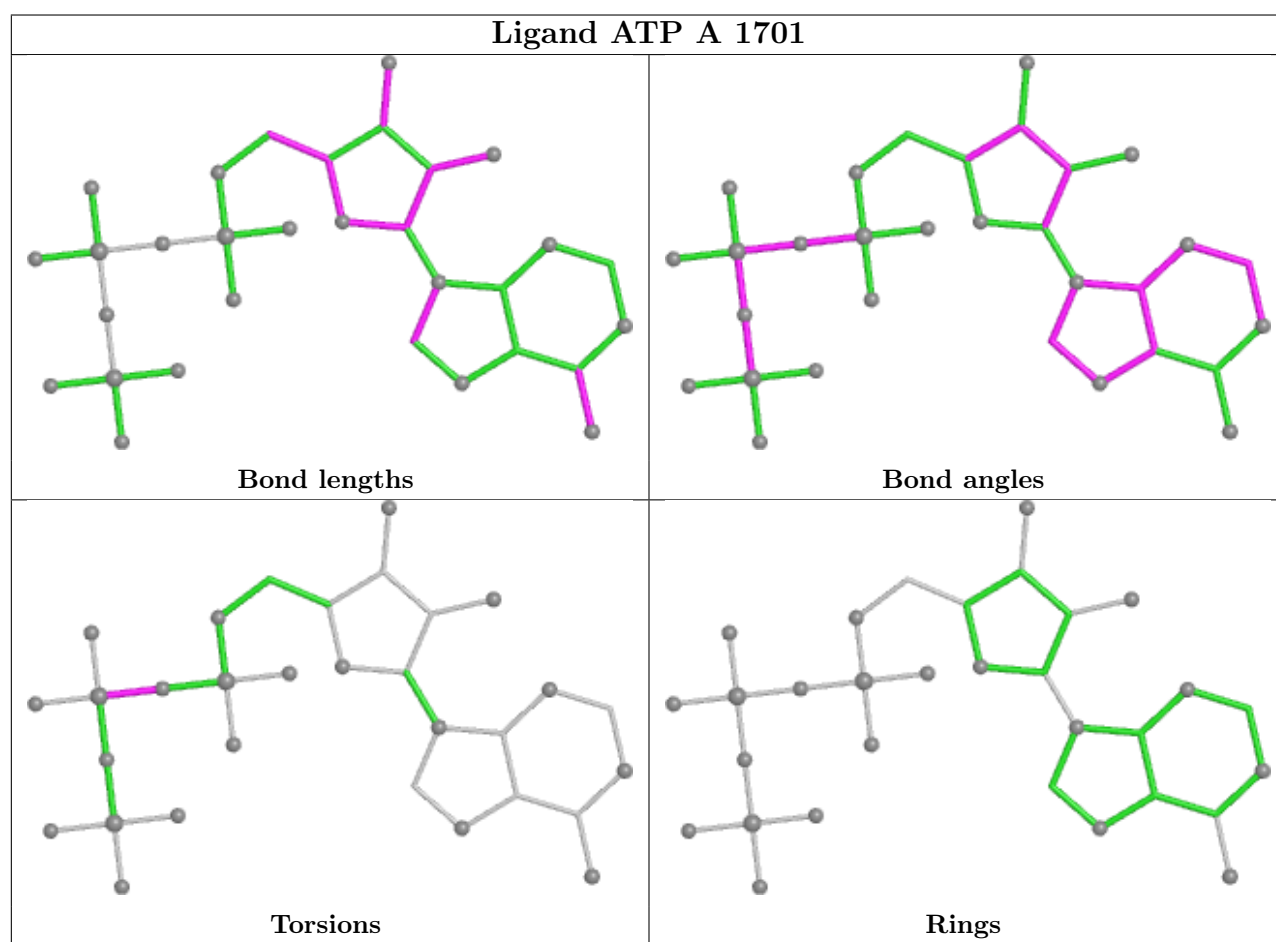
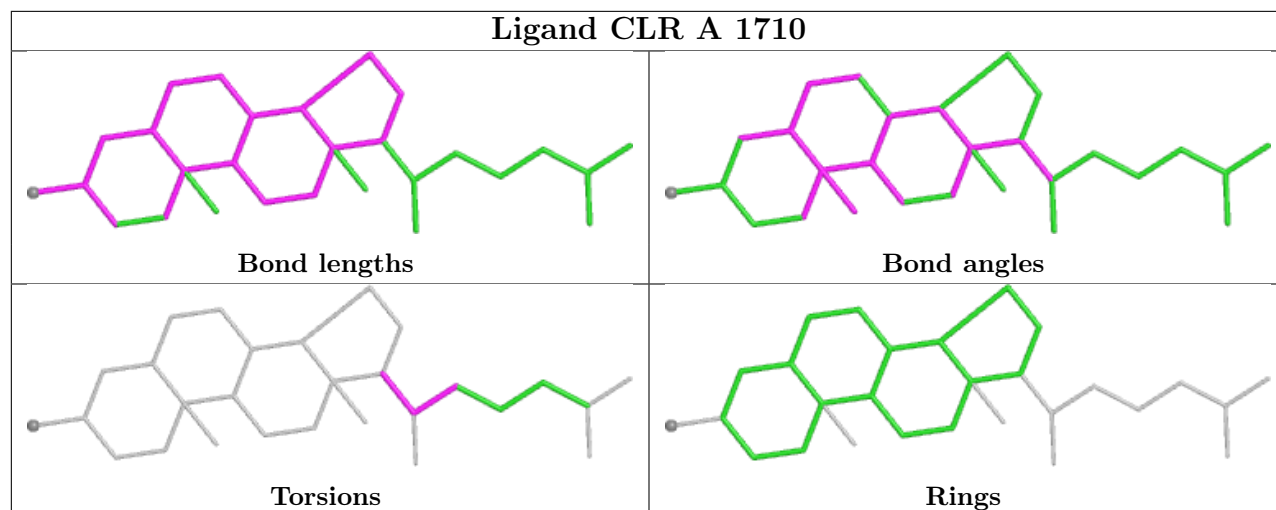
There are no ring outliers.

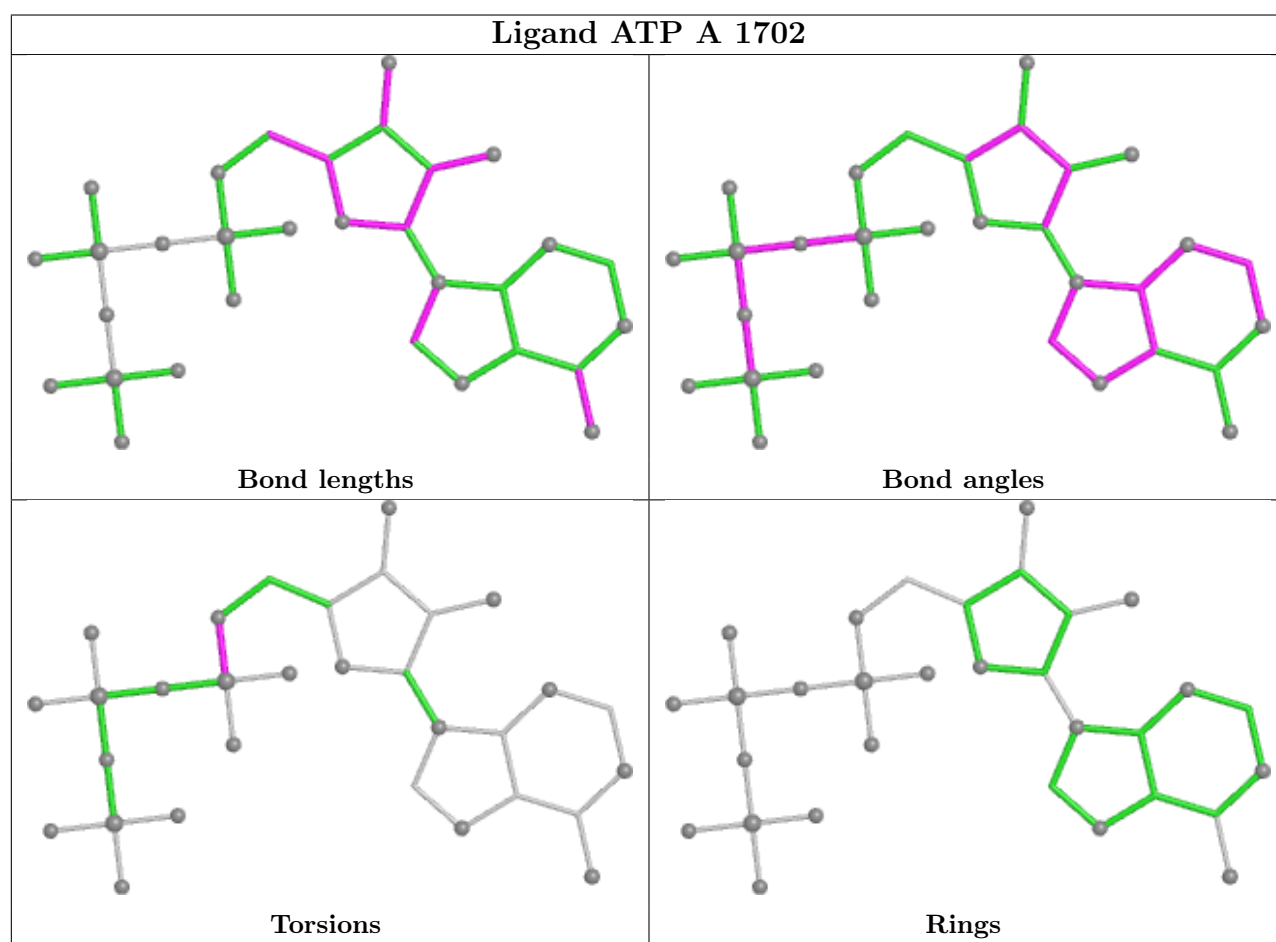
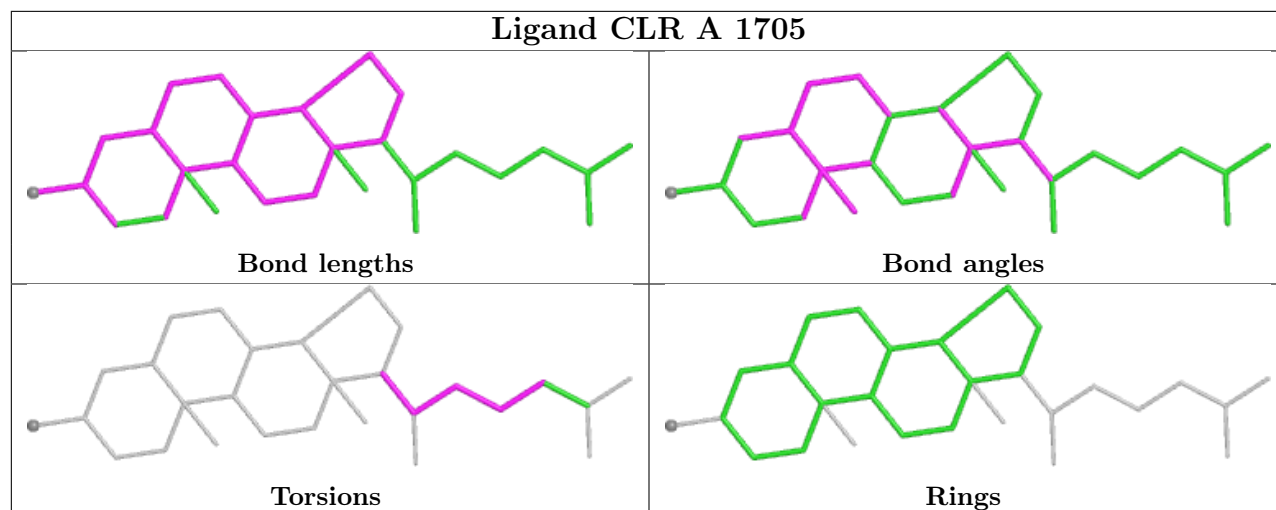
8 monomers are involved in 165 short contacts:

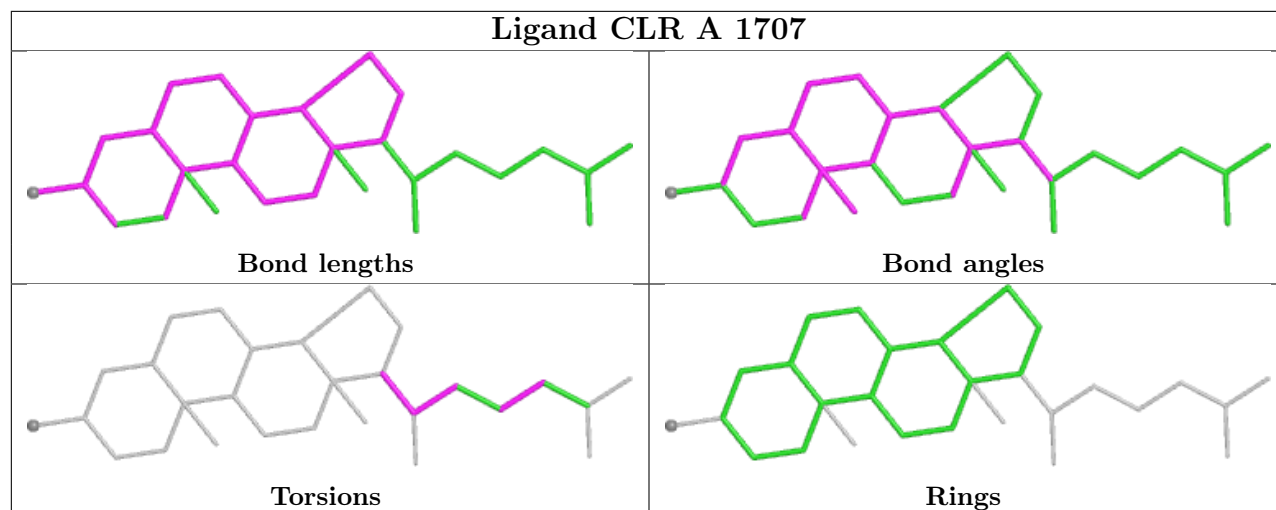
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1706	CLR	22	0
4	A	1708	CLR	22	0
4	A	1709	CLR	28	0
4	A	1710	CLR	29	0
2	A	1701	ATP	1	0
4	A	1705	CLR	32	0
2	A	1702	ATP	1	0
4	A	1707	CLR	30	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

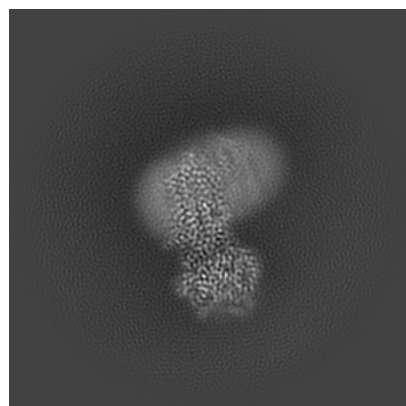
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65915. These allow visual inspection of the internal detail of the map and identification of artifacts.

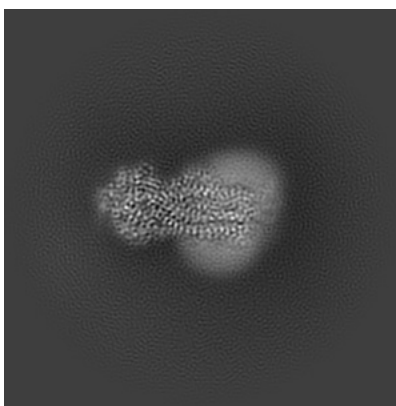
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

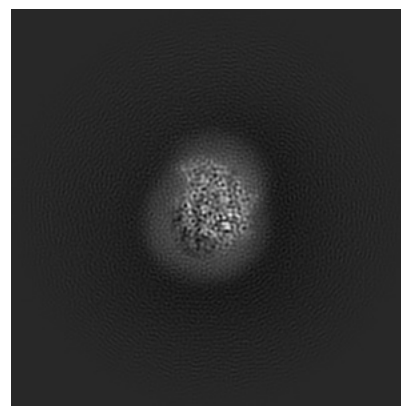
6.1.1 Primary map



X

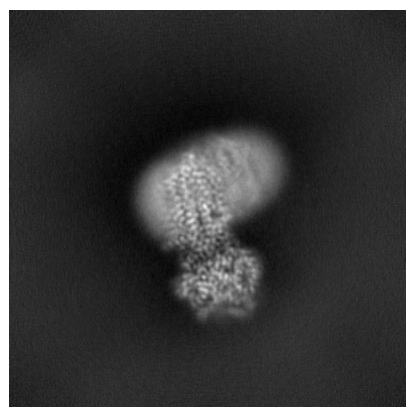


Y

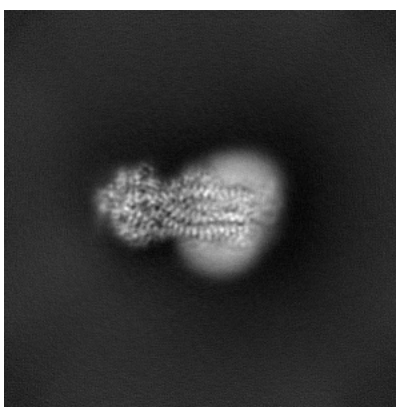


Z

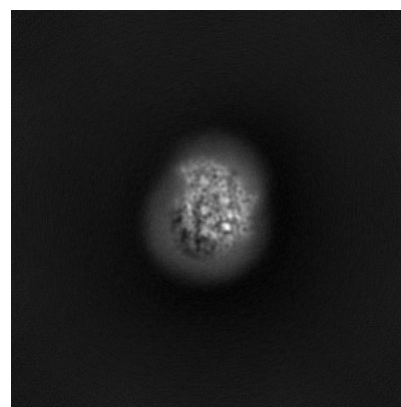
6.1.2 Raw map



X



Y

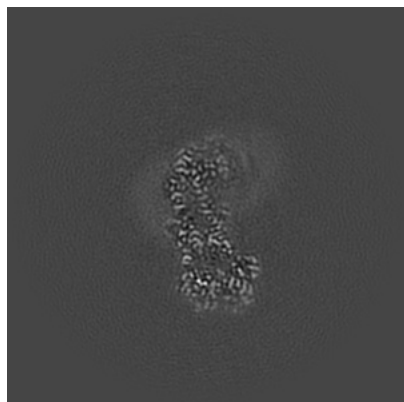


Z

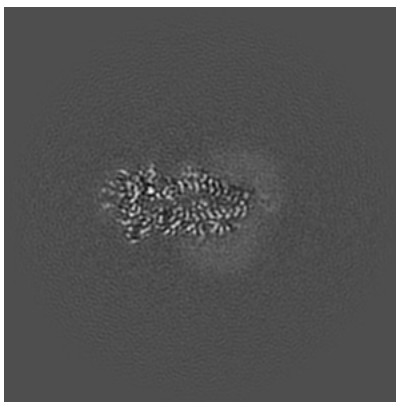
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

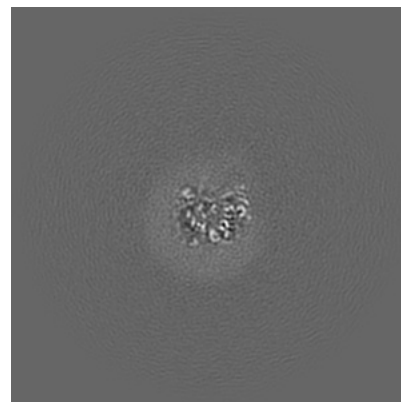
6.2.1 Primary map



X Index: 210

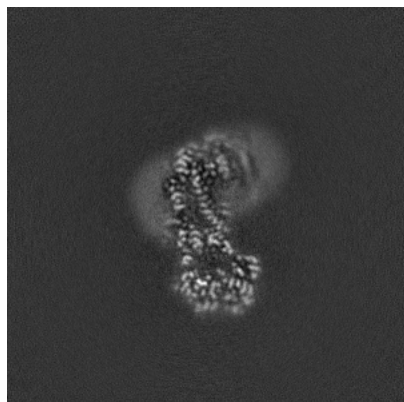


Y Index: 210

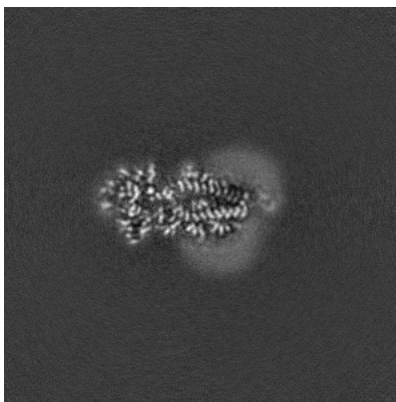


Z Index: 210

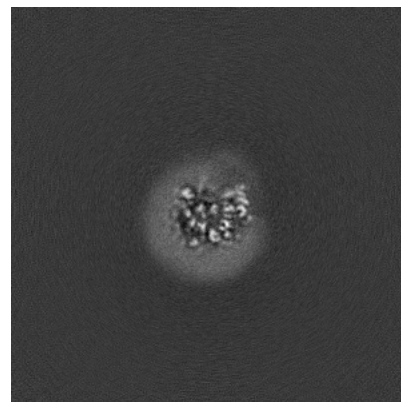
6.2.2 Raw map



X Index: 210



Y Index: 210

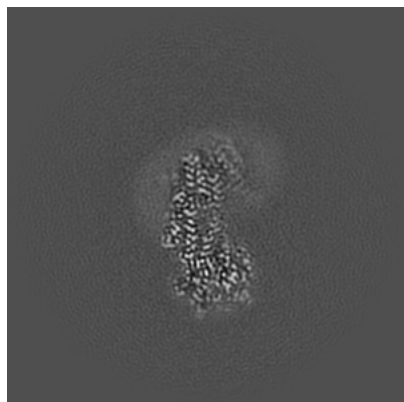


Z Index: 210

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

6.3 Largest variance slices [i](#)

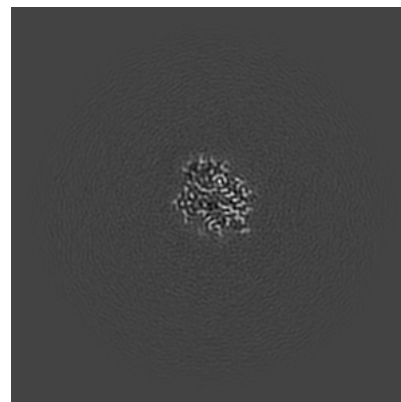
6.3.1 Primary map



X Index: 224

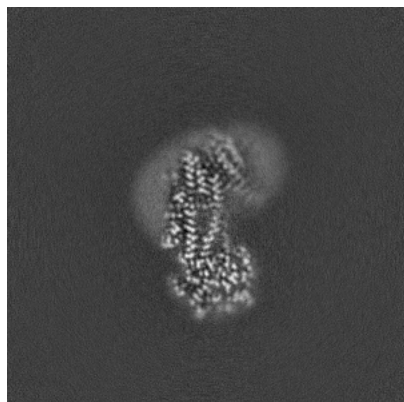


Y Index: 190

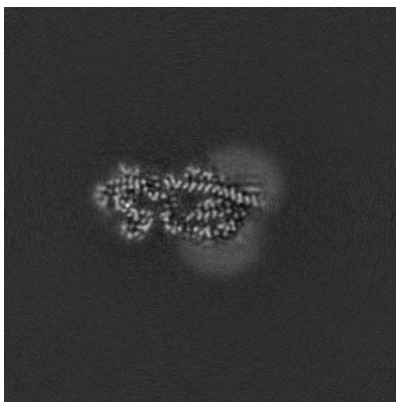


Z Index: 139

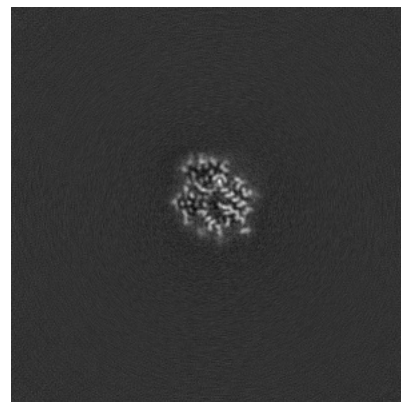
6.3.2 Raw map



X Index: 224



Y Index: 205

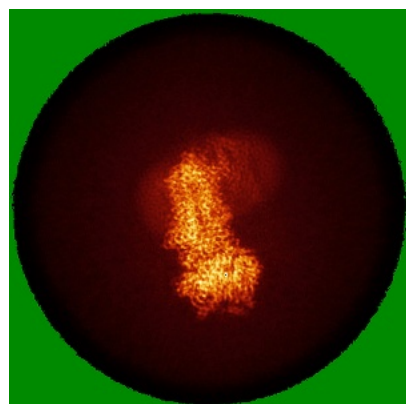


Z Index: 139

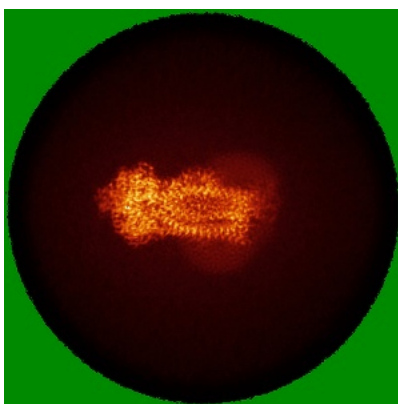
The images above show the largest variance slices of the map in three orthogonal directions.

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

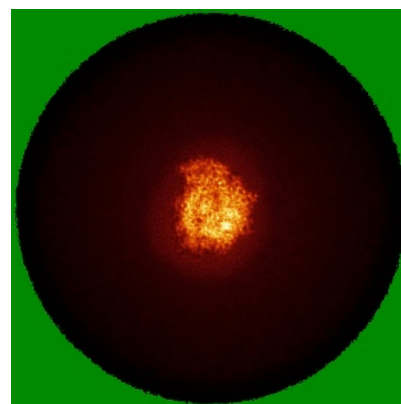
6.4.1 Primary map



X

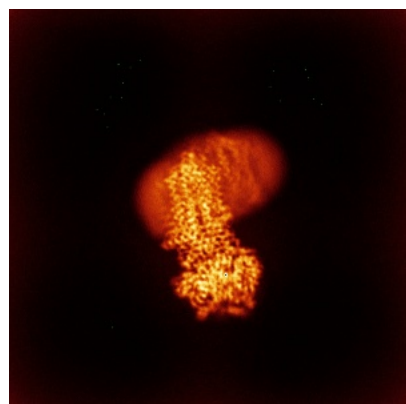


Y

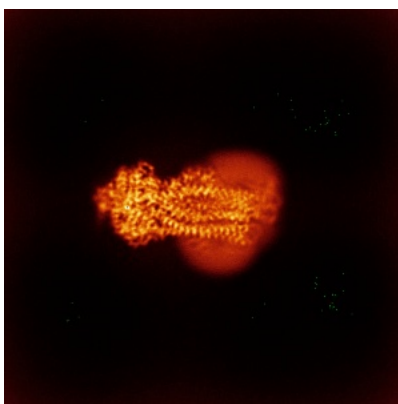


Z

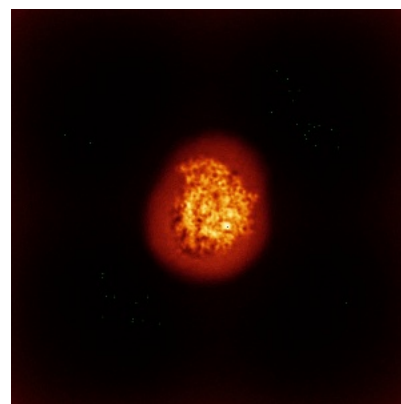
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

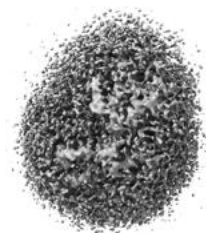
6.5.1 Primary map



X



Y



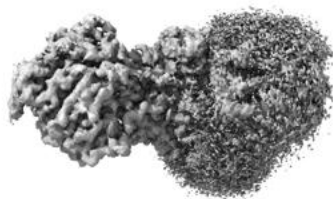
Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

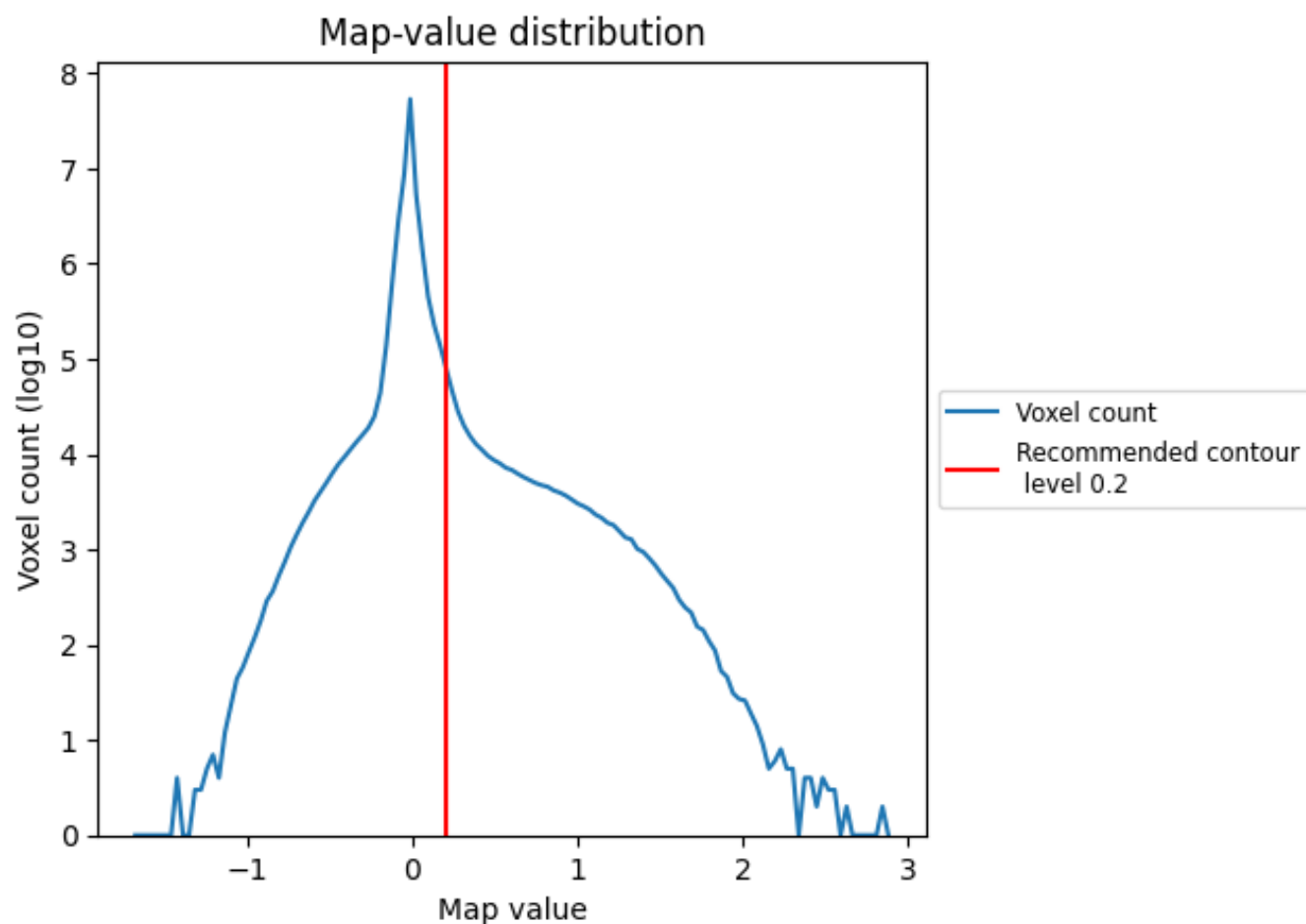
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

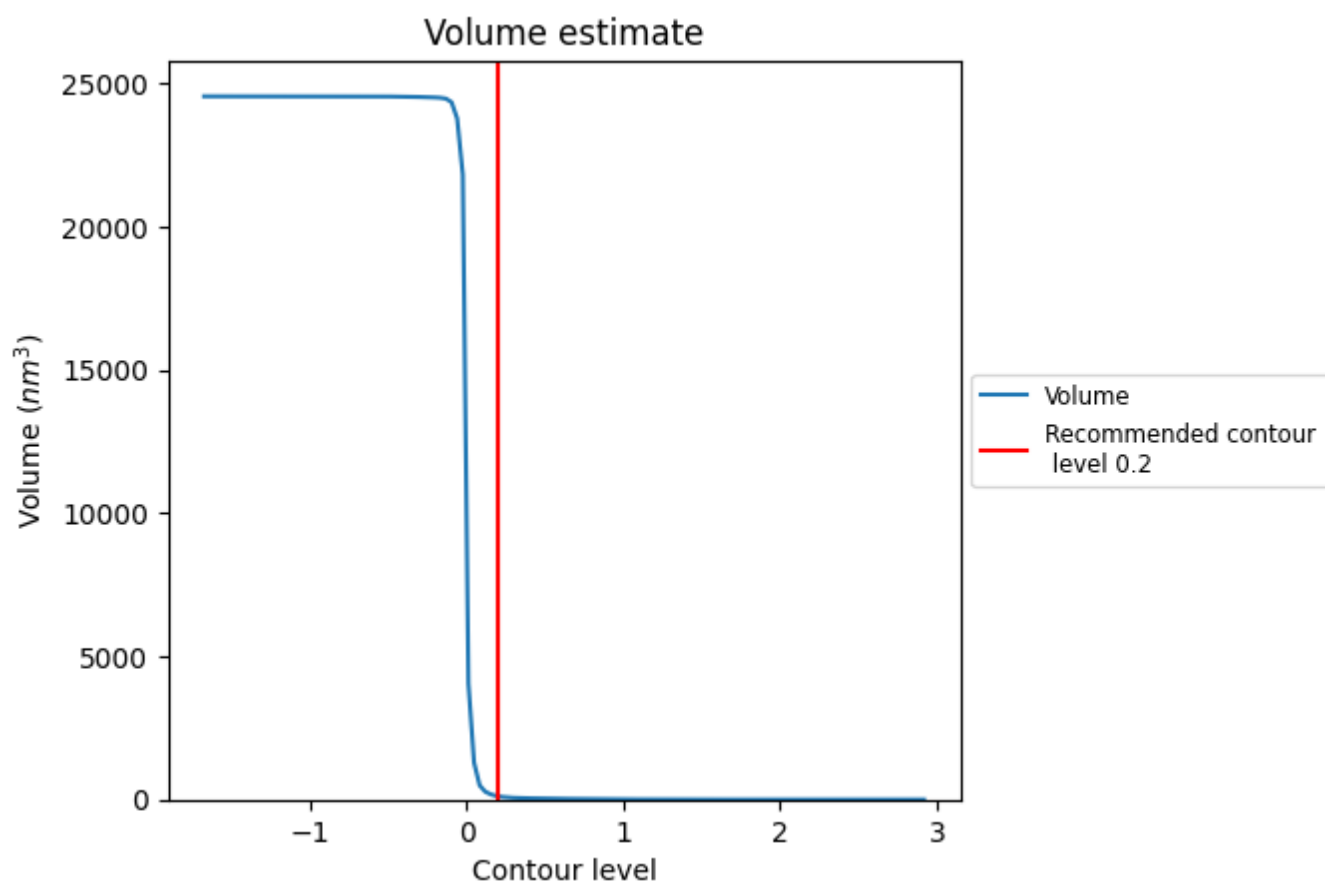
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

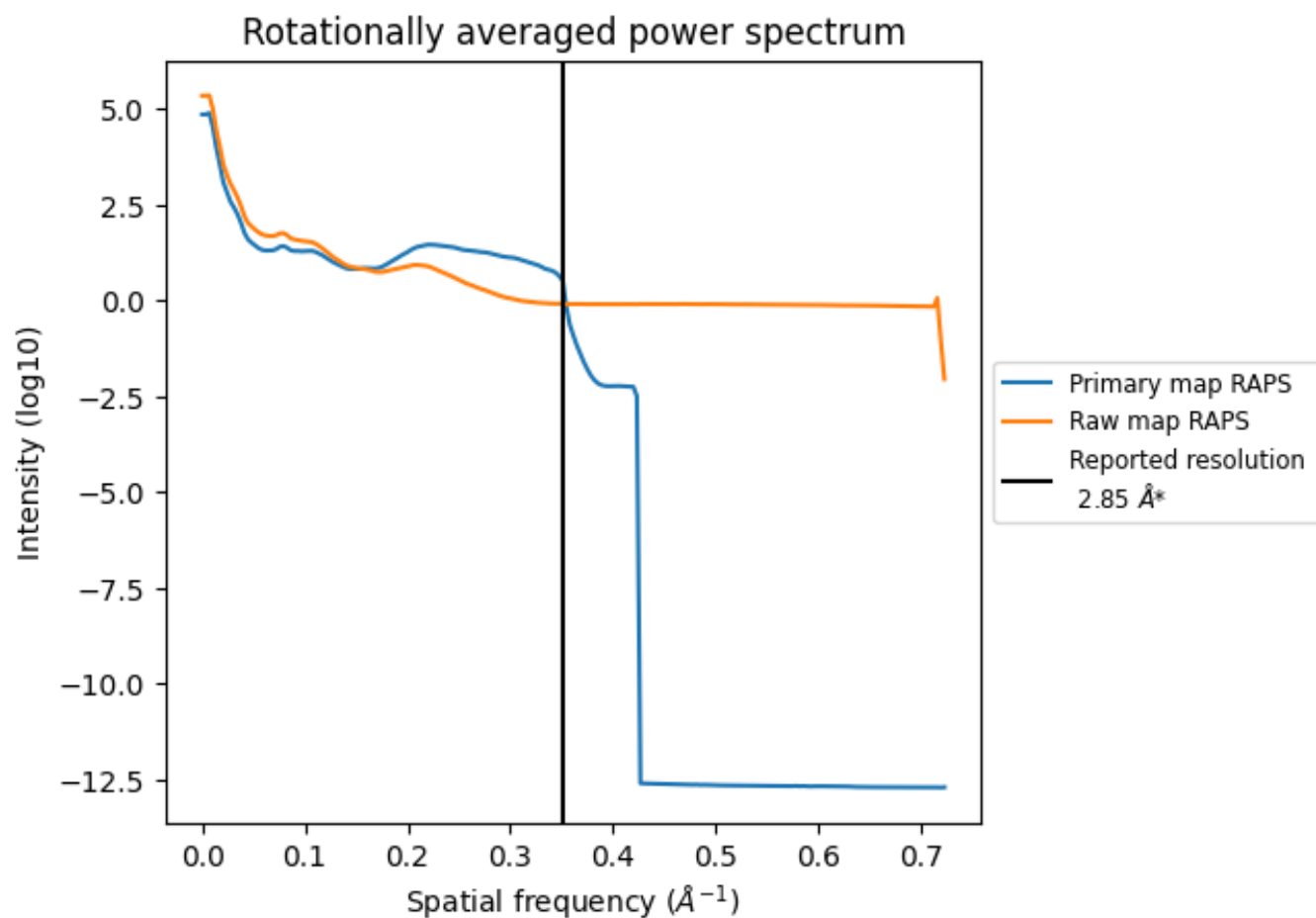
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 115 nm³; this corresponds to an approximate mass of 104 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 ⓘ

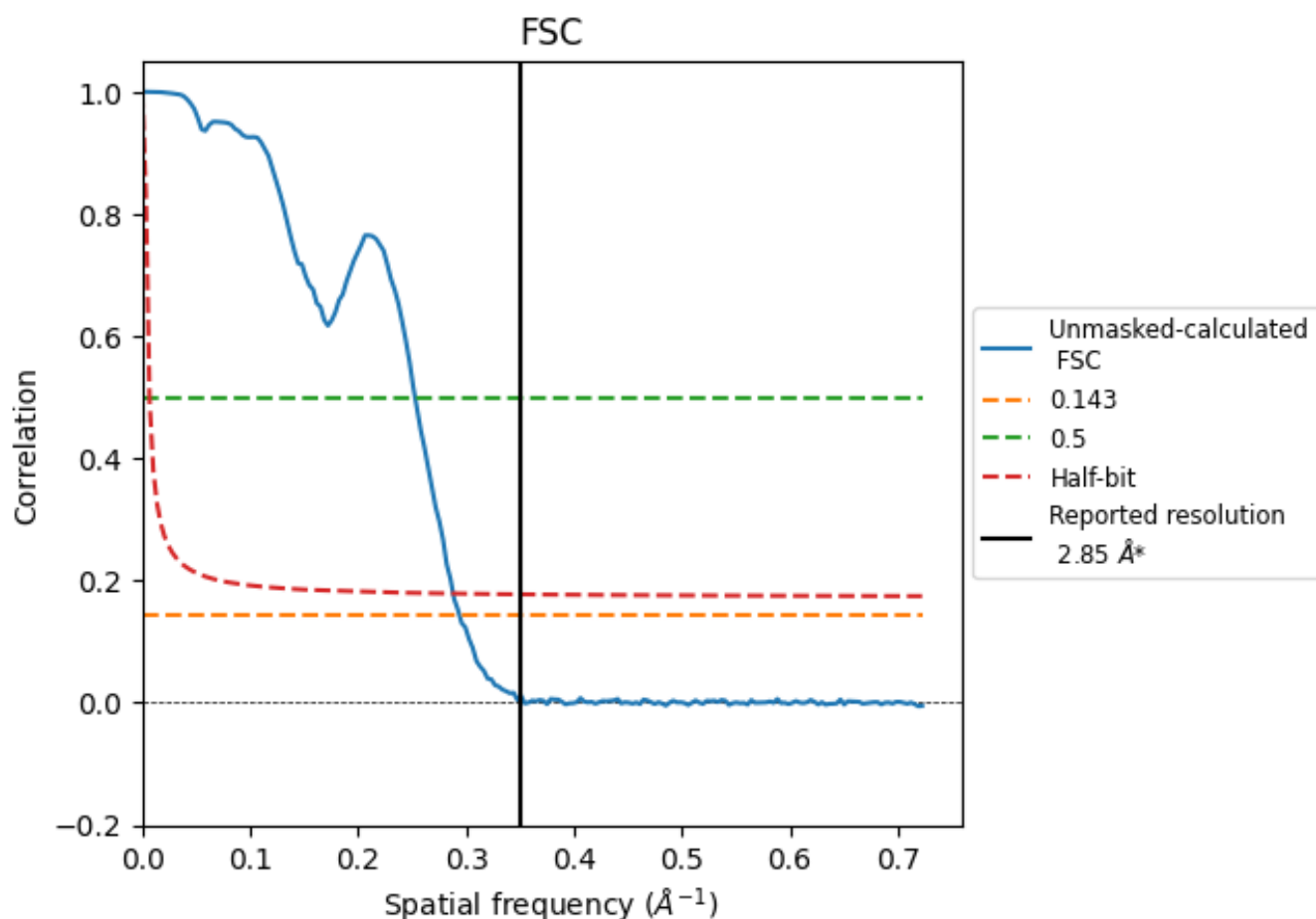


*Reported resolution corresponds to spatial frequency of 0.351 Å⁻¹

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 0.351 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

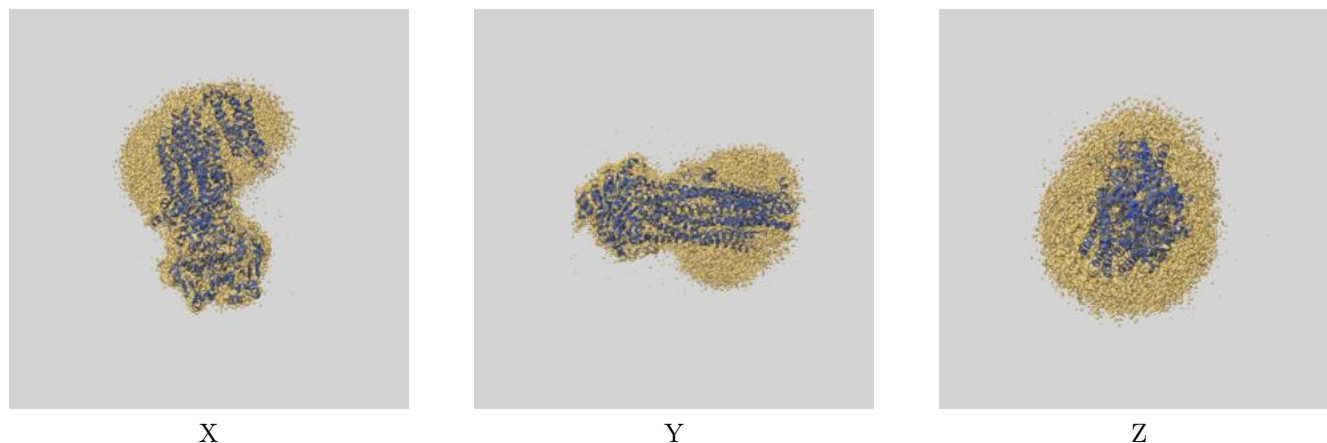
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.40	3.96	3.47

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.40 differs from the reported value 2.85 by more than 10 %

9 Map-model fit [i](#)

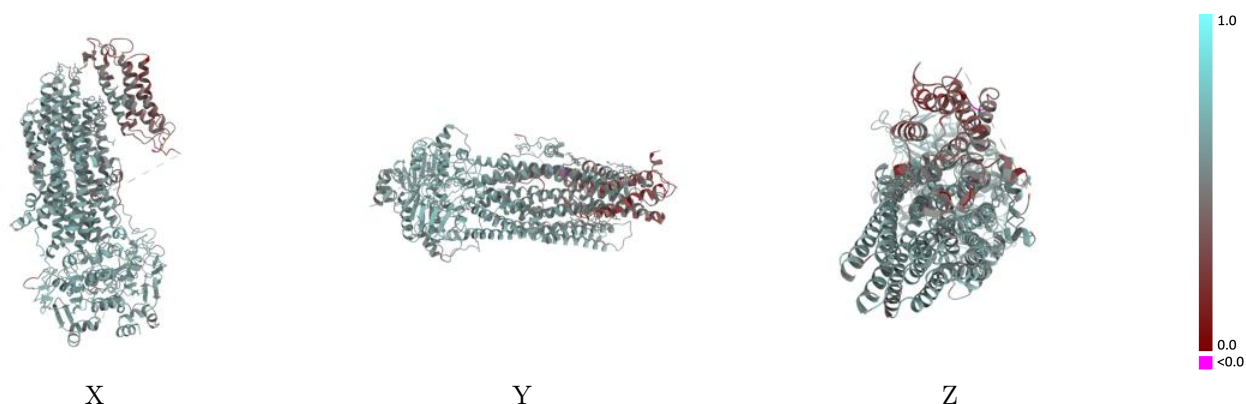
This section contains information regarding the fit between EMDB map EMD-65915 and PDB model 9WET. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



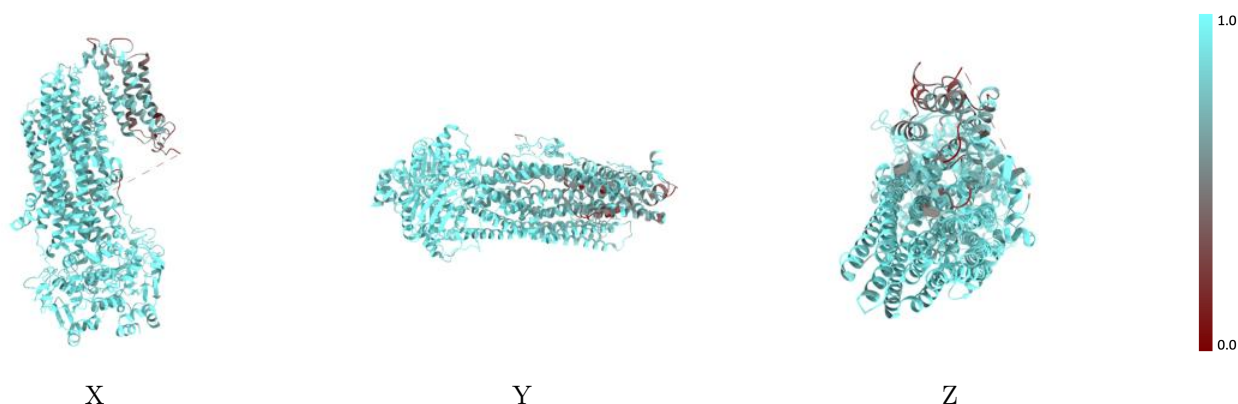
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



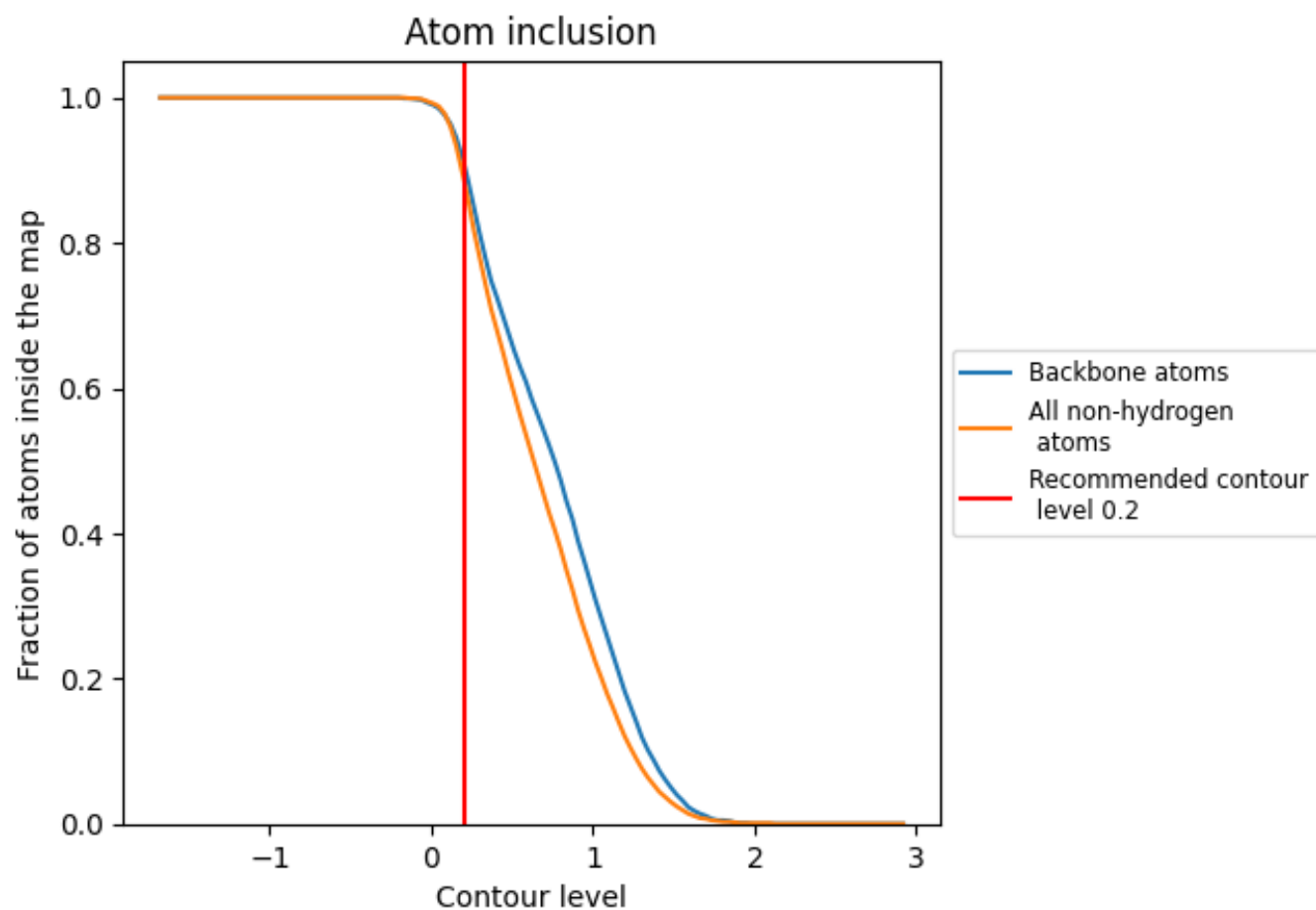
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 89% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8880	0.5540
A	0.8880	0.5540

