



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 03:54 PM UTC

PDB ID : 9LQU / pdb_00009lqu
EMDB ID : EMD-63305
Title : Cryo-EM structure of the JN241-9-bound state 1a of APLNR homodimer
Authors : Ji, S.; Wang, W.; Yang, Y.; Shen, Q.; Zhang, Y.
Deposited on : 2025-01-28
Resolution : 2.70 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

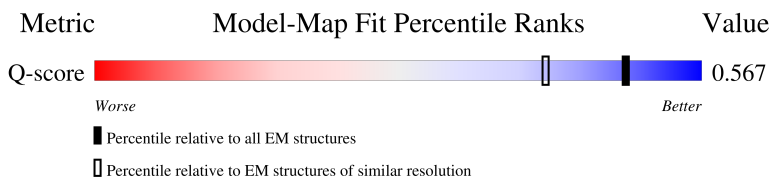
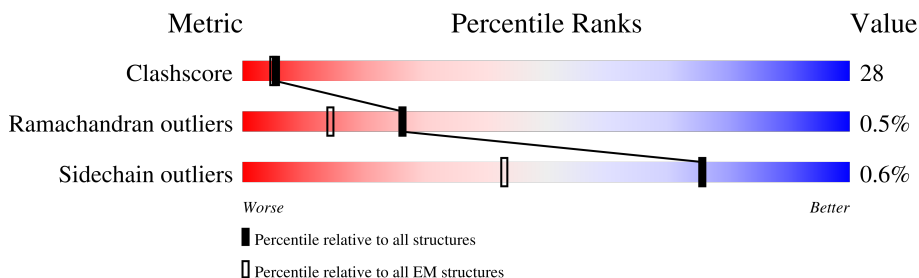
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	C	130	
1	D	130	
2	A	380	
2	B	380	

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	CLR	A	403	-	-	X	-
3	CLR	A	405	-	-	X	-
3	CLR	A	408	-	-	X	-
3	CLR	B	401	-	-	X	-
3	CLR	B	403	-	-	X	-
3	CLR	B	408	-	-	X	-
4	PCF	A	409	-	-	X	-
4	PCF	B	410	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6946 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.

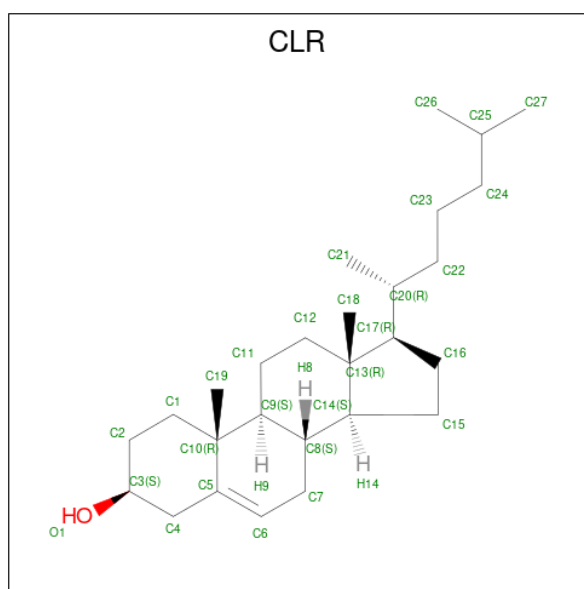
- Molecule 1 is a protein called JN241-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	129	Total	C	N	O	S	0	0
			965	593	170	193	9		
1	C	129	Total	C	N	O	S	0	0
			965	593	170	193	9		

- Molecule 2 is a protein called Apelin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	276	Total	C	N	O	S	0	0
			2184	1458	337	368	21		
2	A	276	Total	C	N	O	S	0	0
			2184	1458	337	368	21		

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



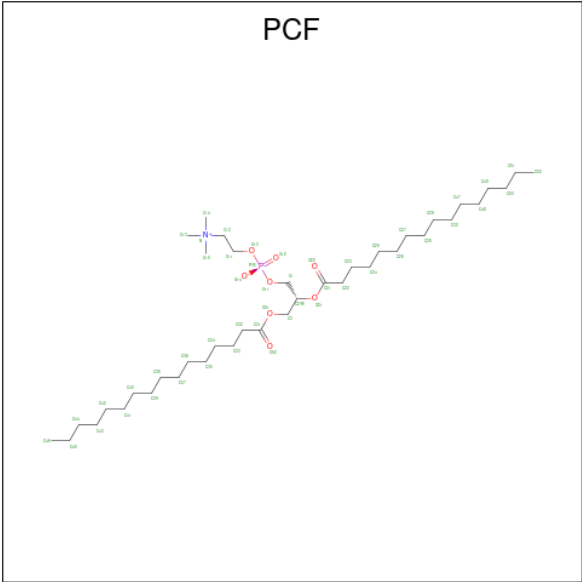
Mol	Chain	Residues	Atoms			AltConf
3	B	1	Total	C	O	0
			28	27	1	

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

- Molecule 4 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (CCD ID: PCF) (formula: $C_{40}H_{80}NO_8P$).



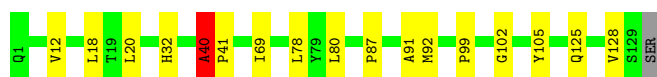
Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			50	40	1	8	1	
4	B	1	Total	C	N	O	P	0
			50	40	1	8	1	
4	A	1	Total	C	N	O	P	0
			50	40	1	8	1	
4	A	1	Total	C	N	O	P	0
			50	40	1	8	1	

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.

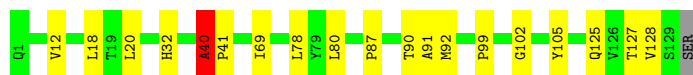
• Molecule 1: JN241-9

Chain D:  86% 12% ..



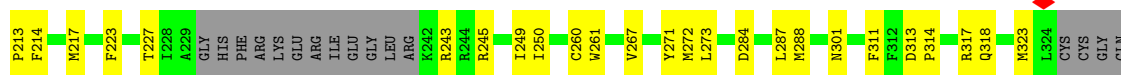
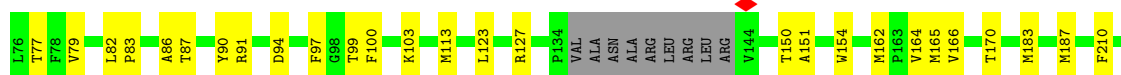
• Molecule 1: JN241-9

Chain C:  85% 14% ..



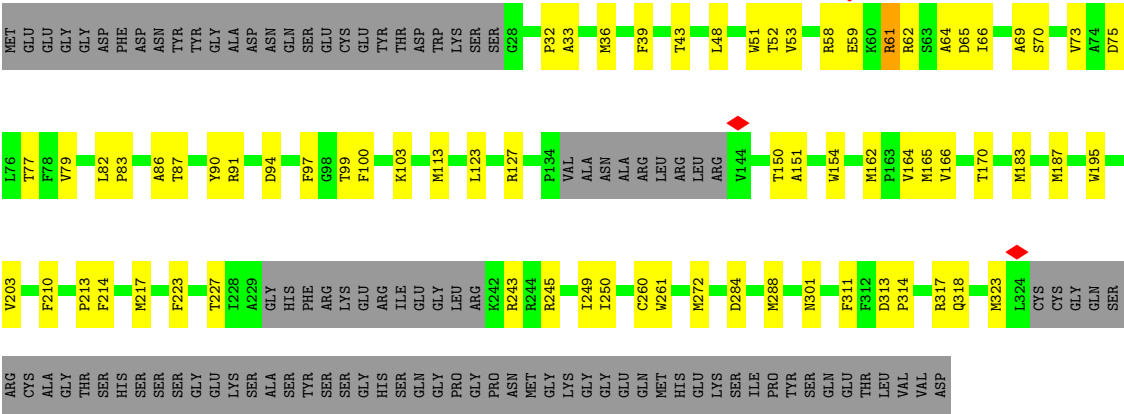
• Molecule 2: Apelin receptor

Chain B:  54% 19% 27%



• Molecule 2: Apelin receptor

Chain A:  54% 18% 27%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97020	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 ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.126	Depositor
Minimum map value	-0.087	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	208.32, 208.32, 208.32	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCF, CLR

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	C	0.16	0/983	0.40	0/1325
1	D	0.16	0/983	0.40	0/1325
2	A	0.15	0/2247	0.38	0/3072
2	B	0.14	0/2247	0.38	0/3072
All	All	0.15	0/6460	0.39	0/8794

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	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	40	ALA	Peptide
1	D	40	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	965	0	925	9	0
1	D	965	0	925	8	0
2	A	2184	0	2190	107	0
2	B	2184	0	2190	106	0
3	A	224	0	368	119	0
3	B	224	0	368	119	0
4	A	100	0	160	70	0
4	B	100	0	160	69	0
All	All	6946	0	7286	395	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 28.

All (395) 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)
2:A:33:ALA:HA	4:A:409:PCF:H491	1.21	1.19
2:B:33:ALA:HA	4:B:410:PCF:H491	1.21	1.18
3:B:403:CLR:H242	4:A:409:PCF:H421	1.44	0.98
4:B:410:PCF:H421	3:A:405:CLR:H242	1.44	0.97
2:A:86:ALA:HB1	4:A:409:PCF:H291	1.55	0.88
2:B:36:MET:HG3	4:B:410:PCF:H482	1.54	0.88
2:A:36:MET:HG3	4:A:409:PCF:H482	1.56	0.88
2:B:86:ALA:HB1	4:B:410:PCF:H291	1.54	0.88
2:B:97:PHE:HE1	3:A:405:CLR:H6	1.39	0.87
4:B:410:PCF:H451	3:A:405:CLR:H221	1.56	0.87
3:B:403:CLR:H221	4:A:409:PCF:H451	1.56	0.87
2:B:33:ALA:HA	4:B:410:PCF:C49	2.06	0.86
3:B:403:CLR:H6	2:A:97:PHE:HE1	1.40	0.85
4:A:409:PCF:H111	4:A:409:PCF:H12	1.57	0.85
4:B:410:PCF:H12	4:B:410:PCF:H111	1.57	0.84
3:A:401:CLR:H17	3:A:403:CLR:H122	1.58	0.84
3:B:406:CLR:H17	3:B:408:CLR:H122	1.58	0.83
2:A:33:ALA:HA	4:A:409:PCF:C49	2.06	0.82
2:A:100:PHE:CD2	3:A:405:CLR:H71	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:PHE:CD2	3:B:403:CLR:H71	2.15	0.81
3:A:406:CLR:H222	3:A:407:CLR:H25	1.63	0.81
2:B:245:ARG:HE	2:B:314:PRO:HG3	1.45	0.81
2:A:90:TYR:CD2	4:A:409:PCF:H251	2.15	0.80
3:B:401:CLR:H231	3:B:405:CLR:H221	1.64	0.80
2:B:90:TYR:CD2	4:B:410:PCF:H251	2.16	0.79
3:B:404:CLR:H222	3:B:405:CLR:H25	1.63	0.79
2:A:245:ARG:HE	2:A:314:PRO:HG3	1.45	0.79
2:A:36:MET:HB3	4:A:409:PCF:H523	1.65	0.78
3:A:407:CLR:H221	3:A:408:CLR:H231	1.64	0.78
4:B:410:PCF:H21	3:A:405:CLR:O1	1.85	0.77
2:B:75:ASP:O	2:B:79:VAL:HG23	1.85	0.77
3:B:403:CLR:O1	4:A:409:PCF:H21	1.85	0.77
2:B:36:MET:HB3	4:B:410:PCF:H523	1.66	0.77
4:B:410:PCF:H463	2:A:100:PHE:HZ	1.49	0.77
3:B:403:CLR:C6	2:A:97:PHE:HE1	1.99	0.75
2:B:97:PHE:HE1	3:A:405:CLR:C6	1.99	0.75
3:B:408:CLR:H222	3:B:408:CLR:H121	1.67	0.75
2:A:75:ASP:O	2:A:79:VAL:HG23	1.85	0.74
4:B:410:PCF:H361	3:A:405:CLR:C12	2.17	0.74
2:A:32:PRO:HB3	4:A:409:PCF:H292	1.68	0.74
3:A:403:CLR:H222	3:A:403:CLR:H121	1.67	0.74
2:B:32:PRO:HB3	4:B:410:PCF:H292	1.68	0.74
1:D:32:HIS:HD2	1:D:99:PRO:HA	1.52	0.74
2:B:100:PHE:HZ	4:A:409:PCF:H463	1.51	0.74
3:B:403:CLR:C12	4:A:409:PCF:H361	2.17	0.74
1:C:32:HIS:HD2	1:C:99:PRO:HA	1.52	0.74
2:B:87:THR:HG23	4:B:410:PCF:H262	1.70	0.73
4:B:410:PCF:H352	3:A:405:CLR:H12	1.70	0.73
3:B:403:CLR:H12	4:A:409:PCF:H352	1.70	0.73
2:A:151:ALA:HB2	3:A:407:CLR:H42	1.70	0.73
2:A:187:MET:HE1	3:A:406:CLR:H41	1.71	0.72
2:A:87:THR:HG23	4:A:409:PCF:H262	1.70	0.72
3:B:407:CLR:H151	3:B:408:CLR:H71	1.70	0.72
3:B:401:CLR:H242	3:B:405:CLR:H241	1.70	0.72
2:B:151:ALA:HB2	3:B:405:CLR:H42	1.70	0.72
3:A:402:CLR:H151	3:A:403:CLR:H71	1.70	0.71
2:B:87:THR:HA	4:B:410:PCF:H262	1.72	0.71
2:B:187:MET:HE1	3:B:404:CLR:H41	1.73	0.71
3:A:407:CLR:H241	3:A:408:CLR:H242	1.70	0.71
2:A:90:TYR:HD2	4:A:409:PCF:H251	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:87:THR:HA	4:A:409:PCF:H262	1.72	0.70
2:B:90:TYR:HD2	4:B:410:PCF:H251	1.57	0.69
2:B:100:PHE:HD1	4:A:409:PCF:H351	1.57	0.69
3:A:401:CLR:H242	3:A:403:CLR:H232	1.75	0.69
3:B:403:CLR:H241	3:B:403:CLR:C21	2.23	0.68
3:B:408:CLR:H181	3:A:408:CLR:H122	1.75	0.68
3:A:405:CLR:H241	3:A:405:CLR:C21	2.23	0.68
2:A:58:ARG:H	2:A:61:ARG:HG2	1.58	0.68
2:B:123:LEU:HB3	2:B:250:ILE:HD13	1.76	0.68
4:B:410:PCF:H351	2:A:100:PHE:HD1	1.58	0.68
3:B:406:CLR:H242	3:B:408:CLR:H232	1.75	0.67
3:B:401:CLR:H122	3:A:403:CLR:H181	1.75	0.67
2:B:58:ARG:H	2:B:61:ARG:HG2	1.57	0.67
2:B:70:SER:OG	2:B:154:TRP:NE1	2.28	0.67
3:B:406:CLR:H263	3:B:408:CLR:H273	1.77	0.67
2:A:123:LEU:HB3	2:A:250:ILE:HD13	1.76	0.67
2:B:97:PHE:CE1	3:A:405:CLR:H6	2.29	0.66
2:A:90:TYR:CB	4:A:409:PCF:H271	2.25	0.66
2:B:100:PHE:CZ	3:B:403:CLR:H14	2.31	0.66
3:B:403:CLR:H112	4:A:409:PCF:H361	1.77	0.66
2:A:70:SER:OG	2:A:154:TRP:NE1	2.28	0.66
4:B:410:PCF:H361	3:A:405:CLR:H112	1.77	0.65
3:A:401:CLR:H263	3:A:403:CLR:H273	1.77	0.65
2:A:36:MET:HG3	4:A:409:PCF:C48	2.26	0.65
3:B:403:CLR:H6	2:A:97:PHE:CE1	2.29	0.65
2:A:87:THR:HA	4:A:409:PCF:H282	1.78	0.65
3:A:405:CLR:H241	3:A:405:CLR:H211	1.77	0.65
2:B:87:THR:HA	4:B:410:PCF:H282	1.79	0.65
3:B:403:CLR:H241	3:B:403:CLR:H211	1.77	0.65
1:D:20:LEU:HD12	1:D:80:LEU:HD23	1.79	0.64
2:B:154:TRP:CB	3:B:405:CLR:H72	2.28	0.64
2:B:90:TYR:CB	4:B:410:PCF:H271	2.27	0.64
2:B:100:PHE:CE1	3:B:403:CLR:H14	2.33	0.64
4:B:409:PCF:C31	4:B:409:PCF:H12	2.27	0.64
2:B:36:MET:HG3	4:B:410:PCF:C48	2.25	0.64
2:B:87:THR:N	4:B:410:PCF:H282	2.12	0.64
2:A:154:TRP:CB	3:A:407:CLR:H72	2.28	0.64
2:B:83:PRO:HB2	3:A:405:CLR:H152	1.80	0.63
2:A:87:THR:N	4:A:409:PCF:H282	2.13	0.63
3:B:401:CLR:H183	3:B:405:CLR:H14	1.79	0.63
2:A:100:PHE:CZ	3:A:405:CLR:H14	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:410:PCF:H12	4:A:410:PCF:C31	2.27	0.63
1:C:20:LEU:HD12	1:C:80:LEU:HD23	1.79	0.63
2:A:39:PHE:HA	2:A:79:VAL:HG13	1.80	0.63
2:A:90:TYR:HB3	4:A:409:PCF:H271	1.81	0.63
2:B:39:PHE:HA	2:B:79:VAL:HG13	1.80	0.63
2:B:86:ALA:C	4:B:410:PCF:H282	2.24	0.63
3:B:403:CLR:C6	2:A:97:PHE:CE1	2.82	0.63
2:A:36:MET:CB	4:A:409:PCF:H523	2.29	0.63
2:A:73:VAL:HG11	3:A:408:CLR:H71	1.81	0.62
2:A:100:PHE:CE1	3:A:405:CLR:H14	2.33	0.62
3:A:407:CLR:C6	3:A:408:CLR:H191	2.30	0.62
3:A:407:CLR:H14	3:A:408:CLR:H183	1.79	0.62
2:A:86:ALA:C	4:A:409:PCF:H282	2.24	0.62
2:B:97:PHE:CE1	3:A:405:CLR:C6	2.82	0.62
2:B:36:MET:CB	4:B:410:PCF:H523	2.30	0.62
3:B:403:CLR:H152	2:A:83:PRO:HB2	1.82	0.62
2:B:154:TRP:HB3	3:B:405:CLR:H151	1.81	0.62
3:B:402:CLR:H122	3:A:403:CLR:H72	1.82	0.61
3:B:403:CLR:H213	4:A:409:PCF:H401	1.83	0.61
2:B:73:VAL:HG11	3:B:401:CLR:H71	1.82	0.61
3:B:401:CLR:H191	3:B:405:CLR:C6	2.30	0.61
2:A:87:THR:CA	4:A:409:PCF:H282	2.31	0.61
4:B:410:PCF:H401	3:A:405:CLR:H213	1.83	0.61
2:B:90:TYR:HB3	4:B:410:PCF:H271	1.83	0.60
2:A:154:TRP:HB3	3:A:407:CLR:H151	1.83	0.60
2:A:73:VAL:O	2:A:77:THR:HG23	2.02	0.60
2:B:99:THR:OG1	4:A:409:PCF:H122	2.01	0.60
4:B:410:PCF:H122	2:A:99:THR:OG1	2.02	0.60
3:B:403:CLR:C11	4:A:409:PCF:H361	2.32	0.60
3:A:401:CLR:H9	3:A:403:CLR:H12	1.84	0.59
3:B:406:CLR:H9	3:B:408:CLR:H12	1.84	0.59
4:B:410:PCF:H361	3:A:405:CLR:C11	2.32	0.59
3:B:401:CLR:H12	3:B:402:CLR:H112	1.85	0.59
3:B:404:CLR:H11	4:A:409:PCF:H341	1.85	0.59
3:B:408:CLR:H72	3:A:404:CLR:H122	1.82	0.59
3:A:407:CLR:H71	3:A:408:CLR:H182	1.83	0.59
2:B:154:TRP:CE2	3:B:401:CLR:H72	2.37	0.59
2:A:154:TRP:CE2	3:A:408:CLR:H72	2.37	0.59
3:A:404:CLR:H112	3:A:408:CLR:H12	1.85	0.59
2:B:73:VAL:O	2:B:77:THR:HG23	2.02	0.59
3:B:401:CLR:H182	3:B:405:CLR:H71	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:91:ARG:NH2	2:A:94:ASP:OD2	2.36	0.59
3:A:403:CLR:H222	3:A:403:CLR:C12	2.30	0.59
4:B:410:PCF:C42	3:A:405:CLR:H242	2.28	0.58
2:B:87:THR:CA	4:B:410:PCF:H282	2.32	0.58
2:B:164:VAL:HA	2:B:183:MET:HE1	1.85	0.58
2:B:165:MET:HE2	4:A:409:PCF:C37	2.34	0.58
2:A:311:PHE:O	2:A:317:ARG:NH2	2.37	0.58
2:A:164:VAL:HA	2:A:183:MET:HE1	1.85	0.58
2:B:311:PHE:O	2:B:317:ARG:NH2	2.37	0.58
3:B:403:CLR:C22	4:A:409:PCF:H451	2.32	0.58
4:B:410:PCF:H341	3:A:406:CLR:H11	1.85	0.57
3:B:403:CLR:H161	4:A:409:PCF:H461	1.86	0.57
3:A:406:CLR:H222	3:A:407:CLR:C25	2.33	0.57
4:B:410:PCF:C37	2:A:165:MET:HE2	2.34	0.57
2:A:53:VAL:HG11	2:A:69:ALA:HB2	1.86	0.57
2:B:249:ILE:HD11	2:B:313:ASP:HA	1.86	0.57
4:B:410:PCF:H461	3:A:405:CLR:H161	1.86	0.57
2:B:91:ARG:NH2	2:B:94:ASP:OD2	2.36	0.57
3:B:403:CLR:H161	4:A:409:PCF:C46	2.35	0.57
4:B:410:PCF:H451	3:A:405:CLR:C22	2.32	0.57
4:B:410:PCF:C46	3:A:405:CLR:H161	2.35	0.57
3:A:407:CLR:H71	3:A:408:CLR:H121	1.87	0.57
2:B:162:MET:HE2	3:B:404:CLR:H152	1.87	0.57
3:B:404:CLR:H222	3:B:405:CLR:C25	2.33	0.57
2:B:53:VAL:HG11	2:B:69:ALA:HB2	1.86	0.56
4:B:410:PCF:H221	3:A:405:CLR:O1	2.05	0.56
3:B:401:CLR:H121	3:B:405:CLR:H71	1.86	0.56
3:A:404:CLR:H11	3:A:408:CLR:H21	1.87	0.56
2:A:249:ILE:HD11	2:A:313:ASP:HA	1.86	0.56
3:B:403:CLR:H122	4:A:409:PCF:H361	1.88	0.56
3:B:403:CLR:O1	4:A:409:PCF:H221	2.05	0.56
3:B:401:CLR:H21	3:B:402:CLR:H11	1.87	0.55
1:D:40:ALA:HA	1:D:91:ALA:HA	1.88	0.55
3:B:408:CLR:H222	3:B:408:CLR:C12	2.30	0.55
1:D:102:GLY:HA3	4:B:409:PCF:H522	1.88	0.55
4:A:409:PCF:H12	4:A:409:PCF:C11	2.34	0.54
3:B:403:CLR:H242	4:A:409:PCF:C42	2.28	0.54
2:B:162:MET:HE1	3:B:404:CLR:H181	1.90	0.54
4:B:410:PCF:H361	3:A:405:CLR:H122	1.88	0.54
2:A:162:MET:HE2	3:A:406:CLR:H152	1.88	0.54
3:B:404:CLR:H112	4:A:409:PCF:H341	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ALA:HA	1:C:91:ALA:HA	1.88	0.53
2:A:162:MET:HE1	3:A:406:CLR:H181	1.91	0.53
4:B:410:PCF:H341	3:A:406:CLR:H112	1.90	0.53
4:B:410:PCF:H221	3:A:405:CLR:C2	2.39	0.53
3:B:403:CLR:C2	4:A:409:PCF:H221	2.39	0.53
4:B:410:PCF:H352	3:A:405:CLR:C1	2.37	0.53
2:A:210:PHE:O	2:A:214:PHE:HB2	2.10	0.52
2:B:210:PHE:O	2:B:214:PHE:HB2	2.10	0.52
1:C:102:GLY:HA3	4:A:410:PCF:H522	1.90	0.52
3:A:407:CLR:H6	3:A:408:CLR:H191	1.91	0.52
3:B:403:CLR:H22	4:A:409:PCF:H221	1.91	0.52
2:B:62:ARG:HH21	2:B:65:ASP:HA	1.75	0.52
3:B:403:CLR:C1	4:A:409:PCF:H352	2.38	0.51
2:A:62:ARG:HH21	2:A:65:ASP:HA	1.75	0.51
2:A:314:PRO:O	2:A:318:GLN:HG2	2.10	0.51
3:B:406:CLR:H122	3:B:408:CLR:H9	1.93	0.51
2:A:66:ILE:HD11	2:A:150:THR:HG21	1.93	0.51
2:B:48:LEU:O	2:B:52:THR:HG23	2.11	0.51
2:B:314:PRO:O	2:B:318:GLN:HG2	2.11	0.51
2:A:58:ARG:N	2:A:61:ARG:HG2	2.25	0.51
3:A:401:CLR:H122	3:A:403:CLR:H9	1.93	0.51
4:B:410:PCF:H221	3:A:405:CLR:H22	1.91	0.51
2:A:48:LEU:O	2:A:52:THR:HG23	2.11	0.51
2:A:154:TRP:CZ2	3:A:408:CLR:H72	2.47	0.50
2:B:39:PHE:HA	2:B:79:VAL:CG1	2.41	0.50
2:B:66:ILE:HD11	2:B:150:THR:HG21	1.93	0.50
2:B:154:TRP:CZ2	3:B:401:CLR:H72	2.47	0.50
2:B:213:PRO:O	2:B:217:MET:HG3	2.12	0.50
3:B:403:CLR:H221	4:A:409:PCF:C45	2.35	0.50
3:B:401:CLR:H191	3:B:405:CLR:H6	1.91	0.50
2:A:103:LYS:NZ	3:A:406:CLR:H192	2.27	0.50
4:B:410:PCF:C45	3:A:405:CLR:H221	2.35	0.50
2:A:39:PHE:HA	2:A:79:VAL:CG1	2.42	0.50
2:A:213:PRO:O	2:A:217:MET:HG3	2.12	0.50
2:B:33:ALA:O	4:B:410:PCF:H511	2.12	0.49
2:B:223:PHE:O	2:B:227:THR:HG23	2.12	0.49
3:B:408:CLR:H8	3:A:408:CLR:H111	1.95	0.49
4:B:410:PCF:H12	4:B:410:PCF:C11	2.34	0.49
3:B:403:CLR:C1	4:A:409:PCF:H331	2.43	0.49
3:B:401:CLR:H111	3:A:403:CLR:H8	1.95	0.49
3:A:408:CLR:H272	3:A:408:CLR:H221	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:403:CLR:H191	2:A:87:THR:OG1	2.13	0.49
4:B:410:PCF:H432	3:A:408:CLR:H261	1.95	0.49
4:B:410:PCF:H331	3:A:405:CLR:C1	2.43	0.49
2:B:87:THR:HG21	3:A:405:CLR:H42	1.94	0.48
4:B:410:PCF:H151	2:A:170:THR:O	2.13	0.48
1:C:69:ILE:HD11	1:C:78:LEU:HD11	1.95	0.48
2:B:103:LYS:NZ	3:B:404:CLR:H192	2.28	0.48
3:B:401:CLR:H261	4:A:409:PCF:H432	1.95	0.48
2:A:33:ALA:O	4:A:409:PCF:H511	2.13	0.48
2:A:223:PHE:O	2:A:227:THR:HG23	2.12	0.48
3:B:404:CLR:H11	4:A:409:PCF:C34	2.44	0.48
3:A:404:CLR:H261	3:A:408:CLR:H271	1.95	0.48
2:B:154:TRP:CH2	3:B:401:CLR:H152	2.48	0.48
4:B:410:PCF:C34	3:A:406:CLR:H11	2.44	0.48
3:B:401:CLR:H272	3:B:401:CLR:H221	1.95	0.48
3:B:408:CLR:H41	3:A:404:CLR:C1	2.44	0.48
1:D:69:ILE:HD11	1:D:78:LEU:HD11	1.95	0.48
2:A:154:TRP:CH2	3:A:408:CLR:H152	2.49	0.48
3:B:401:CLR:H272	3:B:401:CLR:H213	1.96	0.48
3:B:401:CLR:C23	3:B:405:CLR:H221	2.41	0.48
3:B:401:CLR:H271	3:B:402:CLR:H261	1.95	0.48
2:B:51:TRP:HH2	2:B:323:MET:HB2	1.79	0.47
2:B:87:THR:OG1	3:A:405:CLR:H191	2.13	0.47
3:B:403:CLR:H271	3:A:403:CLR:H262	1.96	0.47
3:A:408:CLR:H272	3:A:408:CLR:H213	1.96	0.47
2:A:195:TRP:CZ3	4:A:410:PCF:H332	2.48	0.47
3:B:408:CLR:H262	3:A:405:CLR:H271	1.96	0.47
2:B:170:THR:O	4:A:409:PCF:H151	2.14	0.47
2:B:165:MET:HE2	4:A:409:PCF:H371	1.97	0.47
2:A:51:TRP:HH2	2:A:323:MET:HB2	1.79	0.47
2:A:154:TRP:HB3	3:A:407:CLR:H72	1.96	0.47
2:A:272:MET:HG3	4:A:410:PCF:H511	1.97	0.47
2:B:58:ARG:N	2:B:61:ARG:HG2	2.25	0.47
3:B:403:CLR:H42	2:A:87:THR:HG21	1.95	0.47
3:B:405:CLR:H21	3:A:403:CLR:C19	2.45	0.47
2:B:154:TRP:HB3	3:B:405:CLR:C15	2.45	0.46
3:B:406:CLR:H12	3:B:408:CLR:H21	1.97	0.46
3:B:402:CLR:C1	3:A:403:CLR:H41	2.44	0.46
3:B:408:CLR:H162	3:A:408:CLR:H20	1.96	0.46
3:B:408:CLR:C19	3:A:407:CLR:H21	2.45	0.46
4:B:410:PCF:H371	2:A:165:MET:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:TRP:HB3	3:B:405:CLR:H72	1.96	0.46
3:B:406:CLR:C26	3:A:405:CLR:H25	2.45	0.46
3:A:407:CLR:H71	3:A:408:CLR:C18	2.46	0.46
3:B:403:CLR:H25	3:A:401:CLR:C26	2.45	0.46
1:D:92:MET:HE2	1:D:125:GLN:HB2	1.98	0.46
3:B:401:CLR:H20	3:A:403:CLR:H162	1.96	0.46
4:B:409:PCF:H492	4:B:409:PCF:H301	1.59	0.46
1:C:92:MET:HE2	1:C:125:GLN:HB2	1.98	0.46
2:B:271:TYR:HD2	4:B:409:PCF:C51	2.29	0.46
2:A:284:ASP:O	2:A:288:MET:HG3	2.16	0.46
3:A:401:CLR:H12	3:A:403:CLR:H21	1.97	0.46
4:A:410:PCF:H301	4:A:410:PCF:H492	1.59	0.45
2:A:87:THR:HG23	4:A:409:PCF:C26	2.43	0.45
2:A:154:TRP:CZ3	3:A:408:CLR:H152	2.52	0.45
2:B:154:TRP:CZ3	3:B:401:CLR:H152	2.52	0.45
2:B:284:ASP:O	2:B:288:MET:HG3	2.16	0.45
3:B:401:CLR:C18	3:B:405:CLR:H71	2.46	0.45
2:A:272:MET:HG3	4:A:410:PCF:C51	2.46	0.45
2:A:272:MET:HG2	4:A:410:PCF:H502	1.99	0.45
3:A:408:CLR:C18	3:A:408:CLR:H222	2.47	0.45
2:B:87:THR:HG23	4:B:410:PCF:C26	2.44	0.45
4:B:410:PCF:H332	3:A:406:CLR:H11	1.99	0.45
2:A:62:ARG:HG2	2:A:64:ALA:H	1.82	0.45
2:B:165:MET:HG2	3:B:404:CLR:C18	2.47	0.45
3:B:404:CLR:H11	4:A:409:PCF:H332	1.99	0.45
1:D:87:PRO:HA	1:D:128:VAL:HB	1.99	0.45
3:B:402:CLR:H211	3:B:402:CLR:H231	1.76	0.45
3:B:403:CLR:H112	4:A:409:PCF:C36	2.45	0.45
2:A:87:THR:HA	4:A:409:PCF:C26	2.45	0.45
2:B:62:ARG:HG2	2:B:64:ALA:H	1.82	0.45
2:A:100:PHE:CG	3:A:405:CLR:H71	2.52	0.45
2:A:73:VAL:HG12	3:A:408:CLR:H151	1.99	0.44
1:C:87:PRO:HA	1:C:128:VAL:HB	1.99	0.44
2:A:39:PHE:O	2:A:43:THR:OG1	2.28	0.44
2:A:127:ARG:HG2	2:A:127:ARG:HH11	1.82	0.44
4:B:410:PCF:C36	3:A:405:CLR:H112	2.45	0.44
3:B:401:CLR:C18	3:B:401:CLR:H222	2.47	0.44
2:B:162:MET:CE	3:B:404:CLR:H181	2.48	0.44
4:A:410:PCF:H342	4:A:410:PCF:O32	2.17	0.44
2:B:73:VAL:HG12	3:B:401:CLR:H151	1.98	0.44
2:B:100:PHE:CG	3:B:403:CLR:H71	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:401:CLR:H12	3:B:402:CLR:C11	2.47	0.44
3:B:402:CLR:C12	3:A:403:CLR:H72	2.47	0.44
3:B:405:CLR:H213	3:A:403:CLR:H211	2.00	0.44
2:A:154:TRP:HB3	3:A:407:CLR:C15	2.47	0.44
2:A:165:MET:HG2	3:A:406:CLR:C18	2.47	0.44
1:D:12:VAL:HB	1:D:18:LEU:HD21	2.00	0.44
3:A:404:CLR:H211	3:A:404:CLR:H231	1.76	0.44
3:B:408:CLR:H211	3:A:407:CLR:H213	2.00	0.43
4:B:409:PCF:O32	4:B:409:PCF:H342	2.17	0.43
3:A:404:CLR:C11	3:A:408:CLR:H12	2.47	0.43
3:A:405:CLR:H121	3:A:405:CLR:H212	2.01	0.43
3:A:407:CLR:H221	3:A:408:CLR:C23	2.41	0.43
2:B:82:LEU:HD23	2:B:82:LEU:HA	1.81	0.43
2:A:33:ALA:CA	4:A:409:PCF:H491	2.16	0.43
2:A:103:LYS:HE3	3:A:406:CLR:H22	2.01	0.43
2:A:162:MET:CE	3:A:406:CLR:H181	2.49	0.43
3:A:405:CLR:C21	3:A:405:CLR:C24	2.95	0.43
2:B:127:ARG:HG2	2:B:127:ARG:HH11	1.82	0.43
2:B:165:MET:HE2	4:A:409:PCF:H372	2.01	0.43
3:A:404:CLR:C21	3:A:408:CLR:H17	2.49	0.43
2:B:154:TRP:HB2	3:B:405:CLR:H72	1.99	0.43
2:B:271:TYR:CD2	4:B:409:PCF:H512	2.53	0.43
3:A:401:CLR:H12	3:A:403:CLR:C2	2.48	0.43
1:C:12:VAL:HB	1:C:18:LEU:HD21	2.00	0.43
3:A:401:CLR:H221	3:A:403:CLR:H17	2.00	0.43
2:B:243:ARG:HE	2:B:245:ARG:HG3	1.83	0.43
2:A:154:TRP:HB2	3:A:407:CLR:H72	2.00	0.43
3:B:406:CLR:H221	3:B:408:CLR:H17	2.00	0.42
2:A:203:VAL:HG13	4:A:410:PCF:H463	2.01	0.42
2:B:260:CYS:HB3	2:B:301:ASN:HB2	2.01	0.42
4:B:409:PCF:H111	4:B:409:PCF:H142	1.73	0.42
2:A:58:ARG:H	2:A:61:ARG:CG	2.30	0.42
3:A:401:CLR:H161	3:A:401:CLR:H222	1.98	0.42
2:B:87:THR:HA	4:B:410:PCF:C26	2.45	0.42
2:A:90:TYR:CG	4:A:409:PCF:H271	2.53	0.42
3:B:403:CLR:H121	3:B:403:CLR:H212	2.01	0.42
3:B:406:CLR:H12	3:B:408:CLR:C2	2.48	0.42
3:B:408:CLR:H162	3:B:408:CLR:H212	1.85	0.42
3:B:401:CLR:H17	3:B:402:CLR:C21	2.49	0.42
4:B:410:PCF:H372	2:A:165:MET:HE2	2.01	0.42
2:B:51:TRP:CH2	2:B:323:MET:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:LYS:HE3	3:B:404:CLR:H22	2.01	0.42
3:B:401:CLR:H193	3:A:403:CLR:H191	2.01	0.42
2:A:260:CYS:HB3	2:A:301:ASN:HB2	2.01	0.42
4:B:410:PCF:H112	4:B:410:PCF:H142	1.70	0.42
2:A:243:ARG:HE	2:A:245:ARG:HG3	1.84	0.42
2:B:58:ARG:O	2:B:59:GLU:C	2.61	0.42
3:B:401:CLR:C1	3:B:402:CLR:H112	2.49	0.42
2:A:79:VAL:O	2:A:82:LEU:HB2	2.20	0.42
2:A:113:MET:HE2	2:A:261:TRP:CZ3	2.55	0.42
2:A:245:ARG:HG3	2:A:245:ARG:HH11	1.85	0.42
2:A:36:MET:HB2	4:A:409:PCF:C51	2.50	0.41
2:B:90:TYR:CG	4:B:410:PCF:H271	2.55	0.41
2:B:272:MET:HG2	4:B:409:PCF:H502	2.02	0.41
1:C:90:THR:HG23	1:C:127:THR:HA	2.02	0.41
2:A:58:ARG:O	2:A:59:GLU:C	2.61	0.41
3:A:406:CLR:H221	3:A:406:CLR:H25	1.87	0.41
2:A:82:LEU:N	2:A:83:PRO:HD2	2.36	0.41
2:B:36:MET:HE2	2:B:36:MET:HA	2.02	0.41
2:B:36:MET:HB2	4:B:410:PCF:C51	2.50	0.41
3:B:408:CLR:H191	3:A:408:CLR:H193	2.01	0.41
2:A:36:MET:HA	2:A:36:MET:HE2	2.02	0.41
3:B:408:CLR:H72	3:A:404:CLR:C12	2.47	0.41
3:A:406:CLR:H221	3:A:406:CLR:H162	1.21	0.41
2:B:39:PHE:O	2:B:43:THR:OG1	2.28	0.41
2:B:79:VAL:O	2:B:82:LEU:HB2	2.20	0.41
2:B:273:LEU:HD21	4:B:409:PCF:H402	2.01	0.41
3:B:406:CLR:H161	3:B:406:CLR:H222	1.98	0.41
2:A:51:TRP:CH2	2:A:323:MET:HB2	2.55	0.41
2:A:62:ARG:HE	2:A:65:ASP:N	2.19	0.41
2:A:166:VAL:HA	3:A:406:CLR:H191	2.03	0.41
4:B:410:PCF:H121	4:B:410:PCF:H32	2.03	0.41
2:B:62:ARG:HB3	2:B:65:ASP:OD2	2.21	0.41
2:B:113:MET:HE2	2:B:261:TRP:CZ3	2.55	0.41
2:B:245:ARG:HG3	2:B:245:ARG:HH11	1.85	0.41
3:B:403:CLR:H213	4:A:409:PCF:C40	2.50	0.41
2:A:87:THR:HA	4:A:409:PCF:C28	2.49	0.41
4:A:409:PCF:H32	4:A:409:PCF:H121	2.03	0.41
2:B:62:ARG:HE	2:B:65:ASP:N	2.19	0.40
2:A:62:ARG:HB3	2:A:65:ASP:OD2	2.21	0.40
3:A:404:CLR:H112	3:A:408:CLR:C1	2.49	0.40
2:B:33:ALA:CA	4:B:410:PCF:H491	2.15	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:LEU:N	2:B:83:PRO:HD2	2.36	0.40
3:B:401:CLR:H111	3:B:401:CLR:H193	1.83	0.40
2:B:166:VAL:HA	3:B:404:CLR:H191	2.03	0.40
2:A:166:VAL:HG22	3:A:406:CLR:H72	2.04	0.40
2:B:166:VAL:HG22	3:B:404:CLR:H72	2.04	0.40
2:B:267:VAL:HG13	2:B:287:LEU:HD22	2.04	0.40
3:B:402:CLR:H6	3:A:402:CLR:H12	2.04	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	C	127/130 (98%)	120 (94%)	5 (4%)	2 (2%)	7	20
1	D	127/130 (98%)	120 (94%)	5 (4%)	2 (2%)	7	20
2	A	270/380 (71%)	262 (97%)	8 (3%)	0	100	100
2	B	270/380 (71%)	262 (97%)	8 (3%)	0	100	100
All	All	794/1020 (78%)	764 (96%)	26 (3%)	4 (0%)	26	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	41	PRO
1	C	41	PRO
1	D	40	ALA
1	C	40	ALA

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	C	103/104 (99%)	102 (99%)	1 (1%)	68	86
1	D	103/104 (99%)	102 (99%)	1 (1%)	68	86
2	A	237/327 (72%)	236 (100%)	1 (0%)	84	93
2	B	237/327 (72%)	236 (100%)	1 (0%)	84	93
All	All	680/862 (79%)	676 (99%)	4 (1%)	76	91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	105	TYR
2	B	61	ARG
1	C	105	TYR
2	A	61	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	112	ASN
2	B	180	GLN
2	B	301	ASN
2	A	112	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	CLR	A	408	-	31,31,31	1.16	2 (6%)	48,48,48	1.89	11 (22%)
3	CLR	A	405	-	31,31,31	1.14	2 (6%)	48,48,48	1.39	6 (12%)
3	CLR	A	403	-	31,31,31	1.15	1 (3%)	48,48,48	1.52	8 (16%)
3	CLR	A	406	-	31,31,31	1.13	1 (3%)	48,48,48	1.51	9 (18%)
4	PCF	B	410	-	49,49,49	1.35	5 (10%)	55,57,57	1.17	4 (7%)
3	CLR	A	404	-	31,31,31	1.17	2 (6%)	48,48,48	1.41	8 (16%)
4	PCF	B	409	-	49,49,49	1.31	5 (10%)	55,57,57	1.19	5 (9%)
4	PCF	A	410	-	49,49,49	1.31	5 (10%)	55,57,57	1.19	5 (9%)
3	CLR	B	407	-	31,31,31	1.16	1 (3%)	48,48,48	1.43	10 (20%)
3	CLR	A	407	-	31,31,31	1.13	1 (3%)	48,48,48	1.70	10 (20%)
3	CLR	B	406	-	31,31,31	1.16	1 (3%)	48,48,48	1.49	9 (18%)
3	CLR	A	402	-	31,31,31	1.16	1 (3%)	48,48,48	1.43	10 (20%)
3	CLR	B	404	-	31,31,31	1.14	1 (3%)	48,48,48	1.51	9 (18%)
3	CLR	B	403	-	31,31,31	1.14	2 (6%)	48,48,48	1.38	6 (12%)
3	CLR	B	401	-	31,31,31	1.17	2 (6%)	48,48,48	1.89	11 (22%)
3	CLR	B	405	-	31,31,31	1.13	1 (3%)	48,48,48	1.70	10 (20%)
3	CLR	B	402	-	31,31,31	1.17	1 (3%)	48,48,48	1.41	8 (16%)
3	CLR	B	408	-	31,31,31	1.15	1 (3%)	48,48,48	1.52	8 (16%)
4	PCF	A	409	-	49,49,49	1.35	5 (10%)	55,57,57	1.17	4 (7%)
3	CLR	A	401	-	31,31,31	1.17	1 (3%)	48,48,48	1.49	9 (18%)

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	CLR	A	408	-	-	6/10/68/68	0/4/4/4
3	CLR	A	405	-	-	1/10/68/68	0/4/4/4
3	CLR	A	403	-	-	6/10/68/68	0/4/4/4
3	CLR	A	406	-	-	6/10/68/68	0/4/4/4
4	PCF	B	410	-	-	21/53/53/53	-
3	CLR	A	404	-	-	2/10/68/68	0/4/4/4
4	PCF	B	409	-	-	32/53/53/53	-
4	PCF	A	410	-	-	32/53/53/53	-
3	CLR	B	407	-	-	2/10/68/68	0/4/4/4
3	CLR	A	407	-	-	2/10/68/68	0/4/4/4
3	CLR	B	406	-	-	2/10/68/68	0/4/4/4
3	CLR	A	402	-	-	2/10/68/68	0/4/4/4
3	CLR	B	404	-	-	6/10/68/68	0/4/4/4
3	CLR	B	403	-	-	1/10/68/68	0/4/4/4
3	CLR	B	401	-	-	6/10/68/68	0/4/4/4
3	CLR	B	405	-	-	2/10/68/68	0/4/4/4
3	CLR	B	402	-	-	2/10/68/68	0/4/4/4
3	CLR	B	408	-	-	6/10/68/68	0/4/4/4
4	PCF	A	409	-	-	21/53/53/53	-
3	CLR	A	401	-	-	2/10/68/68	0/4/4/4

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	409	PCF	O21-C21	3.42	1.43	1.34
4	B	410	PCF	O21-C21	3.41	1.43	1.34
4	A	410	PCF	O31-C31	3.38	1.43	1.33
4	B	409	PCF	O31-C31	3.37	1.43	1.33
3	B	401	CLR	C16-C17	3.22	1.61	1.54
3	A	408	CLR	C16-C17	3.19	1.60	1.54
3	B	406	CLR	C16-C17	3.16	1.60	1.54
3	A	401	CLR	C16-C17	3.16	1.60	1.54
3	B	402	CLR	C16-C17	3.13	1.60	1.54
4	A	409	PCF	O31-C31	3.13	1.42	1.33
3	A	404	CLR	C16-C17	3.13	1.60	1.54
4	B	410	PCF	O31-C31	3.13	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	CLR	C16-C17	3.11	1.60	1.54
3	B	407	CLR	C16-C17	3.11	1.60	1.54
3	B	405	CLR	C16-C17	3.08	1.60	1.54
3	B	408	CLR	C16-C17	3.06	1.60	1.54
3	A	403	CLR	C16-C17	3.06	1.60	1.54
3	A	407	CLR	C16-C17	3.04	1.60	1.54
3	B	404	CLR	C16-C17	3.03	1.60	1.54
3	A	406	CLR	C16-C17	3.02	1.60	1.54
4	A	410	PCF	O21-C21	2.99	1.42	1.34
4	B	409	PCF	O21-C21	2.98	1.42	1.34
3	A	405	CLR	C16-C17	2.93	1.60	1.54
3	B	403	CLR	C16-C17	2.92	1.60	1.54
4	A	409	PCF	C22-C21	2.66	1.58	1.50
4	B	410	PCF	C22-C21	2.65	1.58	1.50
4	A	410	PCF	C22-C21	2.60	1.58	1.50
4	B	409	PCF	C22-C21	2.59	1.58	1.50
4	B	409	PCF	O21-C2	-2.38	1.41	1.46
4	A	410	PCF	O21-C2	-2.34	1.41	1.46
4	B	410	PCF	P-O11	2.29	1.68	1.59
4	A	409	PCF	P-O11	2.29	1.68	1.59
4	B	410	PCF	P-O13	2.11	1.67	1.59
4	A	409	PCF	P-O13	2.09	1.67	1.59
3	B	401	CLR	C16-C15	2.08	1.59	1.54
4	A	410	PCF	P-O14	-2.08	1.45	1.55
3	A	408	CLR	C16-C15	2.07	1.59	1.54
4	B	409	PCF	P-O14	-2.07	1.45	1.55
3	A	405	CLR	C16-C15	2.05	1.59	1.54
3	B	403	CLR	C16-C15	2.04	1.59	1.54
3	A	404	CLR	C16-C15	2.00	1.59	1.54

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	408	CLR	C17-C13-C14	-5.06	94.29	100.10
3	B	401	CLR	C17-C13-C14	-5.04	94.31	100.10
3	B	401	CLR	C14-C8-C9	-5.01	102.54	109.09
3	A	408	CLR	C14-C8-C9	-5.00	102.56	109.09
4	A	409	PCF	O21-C21-C22	3.91	119.94	111.48
4	B	410	PCF	O21-C21-C22	3.90	119.92	111.48
3	A	408	CLR	C18-C13-C12	3.63	115.95	110.61
3	B	401	CLR	C18-C13-C12	3.62	115.94	110.61
3	A	407	CLR	C19-C10-C9	-3.50	107.73	111.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	410	PCF	O31-C31-C32	3.50	122.51	111.83
4	B	409	PCF	O31-C31-C32	3.50	122.49	111.83
3	B	405	CLR	C19-C10-C9	-3.49	107.75	111.66
3	B	408	CLR	C15-C14-C13	3.43	107.88	103.84
3	A	403	CLR	C15-C14-C13	3.41	107.85	103.84
3	A	401	CLR	C22-C20-C17	-3.39	103.29	110.33
3	B	406	CLR	C22-C20-C17	-3.39	103.31	110.33
3	B	405	CLR	C22-C20-C17	-3.20	103.69	110.33
3	A	407	CLR	C22-C20-C17	-3.19	103.72	110.33
3	B	408	CLR	C16-C17-C20	-3.19	107.36	112.18
3	A	403	CLR	C16-C17-C20	-3.18	107.37	112.18
4	A	410	PCF	O21-C21-C22	3.15	118.31	111.48
4	B	409	PCF	O21-C21-C22	3.14	118.27	111.48
3	B	405	CLR	C1-C2-C3	3.01	114.46	110.48
3	A	407	CLR	C1-C2-C3	3.00	114.45	110.48
3	B	402	CLR	C22-C20-C17	-2.98	104.15	110.33
3	A	404	CLR	C22-C20-C17	-2.98	104.15	110.33
3	A	408	CLR	C16-C17-C13	-2.97	100.35	103.84
3	B	401	CLR	C16-C17-C13	-2.96	100.36	103.84
3	A	405	CLR	C22-C20-C17	-2.89	104.35	110.33
3	B	403	CLR	C22-C20-C17	-2.87	104.37	110.33
3	A	408	CLR	C21-C20-C22	-2.85	105.92	110.34
3	B	401	CLR	C21-C20-C22	-2.85	105.93	110.34
3	A	401	CLR	C21-C20-C17	2.84	117.14	112.88
3	B	406	CLR	C21-C20-C17	2.83	117.13	112.88
4	B	410	PCF	O31-C31-C32	2.78	120.32	111.83
4	A	409	PCF	O31-C31-C32	2.78	120.32	111.83
3	B	406	CLR	C16-C17-C20	-2.76	108.00	112.18
3	A	404	CLR	C19-C10-C9	-2.76	108.56	111.66
3	A	401	CLR	C16-C17-C20	-2.75	108.01	112.18
3	B	402	CLR	C19-C10-C9	-2.75	108.57	111.66
3	A	402	CLR	C22-C20-C17	-2.74	104.64	110.33
3	A	403	CLR	C12-C13-C14	-2.74	103.15	107.25
3	B	407	CLR	C22-C20-C17	-2.73	104.66	110.33
3	B	408	CLR	C12-C13-C14	-2.71	103.18	107.25
3	A	407	CLR	C3-C4-C5	2.71	116.36	112.05
3	A	406	CLR	C13-C17-C20	-2.69	115.33	119.50
3	B	405	CLR	C3-C4-C5	2.69	116.34	112.05
3	B	404	CLR	C13-C17-C20	-2.69	115.35	119.50
3	B	404	CLR	C22-C20-C17	-2.66	104.81	110.33
3	B	404	CLR	C11-C12-C13	-2.66	108.25	112.74
3	A	406	CLR	C22-C20-C17	-2.66	104.82	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	406	CLR	C11-C12-C13	-2.65	108.26	112.74
4	A	410	PCF	O14-P-O12	-2.65	100.12	112.44
4	B	409	PCF	O14-P-O12	-2.64	100.17	112.44
3	A	406	CLR	C19-C10-C9	-2.64	108.70	111.66
3	B	404	CLR	C19-C10-C9	-2.63	108.71	111.66
3	B	404	CLR	C15-C14-C13	2.62	106.93	103.84
3	A	405	CLR	C7-C8-C14	-2.61	107.23	110.93
3	A	406	CLR	C15-C14-C13	2.61	106.92	103.84
3	B	403	CLR	C7-C8-C14	-2.61	107.23	110.93
3	B	405	CLR	C18-C13-C12	2.61	114.45	110.61
3	A	407	CLR	C18-C13-C12	2.60	114.43	110.61
3	B	402	CLR	C18-C13-C12	2.59	114.43	110.61
3	A	401	CLR	C7-C8-C14	-2.58	107.27	110.93
3	A	404	CLR	C18-C13-C12	2.58	114.41	110.61
3	B	406	CLR	C7-C8-C14	-2.58	107.28	110.93
3	B	403	CLR	C18-C13-C12	2.57	114.39	110.61
3	A	405	CLR	C18-C13-C12	2.56	114.38	110.61
3	A	405	CLR	C13-C17-C20	-2.56	115.55	119.50
3	B	403	CLR	C13-C17-C20	-2.54	115.57	119.50
3	A	408	CLR	C13-C14-C8	-2.52	110.83	114.41
3	B	401	CLR	C13-C14-C8	-2.50	110.86	114.41
3	B	407	CLR	C18-C13-C12	2.50	114.29	110.61
3	B	401	CLR	C12-C11-C9	2.50	117.38	113.14
3	A	408	CLR	C12-C11-C9	2.49	117.37	113.14
3	A	402	CLR	C18-C13-C12	2.49	114.27	110.61
3	B	408	CLR	C7-C8-C14	-2.49	107.41	110.93
3	A	403	CLR	C7-C8-C14	-2.47	107.43	110.93
3	A	406	CLR	C7-C8-C14	-2.44	107.48	110.93
4	A	409	PCF	O14-P-O12	-2.43	101.12	112.44
4	B	410	PCF	O14-P-O12	-2.42	101.17	112.44
3	A	404	CLR	C21-C20-C17	2.41	116.50	112.88
3	B	404	CLR	C7-C8-C14	-2.41	107.52	110.93
3	B	402	CLR	C21-C20-C17	2.40	116.49	112.88
3	B	406	CLR	C18-C13-C12	2.40	114.14	110.61
3	A	408	CLR	C2-C3-C4	-2.39	106.92	110.29
3	B	401	CLR	C2-C3-C4	-2.39	106.93	110.29
3	A	401	CLR	C18-C13-C12	2.39	114.13	110.61
3	A	407	CLR	C11-C12-C13	-2.38	108.73	112.74
3	B	405	CLR	C7-C8-C14	-2.37	107.57	110.93
3	B	405	CLR	C11-C12-C13	-2.37	108.74	112.74
3	B	407	CLR	C21-C20-C17	2.37	116.44	112.88
3	A	407	CLR	C7-C8-C14	-2.36	107.59	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	CLR	C21-C20-C17	2.36	116.42	112.88
4	B	410	PCF	C11-C12-N	-2.34	108.30	115.82
3	B	401	CLR	C4-C5-C6	-2.34	117.40	120.57
3	A	408	CLR	C4-C5-C6	-2.33	117.41	120.57
4	A	409	PCF	C11-C12-N	-2.33	108.35	115.82
3	B	405	CLR	C10-C9-C8	-2.32	109.32	112.71
3	B	404	CLR	C3-C4-C5	2.32	115.75	112.05
3	A	406	CLR	C3-C4-C5	2.31	115.73	112.05
3	A	407	CLR	C10-C9-C8	-2.31	109.34	112.71
3	A	401	CLR	C19-C10-C9	-2.30	109.07	111.66
3	A	405	CLR	C11-C12-C13	-2.30	108.86	112.74
3	B	406	CLR	C19-C10-C9	-2.30	109.08	111.66
3	B	403	CLR	C11-C12-C13	-2.29	108.87	112.74
3	A	402	CLR	C7-C8-C14	-2.27	107.72	110.93
3	A	404	CLR	C7-C8-C14	-2.27	107.72	110.93
3	B	407	CLR	C7-C8-C14	-2.27	107.72	110.93
3	B	402	CLR	C7-C8-C14	-2.27	107.72	110.93
3	A	407	CLR	C16-C17-C20	-2.26	108.76	112.18
3	B	408	CLR	C19-C10-C9	-2.26	109.13	111.66
3	B	405	CLR	C16-C17-C20	-2.26	108.76	112.18
3	B	404	CLR	C24-C23-C22	-2.24	103.22	113.28
3	A	406	CLR	C24-C23-C22	-2.24	103.23	113.28
4	B	409	PCF	C28-C27-C26	-2.24	103.06	114.37
4	A	410	PCF	C28-C27-C26	-2.23	103.09	114.37
3	A	403	CLR	C19-C10-C9	-2.22	109.17	111.66
3	B	402	CLR	C16-C17-C20	-2.21	108.83	112.18
3	B	404	CLR	C18-C13-C12	2.21	113.86	110.61
3	A	404	CLR	C16-C17-C20	-2.20	108.84	112.18
3	B	401	CLR	C8-C7-C6	-2.20	109.71	112.76
3	A	408	CLR	C8-C7-C6	-2.20	109.72	112.76
3	A	402	CLR	C16-C17-C20	-2.19	108.86	112.18
3	A	405	CLR	C3-C4-C5	2.19	115.54	112.05
3	B	407	CLR	C16-C17-C20	-2.18	108.87	112.18
3	B	406	CLR	C21-C20-C22	-2.18	106.97	110.34
3	B	403	CLR	C3-C4-C5	2.18	115.52	112.05
3	A	406	CLR	C18-C13-C12	2.18	113.81	110.61
3	B	406	CLR	C24-C23-C22	-2.17	103.56	113.28
3	A	401	CLR	C24-C23-C22	-2.17	103.56	113.28
3	A	402	CLR	C19-C10-C9	-2.16	109.23	111.66
3	A	401	CLR	C21-C20-C22	-2.16	106.99	110.34
3	B	407	CLR	C19-C10-C9	-2.16	109.24	111.66
3	A	408	CLR	C16-C15-C14	-2.16	100.92	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	CLR	C16-C15-C14	-2.15	100.94	105.14
3	A	404	CLR	C3-C4-C5	2.13	115.45	112.05
3	B	402	CLR	C3-C4-C5	2.13	115.44	112.05
3	A	403	CLR	C24-C23-C22	-2.12	103.80	113.28
3	B	408	CLR	C24-C23-C22	-2.12	103.80	113.28
3	A	402	CLR	C21-C20-C22	-2.11	107.07	110.34
3	B	407	CLR	C21-C20-C22	-2.11	107.07	110.34
3	A	403	CLR	C18-C13-C12	2.11	113.71	110.61
3	B	408	CLR	C18-C13-C12	2.10	113.70	110.61
3	B	407	CLR	C10-C5-C6	2.10	125.99	122.93
3	A	403	CLR	C15-C14-C8	-2.10	115.76	119.10
3	B	408	CLR	C15-C14-C8	-2.09	115.76	119.10
3	B	407	CLR	C24-C23-C22	-2.09	103.93	113.28
3	B	406	CLR	C2-C3-C4	-2.08	107.36	110.29
3	A	401	CLR	C2-C3-C4	-2.08	107.36	110.29
3	A	402	CLR	C24-C23-C22	-2.08	103.96	113.28
3	A	402	CLR	C10-C5-C6	2.07	125.95	122.93
3	B	407	CLR	C3-C4-C5	2.05	115.31	112.05
3	A	402	CLR	C3-C4-C5	2.04	115.31	112.05
3	A	404	CLR	C15-C14-C13	2.04	106.24	103.84
3	B	402	CLR	C15-C14-C13	2.02	106.22	103.84
4	A	410	PCF	O31-C31-O32	-2.02	118.57	123.63
3	B	405	CLR	C21-C20-C17	2.01	115.90	112.88
3	A	407	CLR	C21-C20-C17	2.01	115.90	112.88
4	B	409	PCF	O31-C31-O32	-2.01	118.61	123.63

There are no chirality outliers.

All (160) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	404	CLR	C13-C17-C20-C21
3	B	408	CLR	C13-C17-C20-C22
3	A	403	CLR	C13-C17-C20-C22
3	A	406	CLR	C13-C17-C20-C21
4	B	409	PCF	O13-C11-C12-N
4	B	409	PCF	O32-C31-O31-C3
4	B	409	PCF	C32-C31-O31-C3
4	B	409	PCF	O22-C21-O21-C2
4	B	410	PCF	O13-C11-C12-N
4	B	410	PCF	O22-C21-O21-C2
4	A	409	PCF	O13-C11-C12-N
4	A	409	PCF	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
4	A	410	PCF	O13-C11-C12-N
4	A	410	PCF	O32-C31-O31-C3
4	A	410	PCF	C32-C31-O31-C3
4	A	410	PCF	O22-C21-O21-C2
3	B	404	CLR	C16-C17-C20-C21
3	A	406	CLR	C16-C17-C20-C21
3	B	404	CLR	C13-C17-C20-C22
3	A	406	CLR	C13-C17-C20-C22
4	B	409	PCF	C22-C21-O21-C2
4	B	410	PCF	C22-C21-O21-C2
4	A	409	PCF	C22-C21-O21-C2
4	A	410	PCF	C22-C21-O21-C2
3	B	404	CLR	C16-C17-C20-C22
3	A	406	CLR	C16-C17-C20-C22
3	B	408	CLR	C16-C17-C20-C22
3	A	403	CLR	C16-C17-C20-C22
3	B	402	CLR	C21-C20-C22-C23
3	A	404	CLR	C21-C20-C22-C23
3	B	404	CLR	C21-C20-C22-C23
3	B	408	CLR	C21-C20-C22-C23
3	A	403	CLR	C21-C20-C22-C23
3	A	406	CLR	C21-C20-C22-C23
3	B	404	CLR	C17-C20-C22-C23
3	B	408	CLR	C17-C20-C22-C23
3	A	403	CLR	C17-C20-C22-C23
3	A	406	CLR	C17-C20-C22-C23
3	B	405	CLR	C21-C20-C22-C23
3	A	407	CLR	C21-C20-C22-C23
4	B	409	PCF	C37-C38-C39-C40
4	A	410	PCF	C37-C38-C39-C40
3	B	408	CLR	C16-C17-C20-C21
3	A	403	CLR	C16-C17-C20-C21
3	B	401	CLR	C13-C17-C20-C22
3	A	408	CLR	C13-C17-C20-C22
4	B	409	PCF	C41-C42-C43-C44
4	A	410	PCF	C41-C42-C43-C44
4	B	409	PCF	C24-C25-C26-C27
4	A	410	PCF	C24-C25-C26-C27
3	B	401	CLR	C13-C17-C20-C21
3	A	408	CLR	C13-C17-C20-C21
3	B	401	CLR	C16-C17-C20-C21
3	A	408	CLR	C16-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
4	B	410	PCF	C33-C34-C35-C36
4	B	409	PCF	C27-C28-C29-C30
4	A	409	PCF	C33-C34-C35-C36
4	A	410	PCF	C27-C28-C29-C30
4	B	409	PCF	C34-C35-C36-C37
4	A	410	PCF	C34-C35-C36-C37
4	B	409	PCF	C33-C34-C35-C36
4	A	410	PCF	C33-C34-C35-C36
4	A	410	PCF	C30-C47-C48-C49
4	B	409	PCF	C30-C47-C48-C49
4	B	409	PCF	C40-C41-C42-C43
4	A	410	PCF	C40-C41-C42-C43
3	B	402	CLR	C20-C22-C23-C24
3	A	404	CLR	C20-C22-C23-C24
4	B	409	PCF	C21-C22-C23-C24
4	A	410	PCF	C21-C22-C23-C24
4	B	409	PCF	C1-C2-C3-O31
4	B	410	PCF	C1-C2-C3-O31
4	A	409	PCF	C1-C2-C3-O31
4	A	410	PCF	C1-C2-C3-O31
3	B	407	CLR	C21-C20-C22-C23
3	A	402	CLR	C21-C20-C22-C23
3	B	407	CLR	C17-C20-C22-C23
4	B	410	PCF	C40-C41-C42-C43
3	A	402	CLR	C17-C20-C22-C23
4	A	409	PCF	C40-C41-C42-C43
4	B	409	PCF	O11-C1-C2-O21
4	A	410	PCF	O11-C1-C2-O21
4	B	410	PCF	C32-C33-C34-C35
4	A	409	PCF	C32-C33-C34-C35
3	B	406	CLR	C21-C20-C22-C23
3	A	401	CLR	C21-C20-C22-C23
3	B	401	CLR	C16-C17-C20-C22
3	A	408	CLR	C16-C17-C20-C22
4	A	410	PCF	C47-C48-C49-C50
3	B	406	CLR	C17-C20-C22-C23
3	A	401	CLR	C17-C20-C22-C23
4	B	409	PCF	C47-C48-C49-C50
4	A	410	PCF	C35-C36-C37-C38
4	B	409	PCF	C35-C36-C37-C38
4	B	409	PCF	C49-C50-C51-C52
4	A	410	PCF	C49-C50-C51-C52

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Mol	Chain	Res	Type	Atoms
4	B	410	PCF	C34-C35-C36-C37
4	A	409	PCF	C34-C35-C36-C37
4	B	410	PCF	C2-C1-O11-P
4	A	409	PCF	C2-C1-O11-P
3	B	401	CLR	C22-C23-C24-C25
3	A	408	CLR	C22-C23-C24-C25
4	B	409	PCF	O21-C2-C3-O31
4	B	410	PCF	O21-C2-C3-O31
4	A	409	PCF	O21-C2-C3-O31
4	A	410	PCF	O21-C2-C3-O31
4	A	410	PCF	C29-C30-C47-C48
4	B	409	PCF	C29-C30-C47-C48
4	B	409	PCF	O11-C1-C2-C3
4	A	410	PCF	O11-C1-C2-C3
3	B	403	CLR	C20-C22-C23-C24
3	A	405	CLR	C20-C22-C23-C24
4	B	409	PCF	C12-C11-O13-P
4	A	410	PCF	C12-C11-O13-P
3	B	408	CLR	C13-C17-C20-C21
3	A	403	CLR	C13-C17-C20-C21
4	B	410	PCF	O11-C1-C2-C3
4	A	409	PCF	O11-C1-C2-C3
4	A	410	PCF	C48-C49-C50-C51
4	B	410	PCF	O11-C1-C2-O21
4	A	409	PCF	O11-C1-C2-O21
4	B	409	PCF	C48-C49-C50-C51
4	A	409	PCF	C35-C36-C37-C38
4	A	410	PCF	C22-C23-C24-C25
4	B	410	PCF	C35-C36-C37-C38
4	B	409	PCF	C22-C23-C24-C25
4	B	409	PCF	C1-O11-P-O12
4	B	409	PCF	C11-O13-P-O12
4	B	410	PCF	C1-O11-P-O12
4	B	410	PCF	C1-O11-P-O13
4	B	410	PCF	C1-O11-P-O14
4	A	409	PCF	C1-O11-P-O12
4	A	409	PCF	C1-O11-P-O13
4	A	409	PCF	C1-O11-P-O14
4	A	410	PCF	C1-O11-P-O12
4	A	410	PCF	C11-O13-P-O12
4	B	409	PCF	C2-C1-O11-P
4	A	410	PCF	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
4	B	409	PCF	C1-C2-O21-C21
4	B	410	PCF	C1-C2-O21-C21
4	A	409	PCF	C1-C2-O21-C21
4	A	410	PCF	C1-C2-O21-C21
4	B	410	PCF	C49-C50-C51-C52
4	A	409	PCF	C49-C50-C51-C52
3	B	405	CLR	C13-C17-C20-C21
3	A	407	CLR	C13-C17-C20-C21
4	B	410	PCF	C48-C49-C50-C51
4	A	409	PCF	C48-C49-C50-C51
4	B	409	PCF	O21-C21-C22-C23
4	A	410	PCF	O21-C21-C22-C23
3	B	401	CLR	C20-C22-C23-C24
3	A	408	CLR	C20-C22-C23-C24
4	B	410	PCF	C47-C48-C49-C50
4	A	409	PCF	C47-C48-C49-C50
4	A	409	PCF	C23-C24-C25-C26
4	B	410	PCF	C23-C24-C25-C26
4	B	409	PCF	O22-C21-C22-C23
4	A	410	PCF	O22-C21-C22-C23
4	A	410	PCF	C32-C33-C34-C35
4	B	409	PCF	C32-C33-C34-C35

There are no ring outliers.

20 monomers are involved in 303 short contacts:

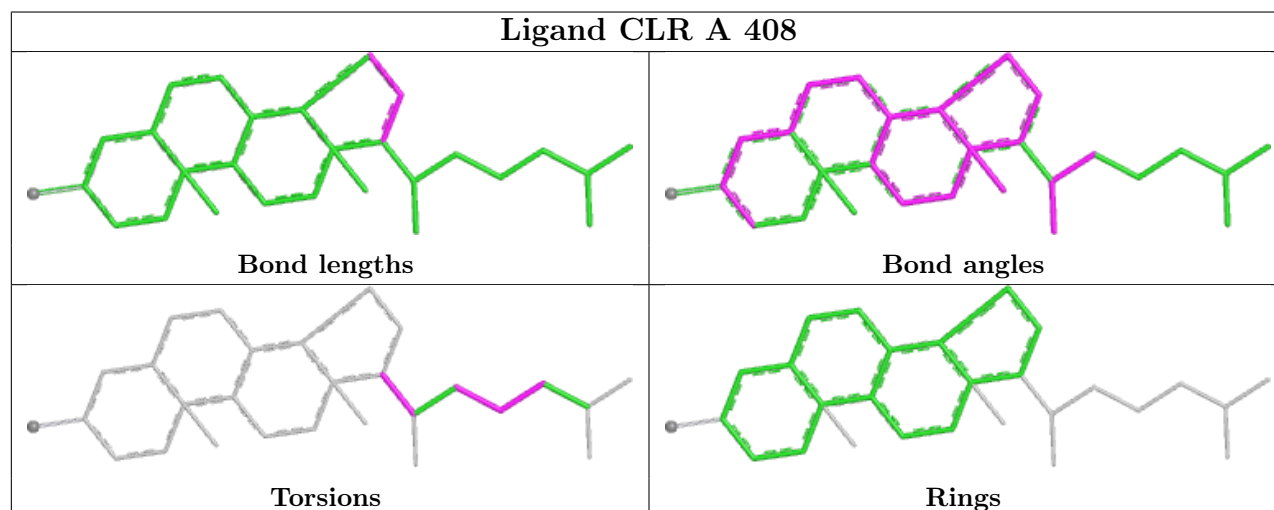
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	408	CLR	29	0
3	A	405	CLR	37	0
3	A	403	CLR	21	0
3	A	406	CLR	17	0
4	B	410	PCF	60	0
3	A	404	CLR	10	0
4	B	409	PCF	9	0
4	A	410	PCF	9	0
3	B	407	CLR	1	0
3	A	407	CLR	19	0
3	B	406	CLR	10	0
3	A	402	CLR	2	0
3	B	404	CLR	15	0
3	B	403	CLR	37	0
3	B	401	CLR	30	0

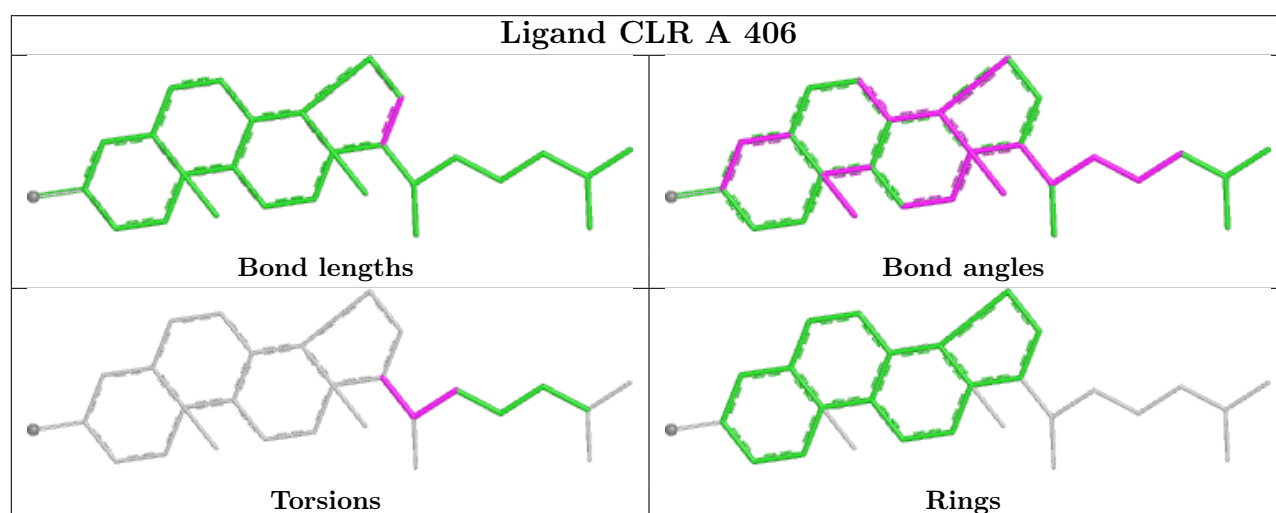
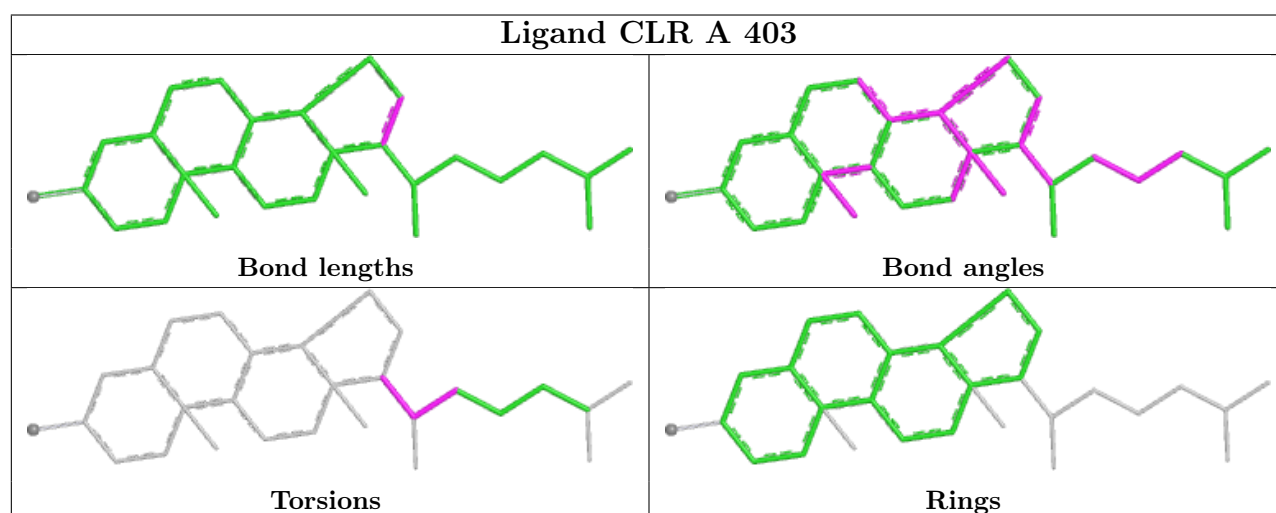
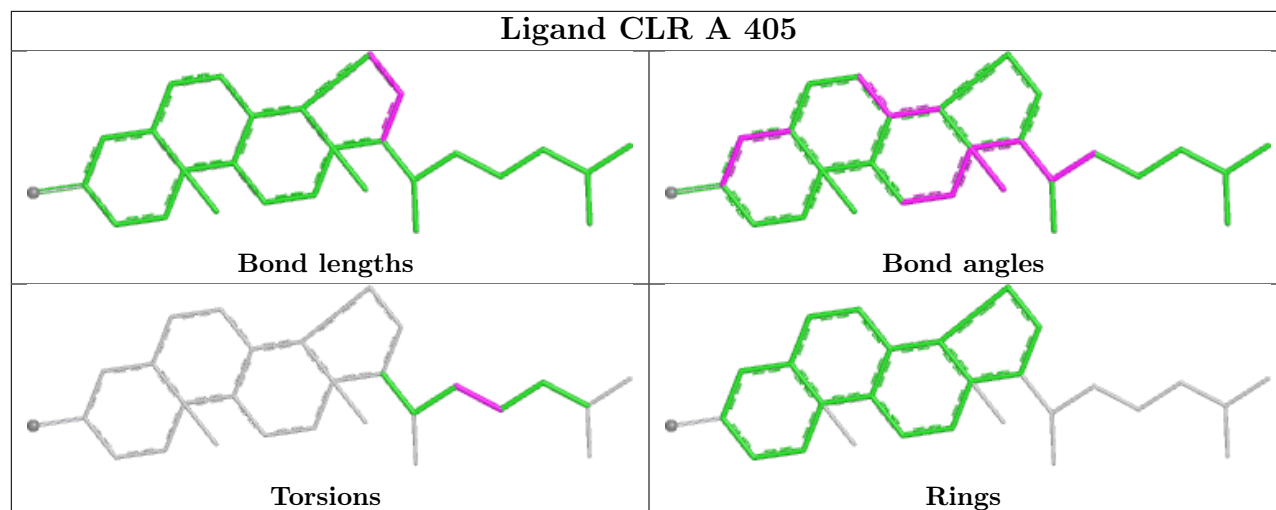
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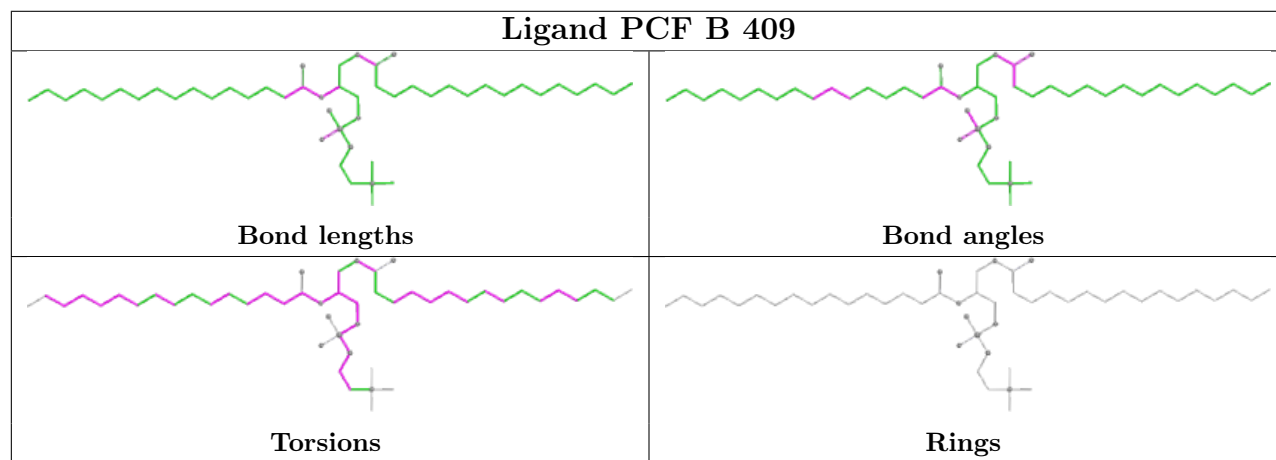
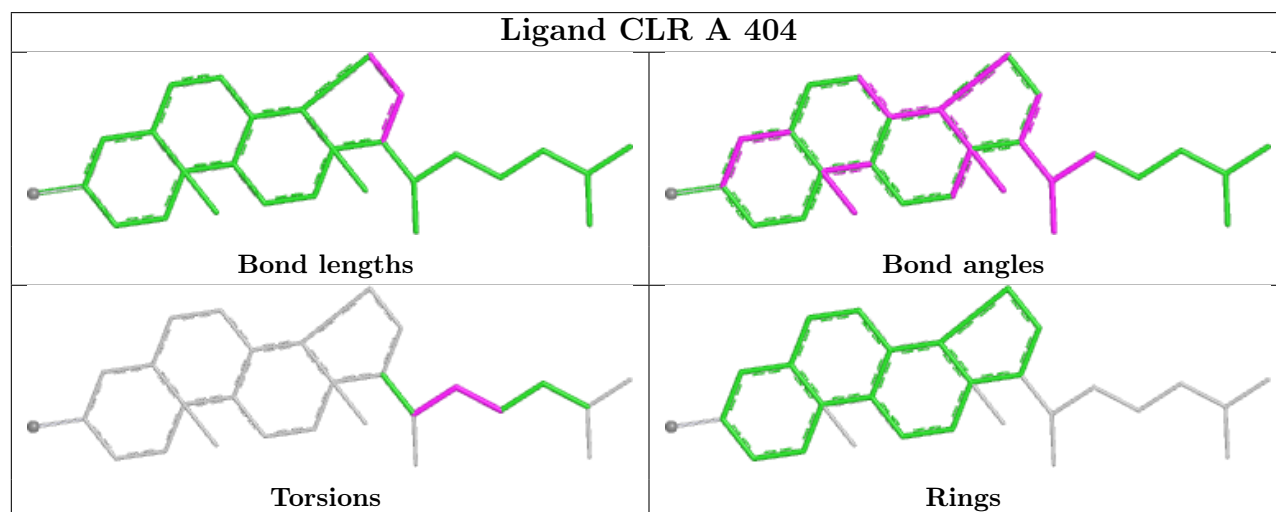
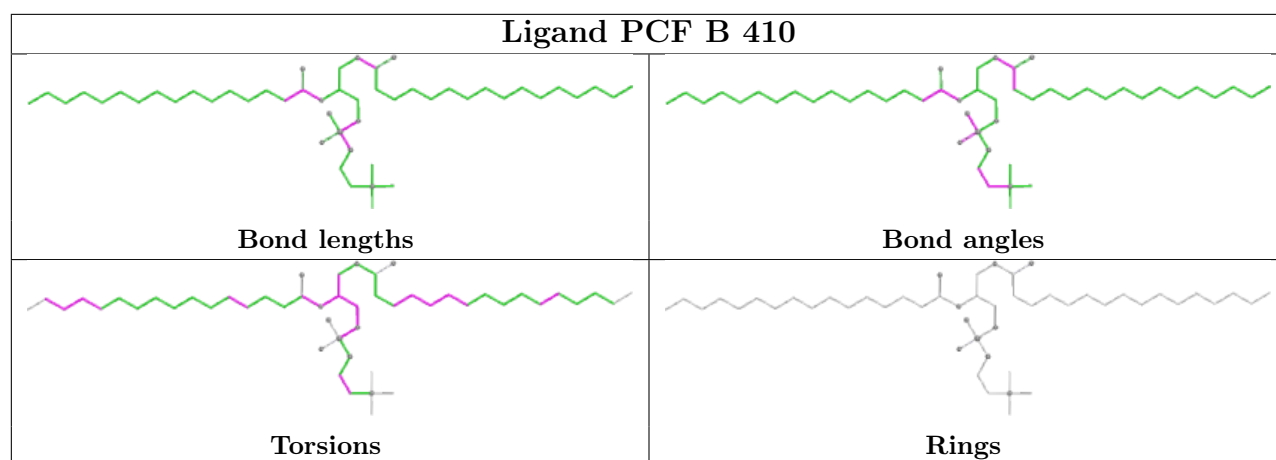
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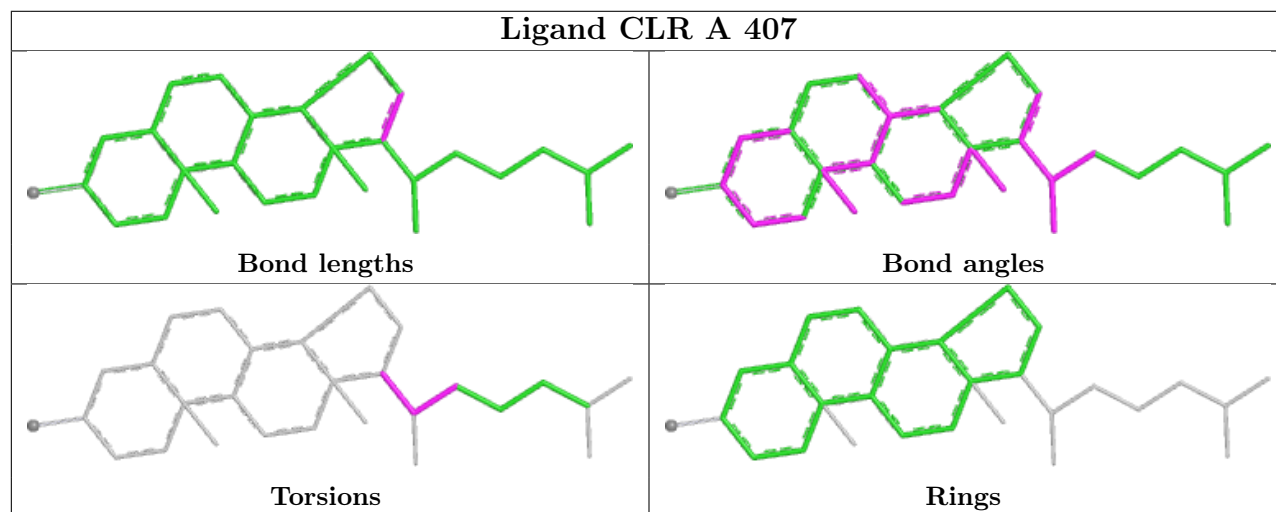
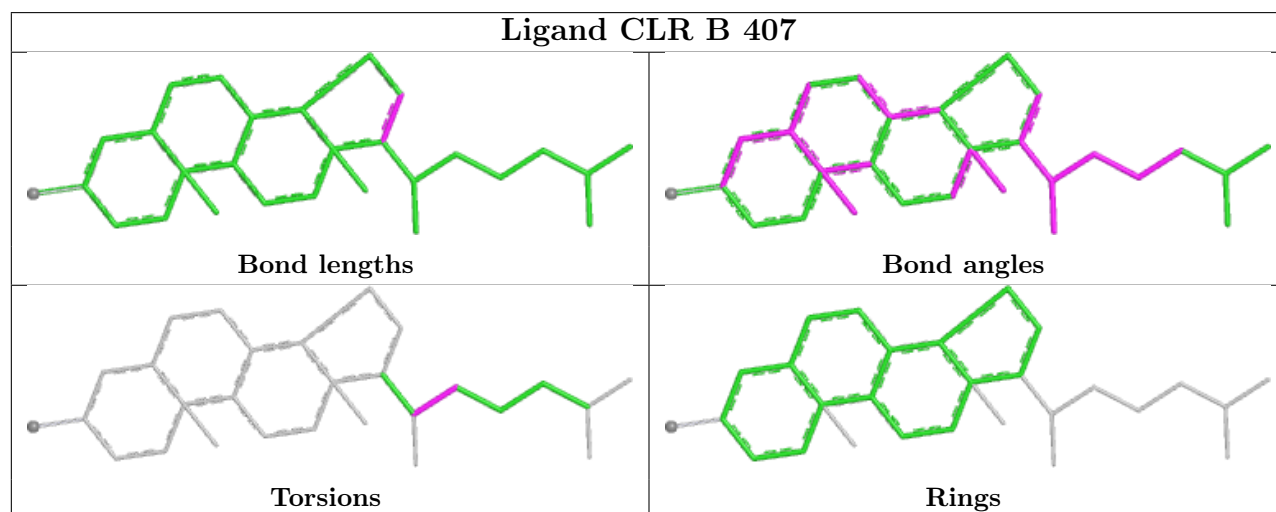
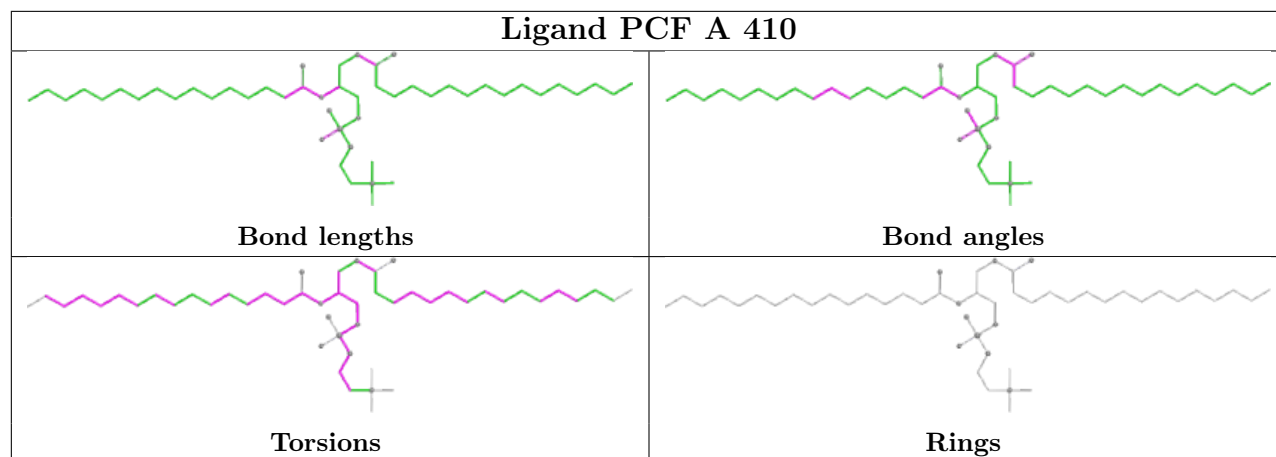
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	405	CLR	19	0
3	B	402	CLR	11	0
3	B	408	CLR	22	0
4	A	409	PCF	61	0
3	A	401	CLR	10	0

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

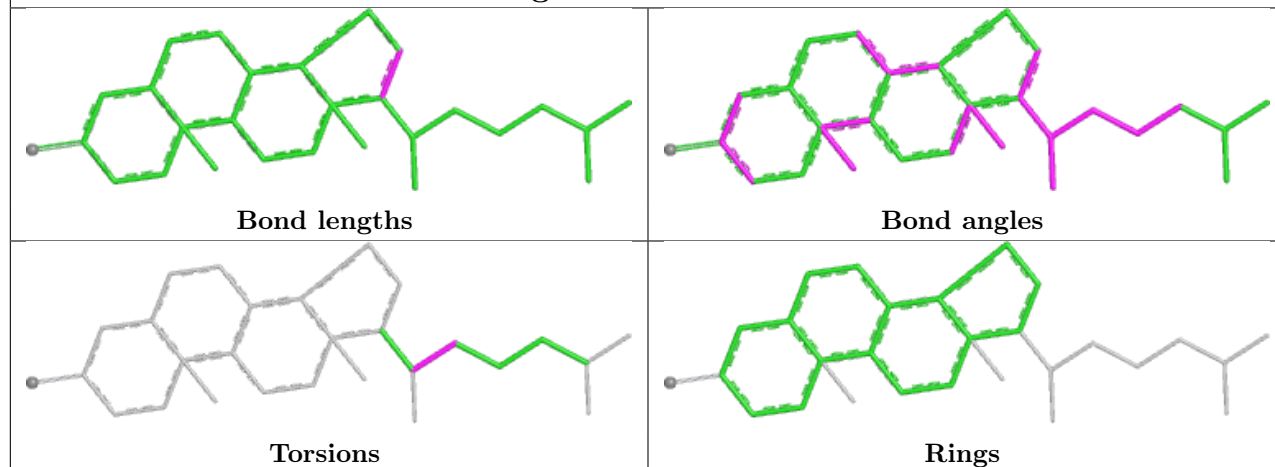




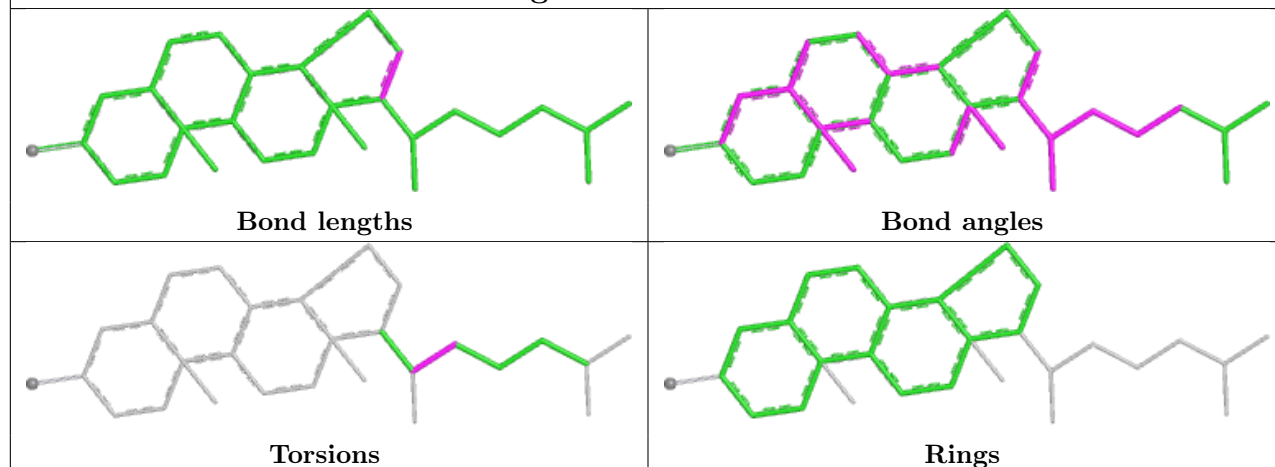




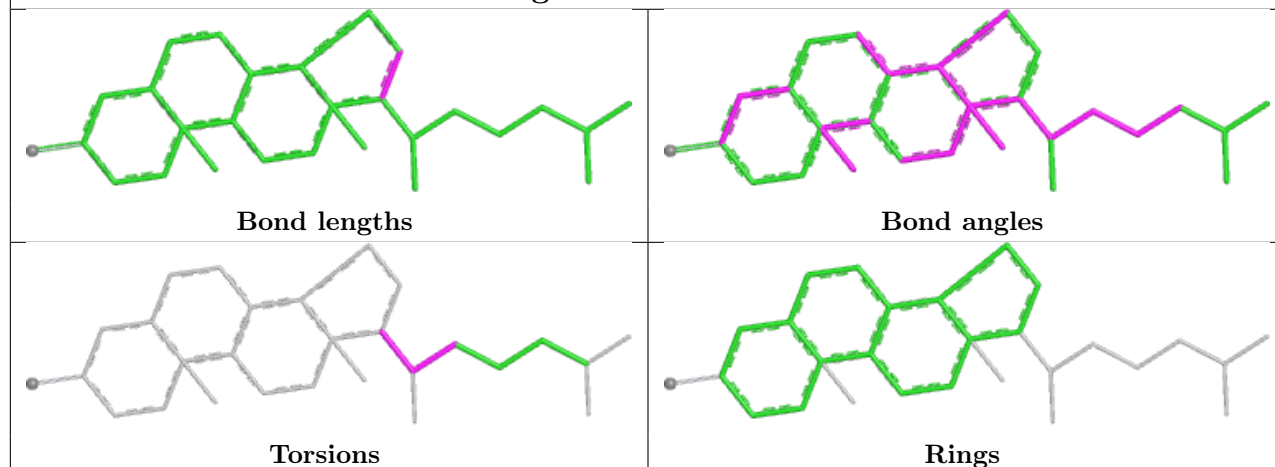
Ligand CLR B 406

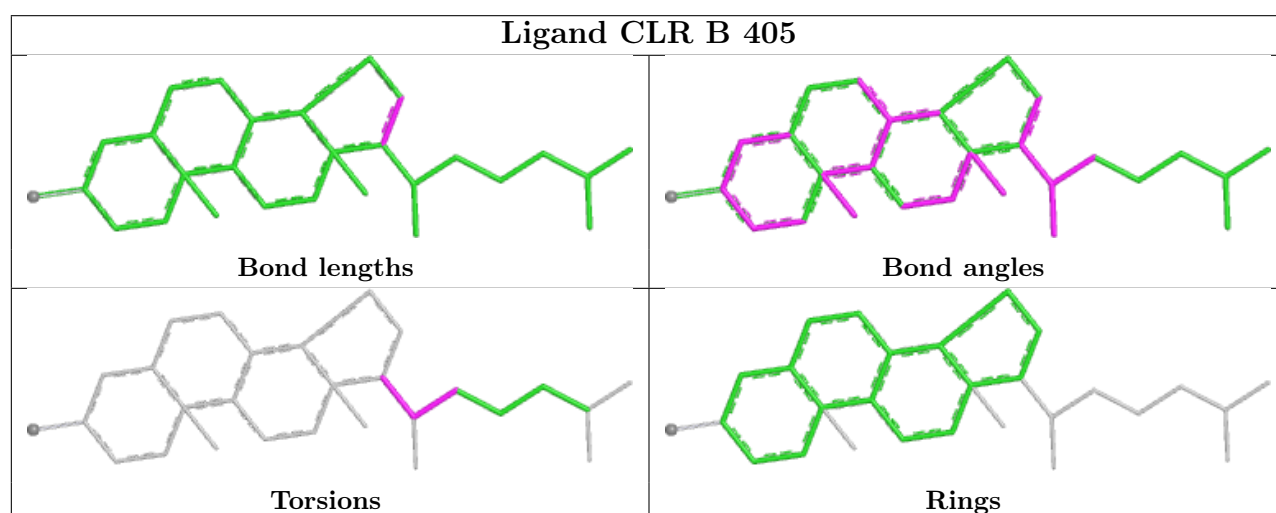
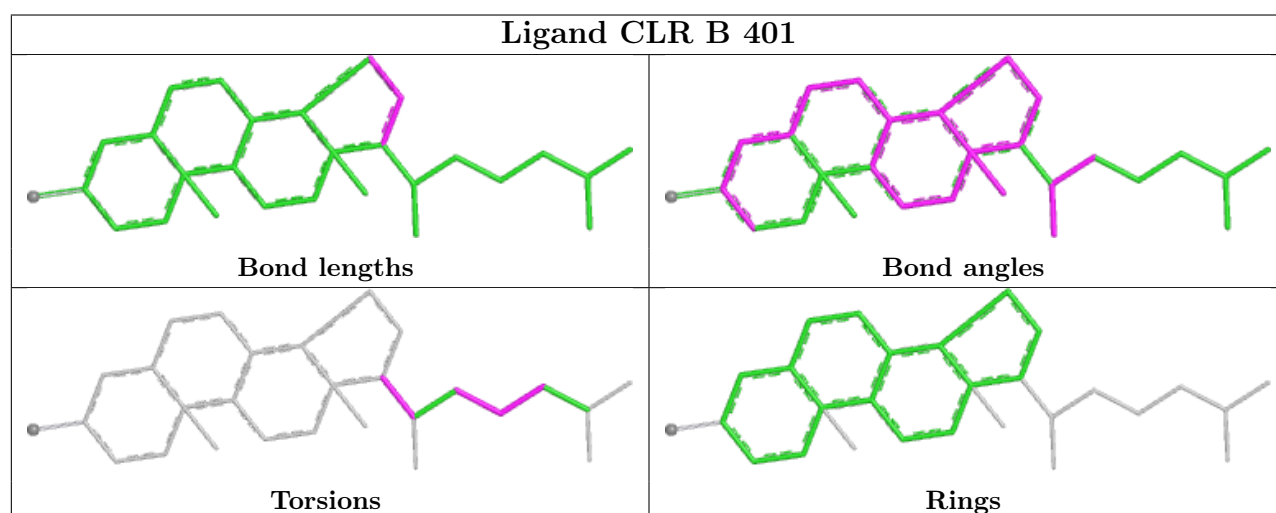
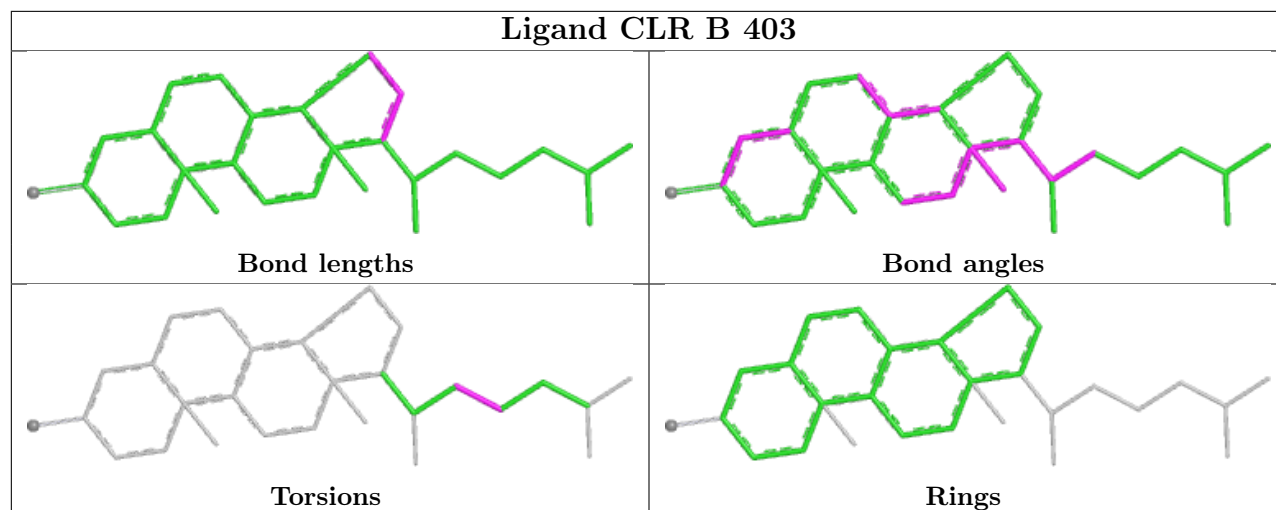


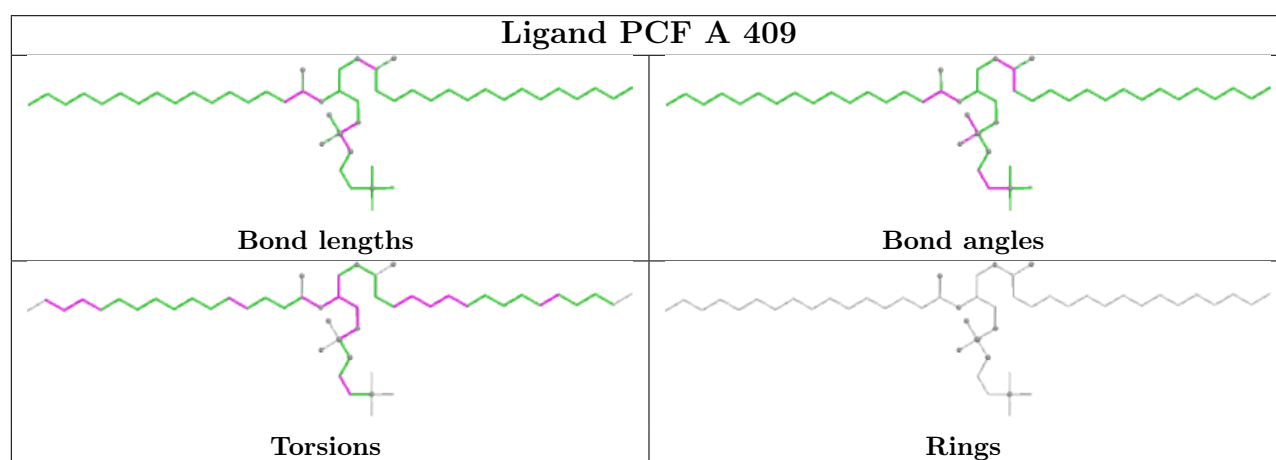
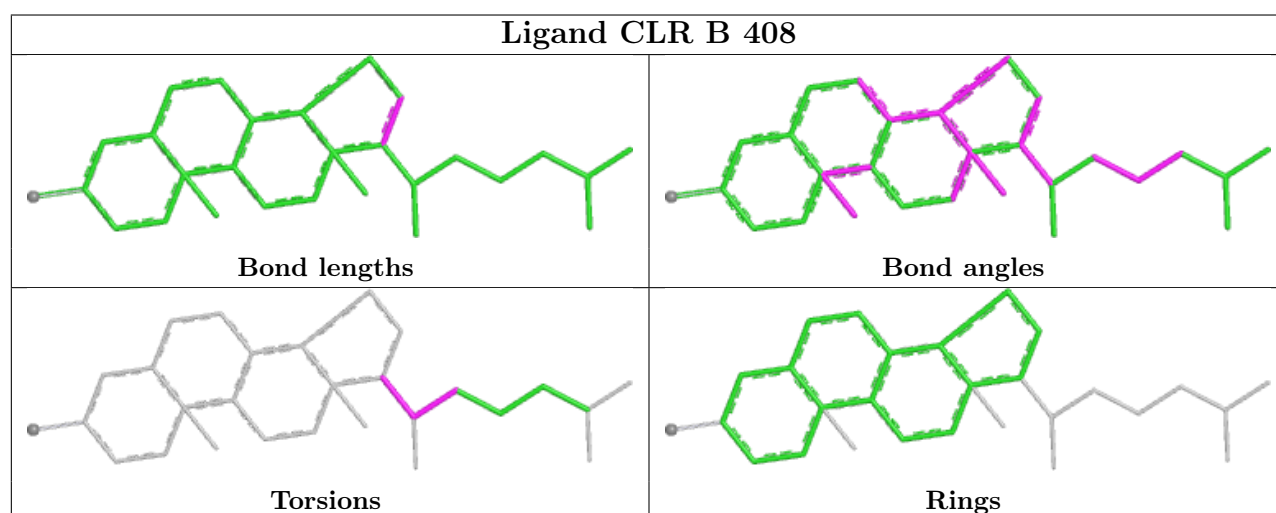
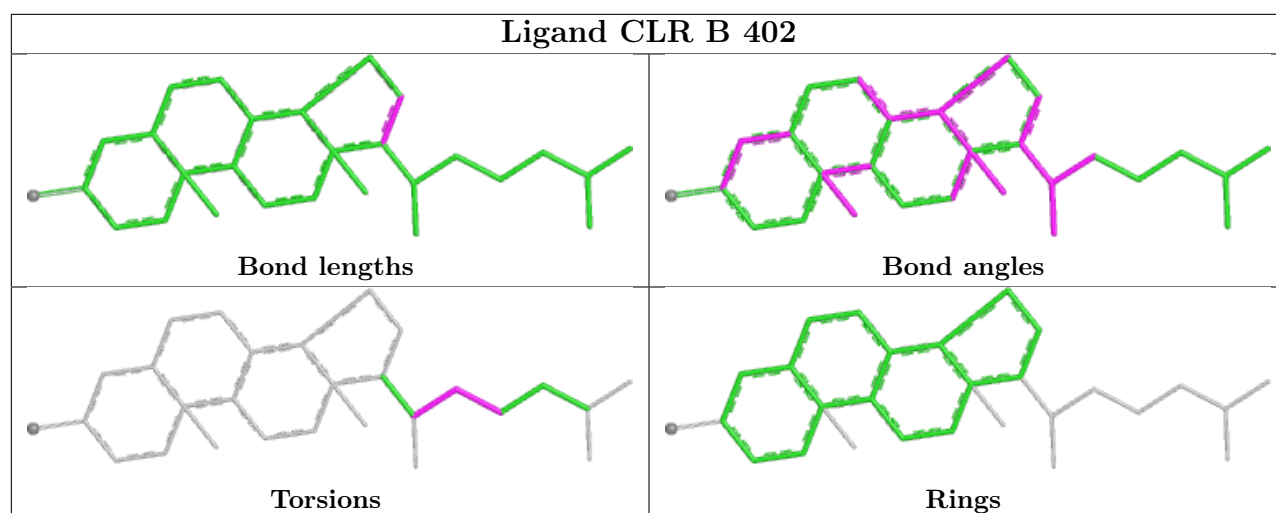
Ligand CLR A 402

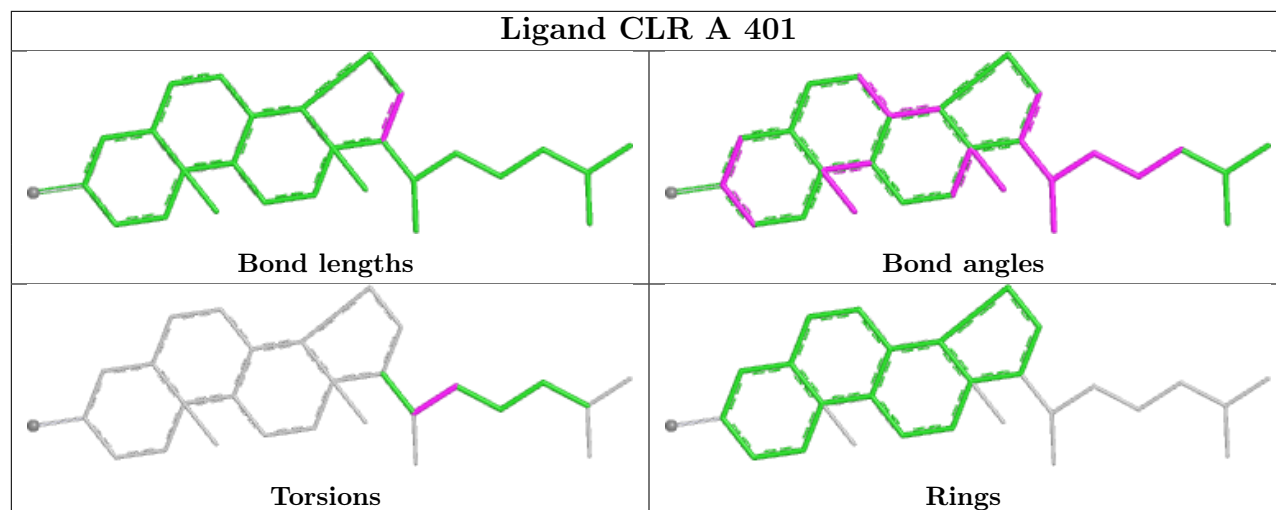


Ligand CLR B 404









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.

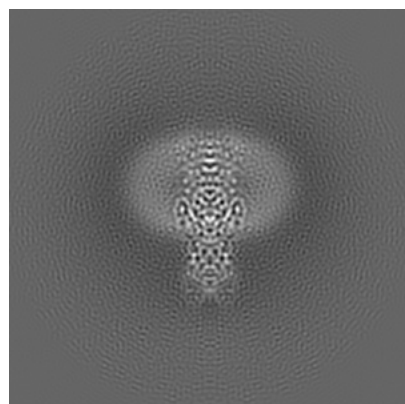
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63305. These allow visual inspection of the internal detail of the map and identification of artifacts.

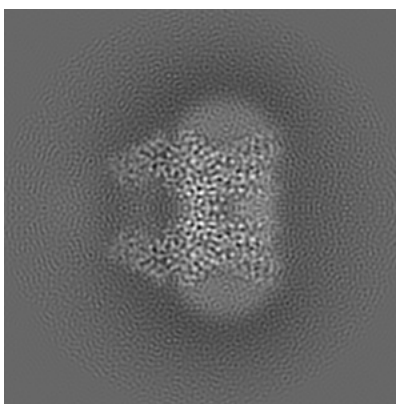
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

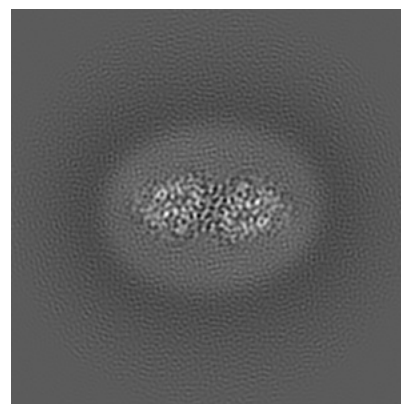
6.1.1 Primary map



X

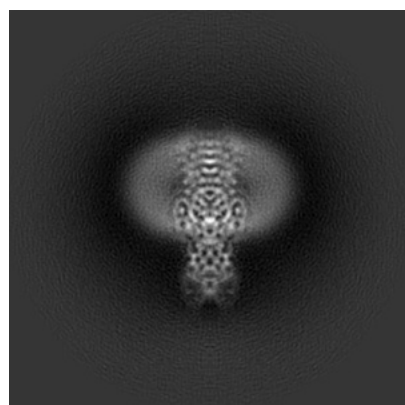


Y

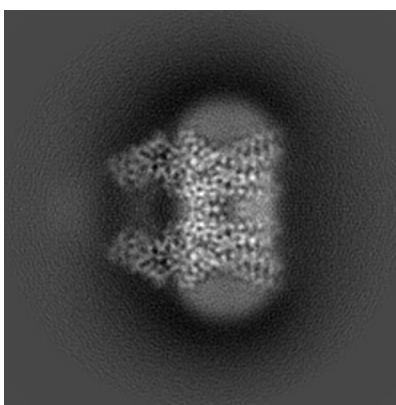


Z

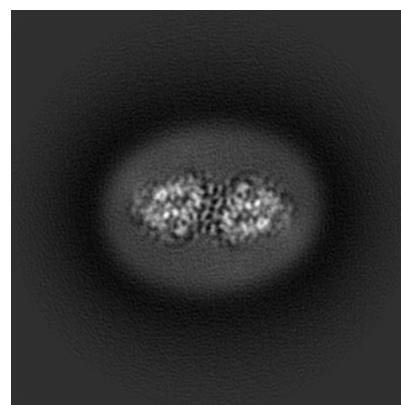
6.1.2 Raw map



X



Y

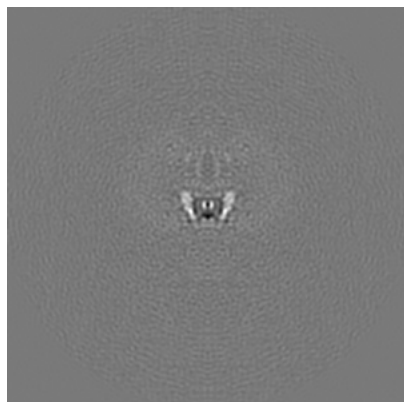


Z

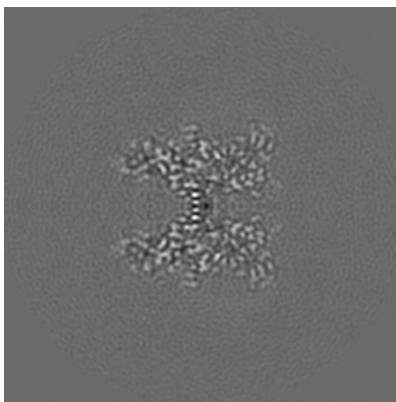
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

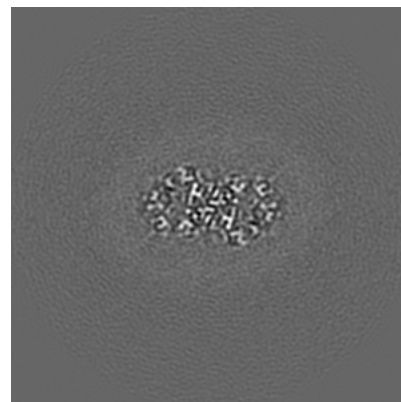
6.2.1 Primary map



X Index: 112

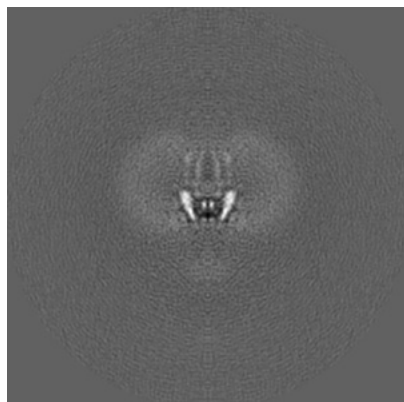


Y Index: 112

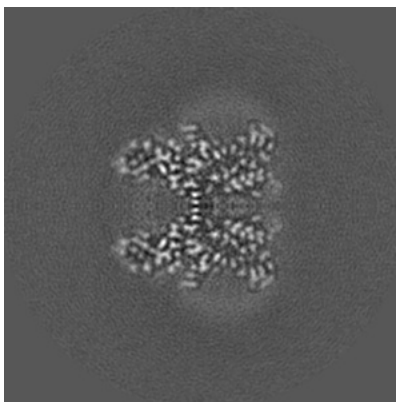


Z Index: 112

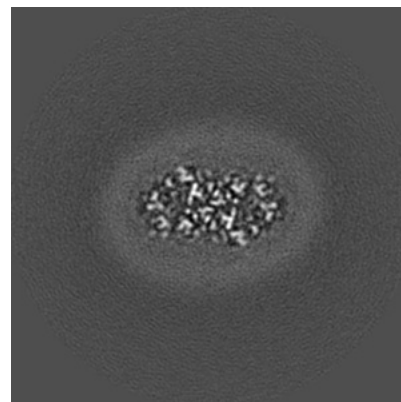
6.2.2 Raw map



X Index: 112



Y Index: 112

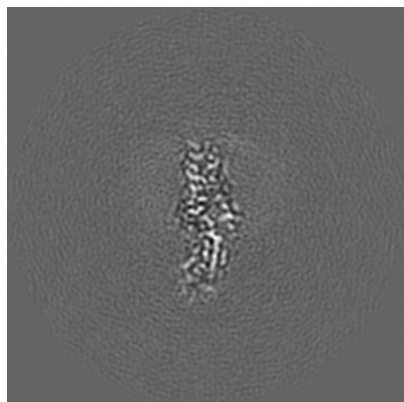


Z Index: 112

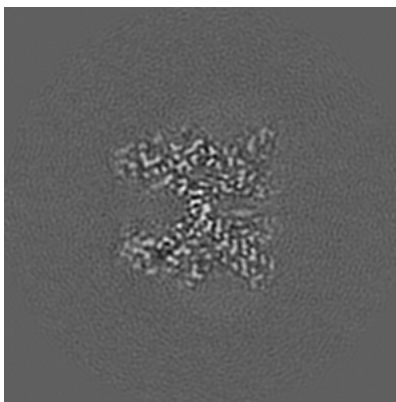
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

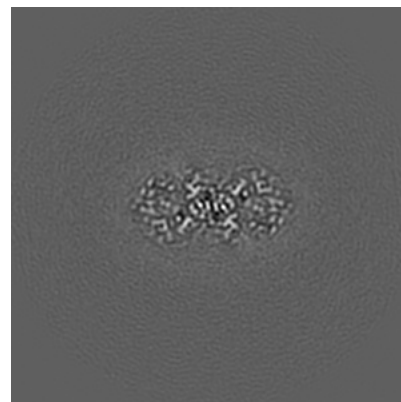
6.3.1 Primary map



X Index: 138

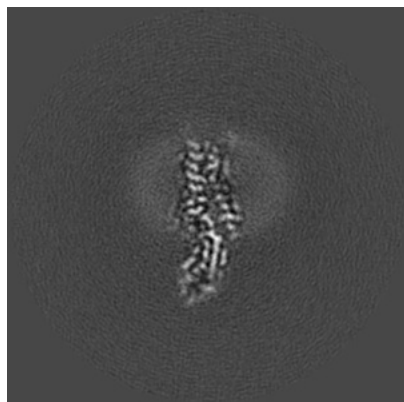


Y Index: 110

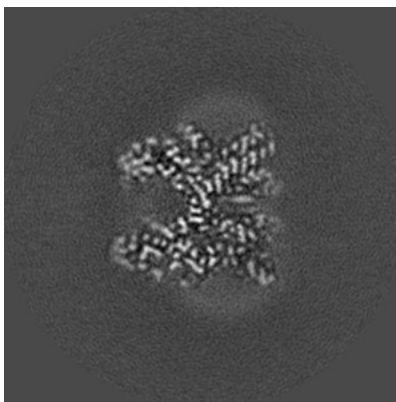


Z Index: 107

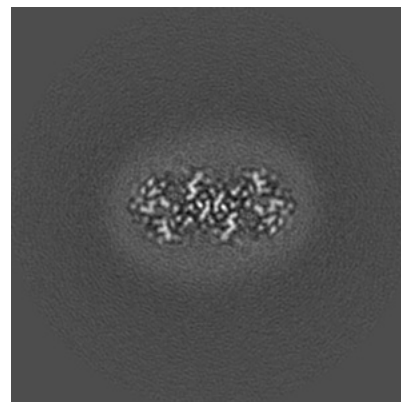
6.3.2 Raw map



X Index: 138



Y Index: 114

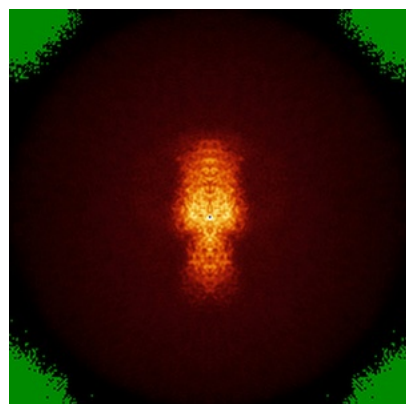


Z Index: 106

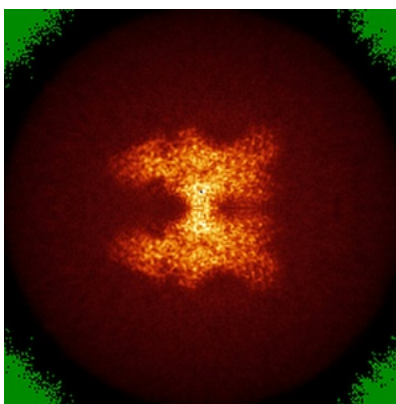
The images above show the largest variance slices of the map in three orthogonal directions.

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

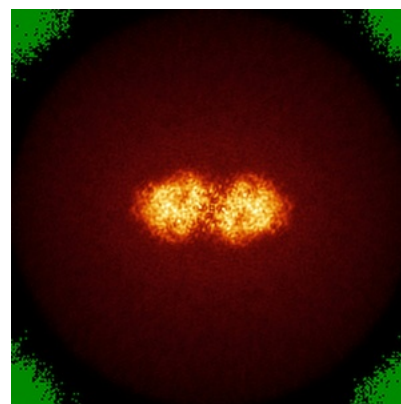
6.4.1 Primary map



X

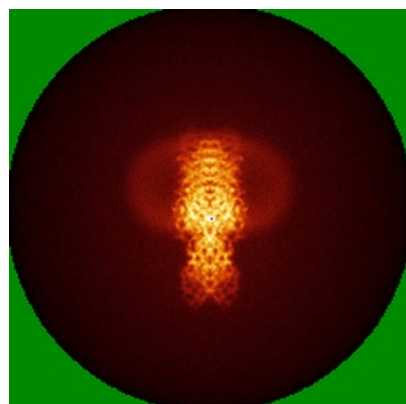


Y

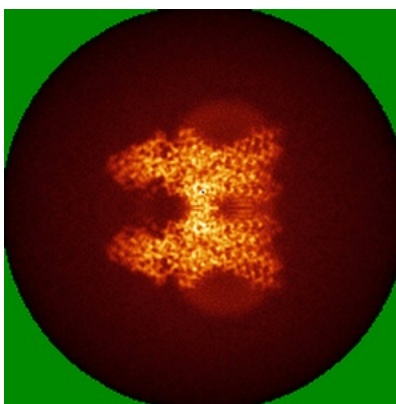


Z

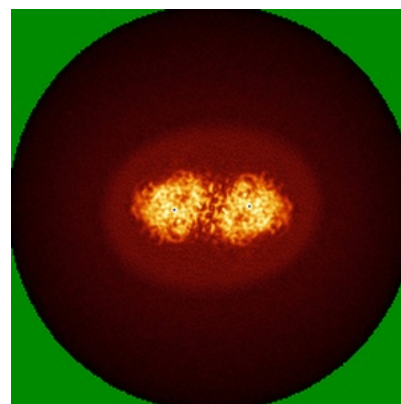
6.4.2 Raw map



X



Y

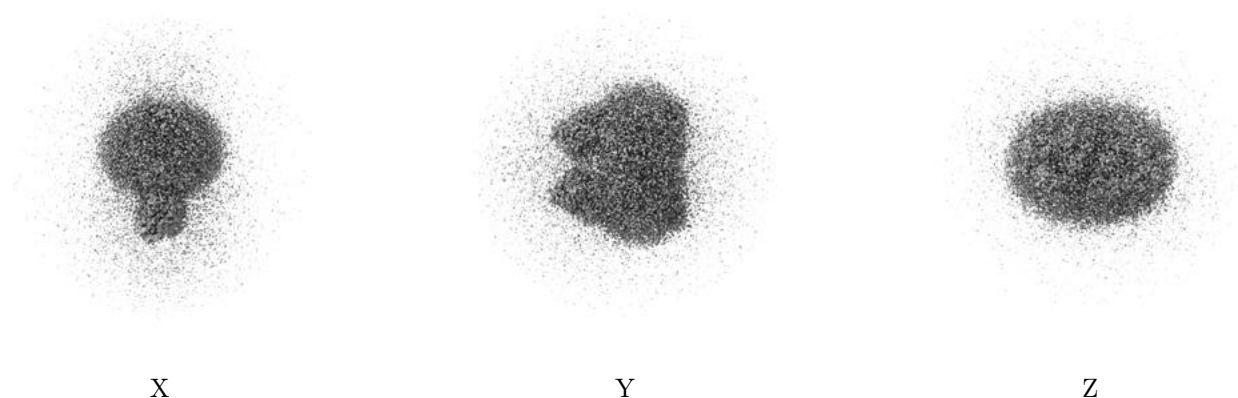


Z

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

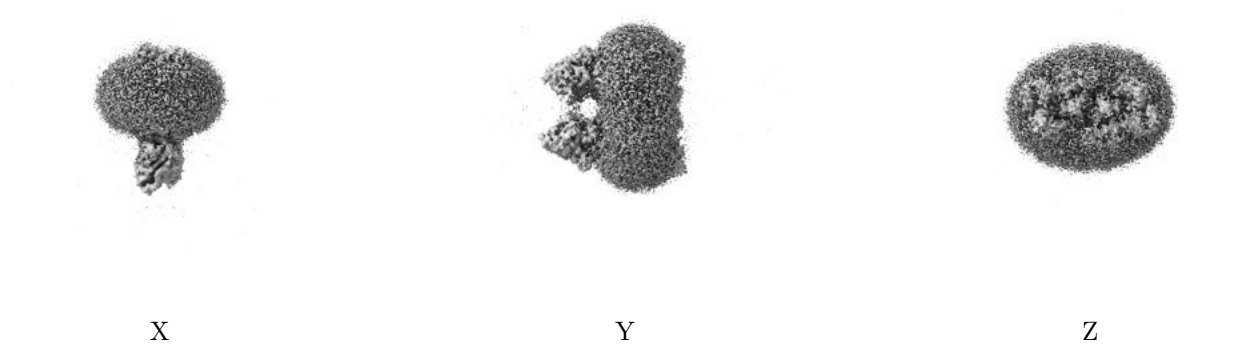
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

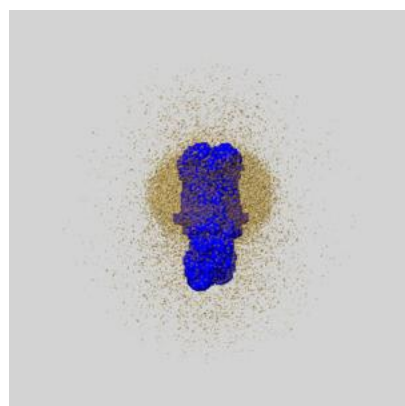
6.6 Mask visualisation [i](#)

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

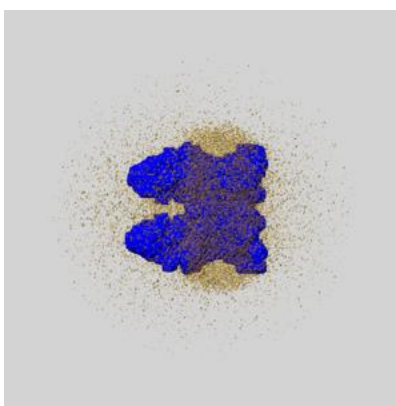
A mask typically either:

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

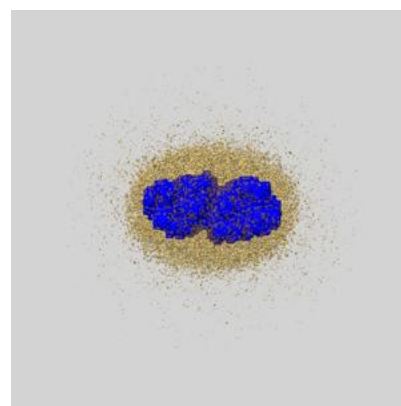
6.6.1 emd_63305_msk_1.map [i](#)



X



Y

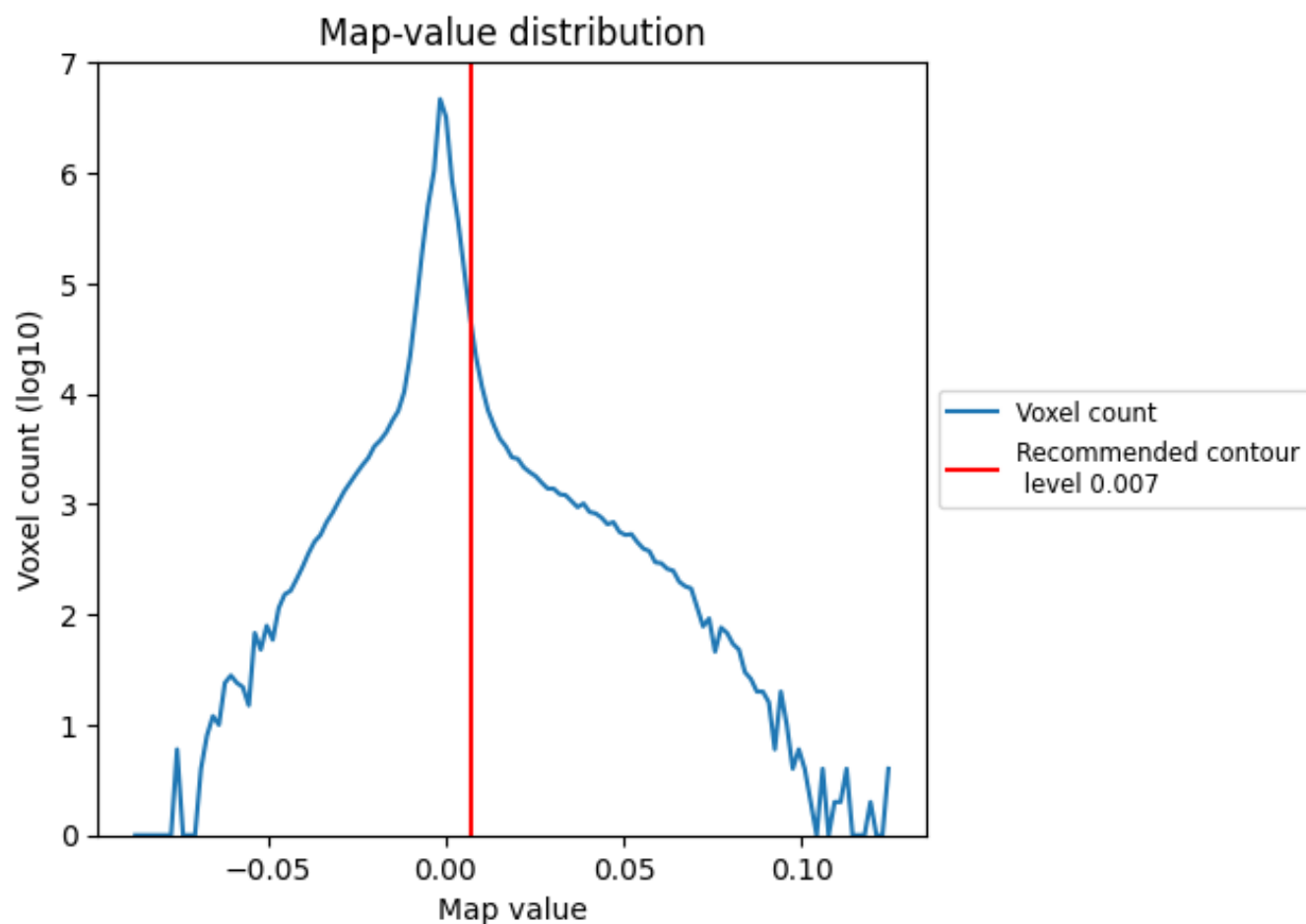


Z

7 Map analysis [i](#)

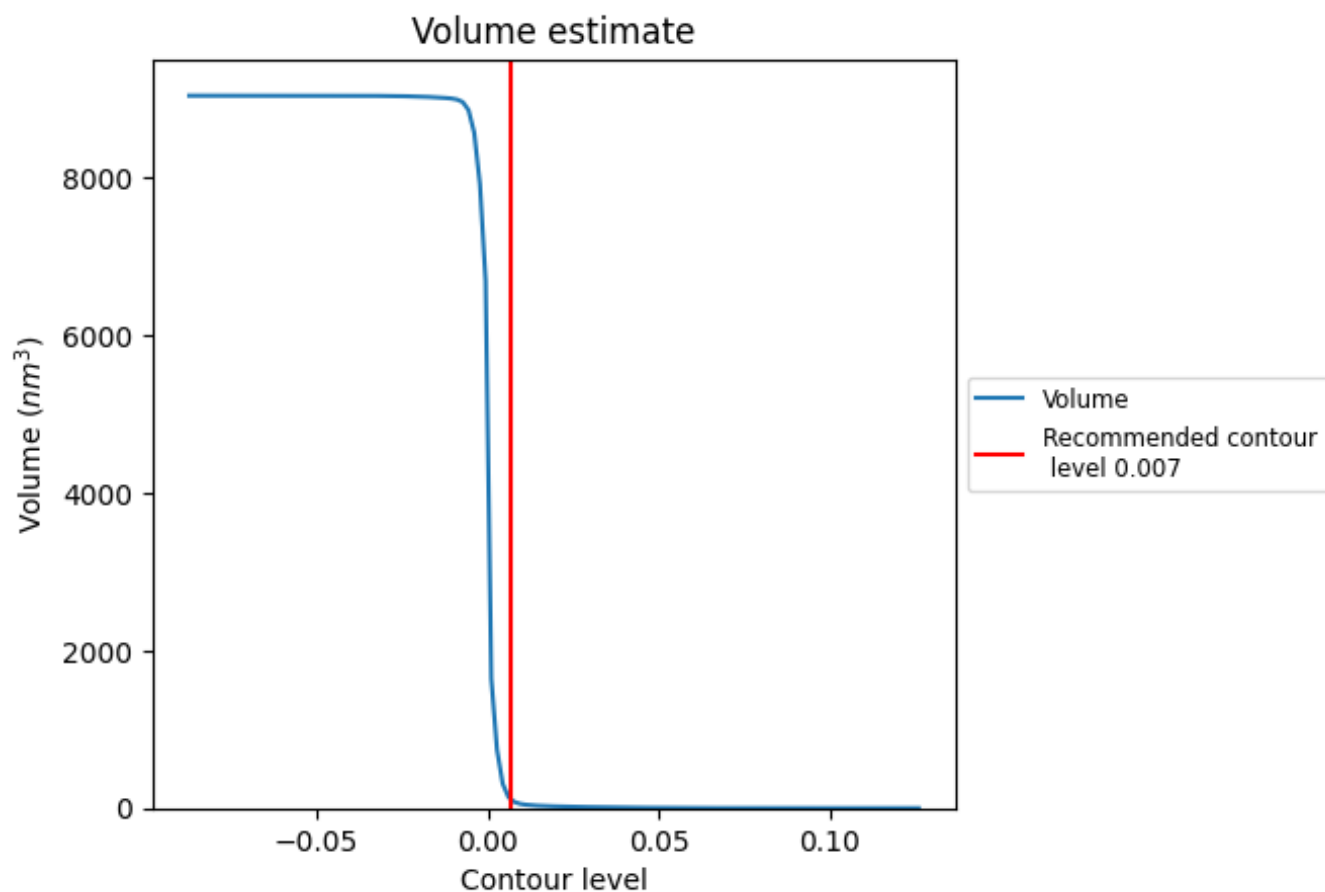
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

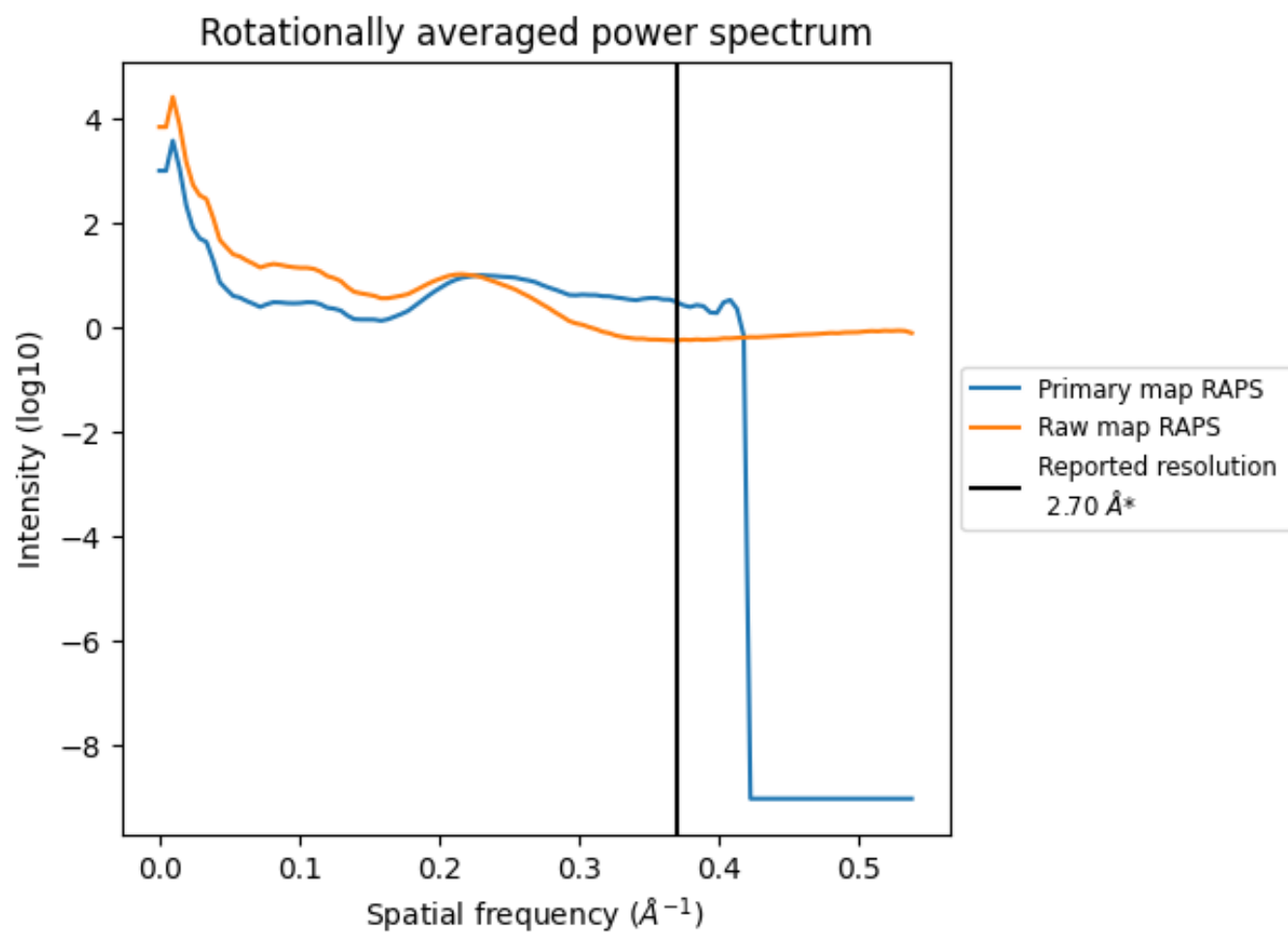
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 108 nm^3 ; this corresponds to an approximate mass of 98 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 ⓘ

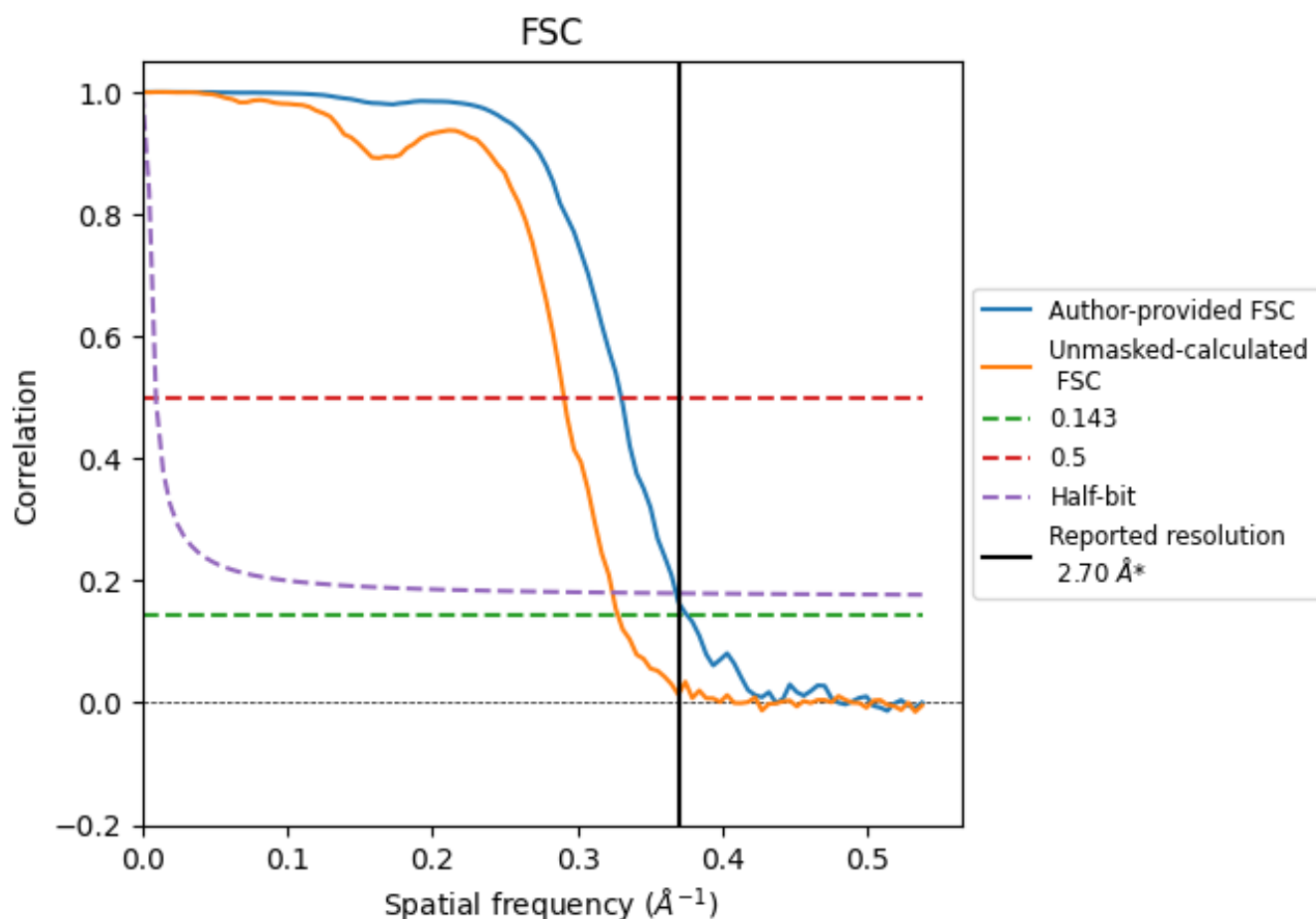


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

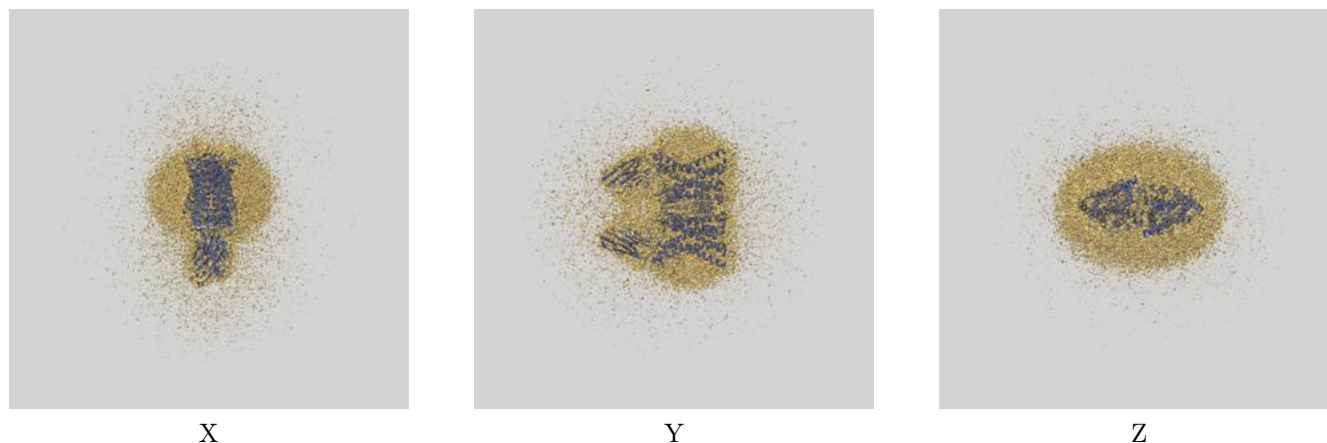
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.66	3.03	2.72
Unmasked-calculated*	3.05	3.44	3.08

*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 3.05 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

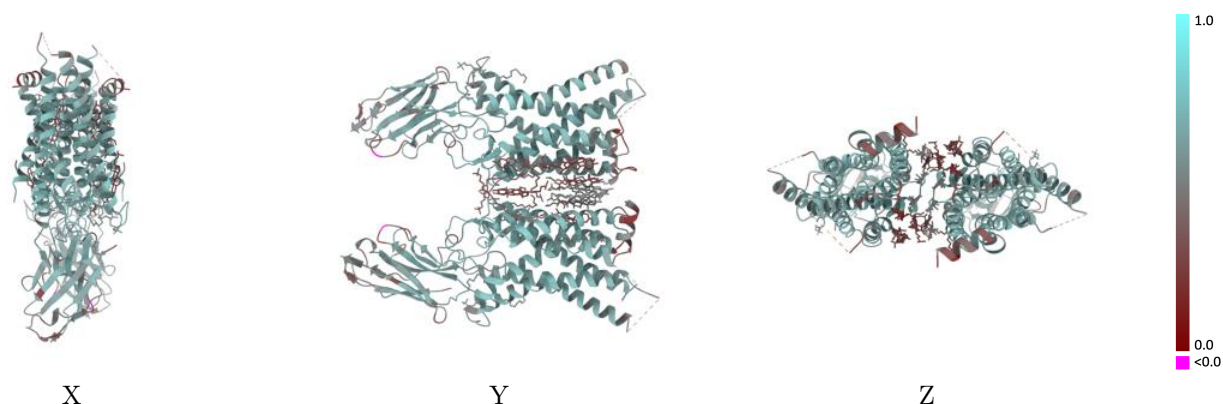
This section contains information regarding the fit between EMDB map EMD-63305 and PDB model 9LQU. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



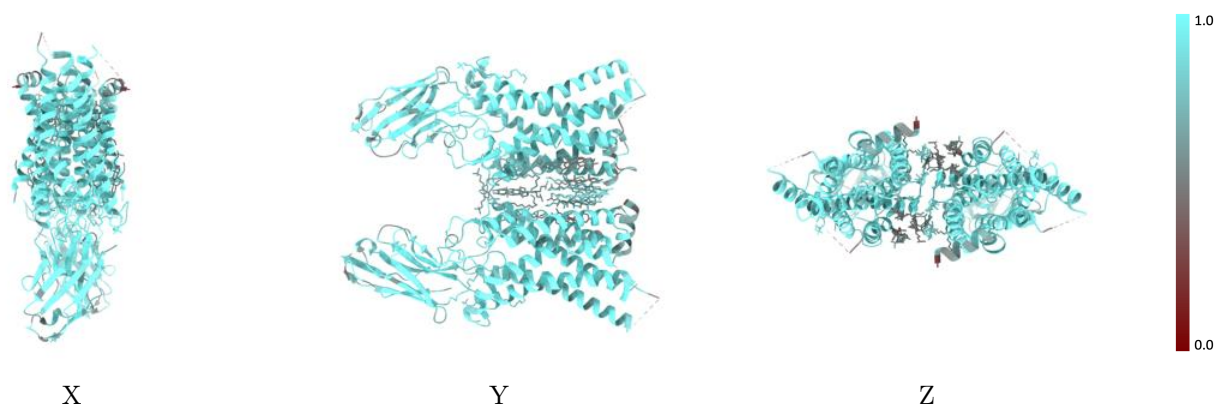
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



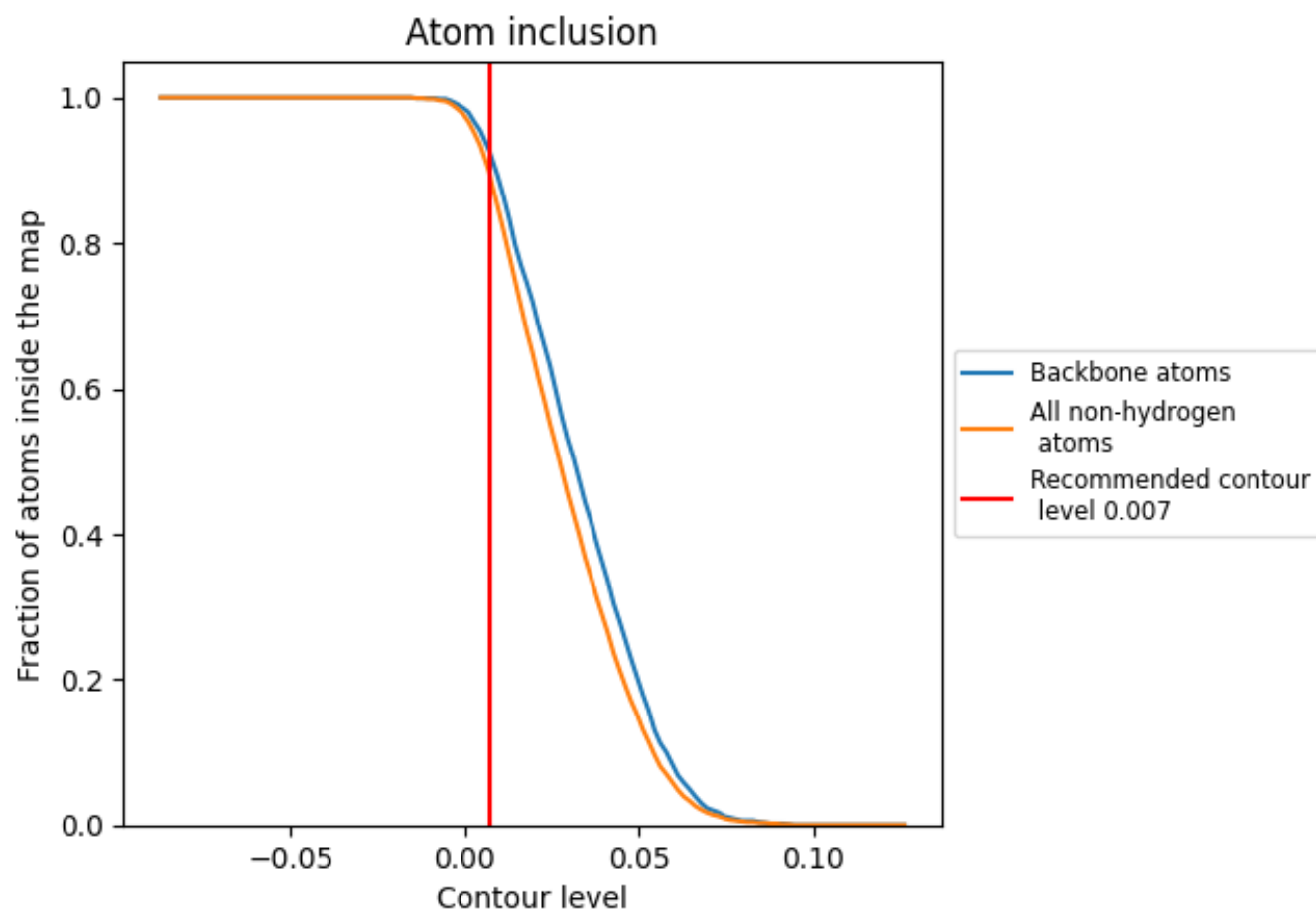
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 90% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8990	0.5670
A	0.9060	0.5780
B	0.9060	0.5780
C	0.8830	0.5390
D	0.8760	0.5400

