



Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 02:15 AM EST

PDB ID : 7SK8
EMDB ID : EMD-25176
Title : Cryo-EM structure of human ACKR3 in complex with CXCL12, a small molecule partial agonist CCX662, an extracellular Fab, and an intracellular Fab
Authors : Yen, Y.C.; Schafer, C.T.; Gustavsson, M.; Handel, T.M.; Tesmer, J.J.G.
Deposited on : 2021-10-19
Resolution : 3.30 Å(reported)

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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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

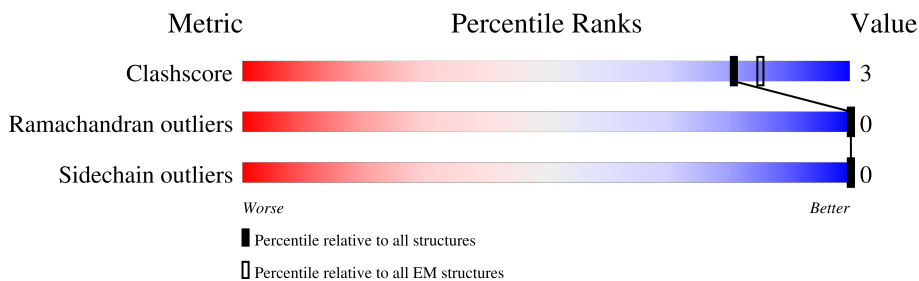
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	393	
2	B	68	
3	C	215	
4	D	236	
5	E	215	
6	F	238	

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 13761 atoms, of which 6885 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 Atypical chemokine receptor 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	306	5020	1656	2534	393	416	21	1	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	cloning artifact	UNP P25106
A	0	ALA	-	cloning artifact	UNP P25106
A	1	PRO	-	cloning artifact	UNP P25106
A	363	GLY	-	expression tag	UNP P25106
A	364	ARG	-	expression tag	UNP P25106
A	365	PRO	-	expression tag	UNP P25106
A	366	LEU	-	expression tag	UNP P25106
A	367	GLU	-	expression tag	UNP P25106
A	368	VAL	-	expression tag	UNP P25106
A	369	LEU	-	expression tag	UNP P25106
A	370	PHE	-	expression tag	UNP P25106
A	371	GLN	-	expression tag	UNP P25106
A	372	GLY	-	expression tag	UNP P25106
A	373	PRO	-	expression tag	UNP P25106
A	374	HIS	-	expression tag	UNP P25106
A	375	HIS	-	expression tag	UNP P25106
A	376	HIS	-	expression tag	UNP P25106
A	377	HIS	-	expression tag	UNP P25106
A	378	HIS	-	expression tag	UNP P25106
A	379	HIS	-	expression tag	UNP P25106
A	380	HIS	-	expression tag	UNP P25106
A	381	HIS	-	expression tag	UNP P25106
A	382	HIS	-	expression tag	UNP P25106
A	383	HIS	-	expression tag	UNP P25106
A	384	ASP	-	expression tag	UNP P25106
A	385	TYR	-	expression tag	UNP P25106
A	386	LYS	-	expression tag	UNP P25106
A	387	ASP	-	expression tag	UNP P25106

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Chain	Residue	Modelled	Actual	Comment	Reference
A	388	ASP	-	expression tag	UNP P25106
A	389	ASP	-	expression tag	UNP P25106
A	390	ASP	-	expression tag	UNP P25106
A	391	LYS	-	expression tag	UNP P25106

- Molecule 2 is a protein called Stromal cell-derived factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	B	62	1040	328	524	99	85	4	0	0

- Molecule 3 is a protein called CID25 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	C	108	1653	530	818	138	164	3	0	0

- Molecule 4 is a protein called CID25 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	D	127	1934	645	933	163	190	3	0	0

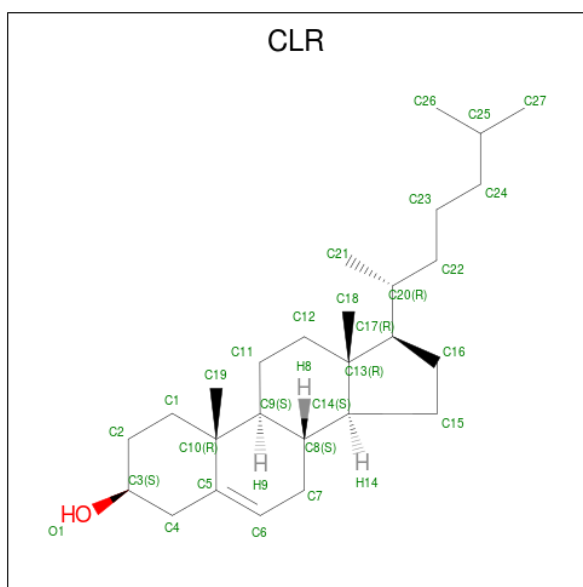
- Molecule 5 is a protein called CID24 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	E	107	1618	518	798	134	165	3	0	0

- Molecule 6 is a protein called CID24 Fab heavy chain.

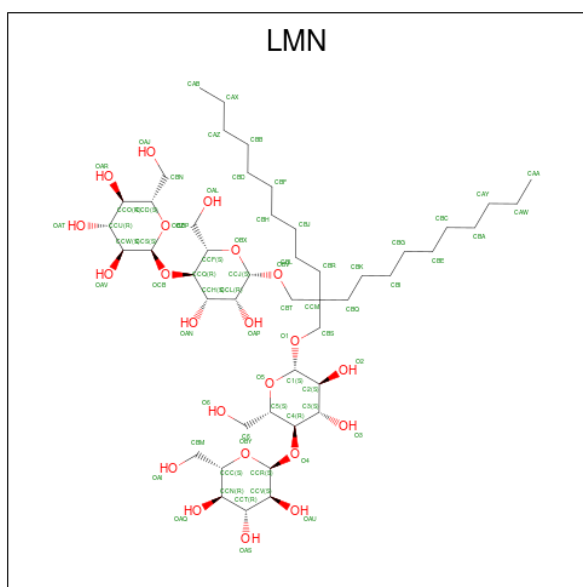
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	F	125	1871	613	906	161	187	4	0	0

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O) (labeled as "Ligand of Interest" by depositor).



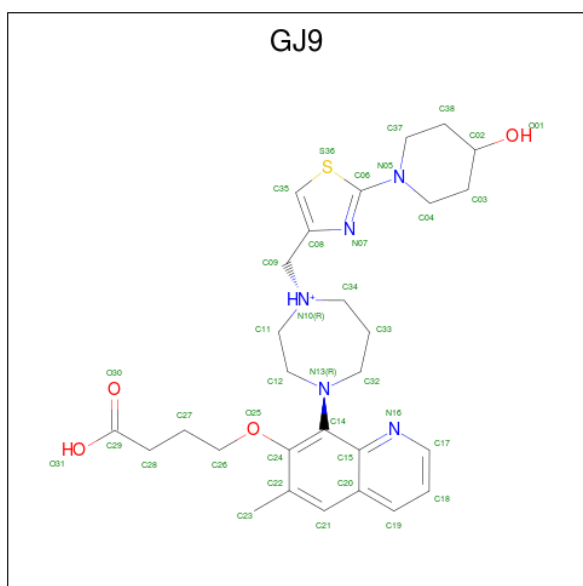
Mol	Chain	Residues	Atoms			AltConf	
			Total	C	H		O
7	A	1	444	162	276	6	0
7	A	1	444	162	276	6	0
7	A	1	444	162	276	6	0
7	A	1	444	162	276	6	0
7	A	1	444	162	276	6	0
7	A	1	444	162	276	6	0

- Molecule 8 is Lauryl Maltose Neopentyl Glycol (three-letter code: LMN) (formula: $C_{47}H_{88}O_{22}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
8	A	1	106	35	59	12	0

- Molecule 9 is (1R)-4-[7-(3-carboxypropoxy)-6-methylquinolin-8-yl]-1-{{2-(4-hydroxypiperidin-1-yl)-1,3-thiazol-4-yl}methyl}-1,4-diazepan-1-ium (three-letter code: GJ9) (formula: $C_{28}H_{38}N_5O_4S$) (labeled as "Ligand of Interest" by depositor).

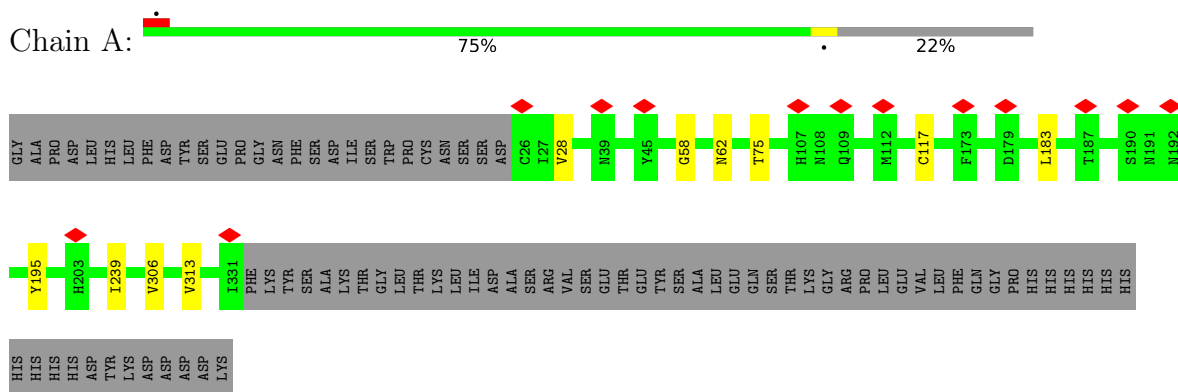


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		S
9	A	1	75	28	37	5	4	1	0

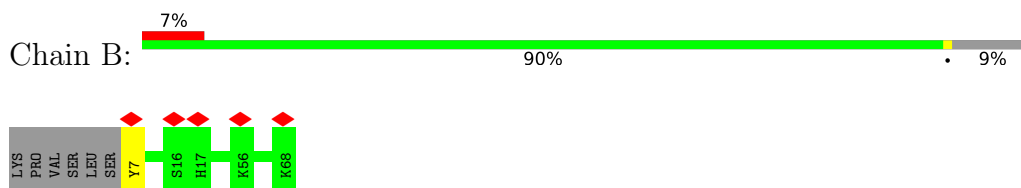
3 Residue-property plots [i](#)

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.

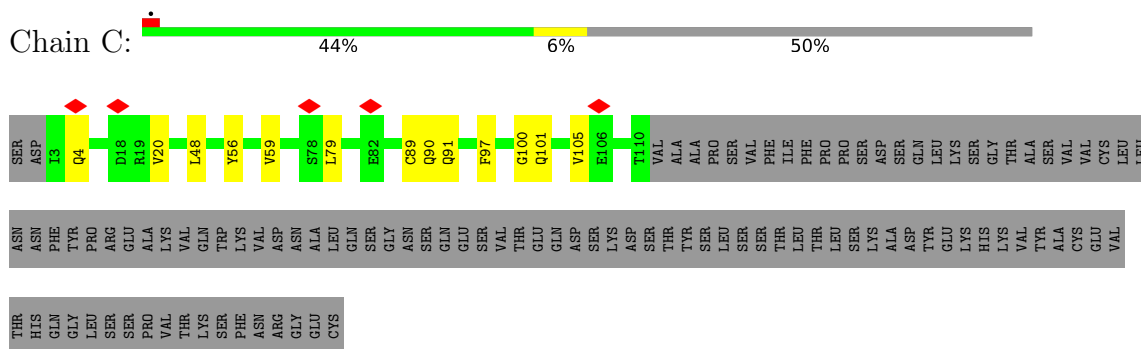
- Molecule 1: Atypical chemokine receptor 3



- Molecule 2: Stromal cell-derived factor 1



- Molecule 3: CID25 Fab light chain



- Molecule 4: CID25 Fab heavy chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	605556	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.123	Depositor
Minimum map value	-4.321	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.86	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GJ9, LMN, 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	A	0.27	0/2562	0.41	0/3502
2	B	0.27	0/526	0.50	0/707
3	C	0.30	0/855	0.51	0/1160
4	D	0.32	0/1033	0.49	0/1408
5	E	0.31	0/839	0.50	0/1139
6	F	0.29	0/993	0.50	0/1353
All	All	0.29	0/6808	0.47	0/9269

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2486	2534	2534	8	0
2	B	516	524	534	1	0
3	C	835	818	818	9	0
4	D	1001	933	933	11	0
5	E	820	798	798	4	0
6	F	965	906	906	3	0
7	A	168	276	276	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	47	59	66	0	0
9	A	38	37	0	0	0
All	All	6876	6885	6865	35	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 3.

All (35) 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)
3:C:20:VAL:HG21	3:C:79:LEU:HD22	1.65	0.77
3:C:101:GLN:N	3:C:101:GLN:OE1	2.29	0.65
4:D:52:ALA:HB3	4:D:73:ILE:HD11	1.84	0.60
5:E:20:VAL:HG21	5:E:79:LEU:HD22	1.90	0.54
4:D:15:VAL:HG11	4:D:89:LEU:HD12	1.90	0.53
4:D:86:MET:HE2	4:D:89:LEU:HD11	1.91	0.53
4:D:22:ARG:NE	4:D:85:GLN:OE1	2.42	0.53
3:C:89:CYS:O	3:C:100:GLY:N	2.43	0.52
5:E:62:ARG:NH2	5:E:82:GLU:OE2	2.41	0.52
1:A:195:TYR:CD2	2:B:7:TYR:HB2	2.45	0.51
1:A:239:ILE:HD11	6:F:106:ASP:OD2	2.11	0.50
3:C:48:LEU:HA	3:C:59:VAL:HG11	1.96	0.48
6:F:118:ASP:N	6:F:118:ASP:OD1	2.46	0.47
1:A:58:GLY:O	1:A:62:ASN:ND2	2.43	0.47
4:D:7:LEU:HD22	4:D:25:CYS:SG	2.55	0.46
1:A:117:CYS:SG	1:A:183:LEU:HD21	2.56	0.45
1:A:75:THR:HG22	1:A:75:THR:O	2.16	0.45
1:A:313:VAL:HG12	1:A:313:VAL:O	2.16	0.45
4:D:52:ALA:CB	4:D:73:ILE:HD11	2.47	0.45
4:D:102:VAL:HG12	4:D:103:TYR:N	2.33	0.44
1:A:306:VAL:HG12	1:A:306:VAL:O	2.18	0.44
4:D:103:TYR:O	4:D:105:TRP:N	2.50	0.43
6:F:107:TRP:CE3	6:F:108:THR:HG23	2.53	0.43
3:C:56:TYR:HB3	3:C:59:VAL:HG13	2.01	0.43
5:E:49:ILE:HD12	5:E:74:LEU:HD13	2.00	0.43
4:D:23:LEU:HD22	4:D:122:THR:HG21	2.00	0.43
4:D:5:VAL:HG13	4:D:30:PHE:CD1	2.54	0.42
5:E:20:VAL:CG2	5:E:79:LEU:HD22	2.49	0.42
7:A:402:CLR:H212	7:A:402:CLR:H121	2.01	0.42
3:C:4:GLN:OE1	3:C:4:GLN:N	2.53	0.42
3:C:97:PHE:N	3:C:97:PHE:CD1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:5:VAL:HG13	4:D:30:PHE:HD1	1.85	0.41
3:C:90:GLN:HG2	3:C:91:GLN:N	2.36	0.41
1:A:28:VAL:HG23	1:A:28:VAL:O	2.21	0.41
3:C:105:VAL:O	3:C:105:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	305/393 (78%)	297 (97%)	8 (3%)	0	100	100
2	B	60/68 (88%)	58 (97%)	2 (3%)	0	100	100
3	C	106/215 (49%)	96 (91%)	10 (9%)	0	100	100
4	D	125/236 (53%)	112 (90%)	13 (10%)	0	100	100
5	E	105/215 (49%)	99 (94%)	6 (6%)	0	100	100
6	F	123/238 (52%)	119 (97%)	4 (3%)	0	100	100
All	All	824/1365 (60%)	781 (95%)	43 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	286/363 (79%)	286 (100%)	0	100	100
2	B	57/63 (90%)	57 (100%)	0	100	100
3	C	94/190 (50%)	94 (100%)	0	100	100
4	D	102/198 (52%)	102 (100%)	0	100	100
5	E	93/190 (49%)	93 (100%)	0	100	100
6	F	101/200 (50%)	101 (100%)	0	100	100
All	All	733/1204 (61%)	733 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
7	CLR	A	407	-	31,31,31	1.04	0	48,48,48	1.38	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	CLR	A	401	-	31,31,31	1.05	2 (6%)	48,48,48	1.31	6 (12%)
7	CLR	A	404	-	31,31,31	1.03	1 (3%)	48,48,48	1.37	5 (10%)
7	CLR	A	405	-	31,31,31	1.06	0	48,48,48	1.35	5 (10%)
7	CLR	A	403	-	31,31,31	1.02	2 (6%)	48,48,48	1.31	5 (10%)
7	CLR	A	402	-	31,31,31	1.04	1 (3%)	48,48,48	1.31	6 (12%)
9	GJ9	A	408	-	37,42,42	1.71	9 (24%)	47,58,58	1.83	12 (25%)
8	LMN	A	406	-	48,48,72	1.94	14 (29%)	60,62,98	0.93	1 (1%)

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
7	CLR	A	407	-	-	3/10/68/68	0/4/4/4
7	CLR	A	401	-	-	2/10/68/68	0/4/4/4
7	CLR	A	404	-	-	3/10/68/68	0/4/4/4
7	CLR	A	405	-	-	1/10/68/68	0/4/4/4
7	CLR	A	403	-	-	1/10/68/68	0/4/4/4
7	CLR	A	402	-	-	2/10/68/68	0/4/4/4
9	GJ9	A	408	-	-	6/17/40/40	0/5/5/5
8	LMN	A	406	-	-	16/38/78/130	0/2/2/4

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	406	LMN	CBT-CCM	5.12	1.65	1.53
9	A	408	GJ9	C12-N13	4.62	1.52	1.46
8	A	406	LMN	O5-C1	4.49	1.53	1.41
9	A	408	GJ9	C06-N05	4.14	1.38	1.32
9	A	408	GJ9	C09-N10	4.14	1.55	1.47
8	A	406	LMN	CBQ-CCM	3.90	1.61	1.54
8	A	406	LMN	CBR-CCM	3.62	1.60	1.54
8	A	406	LMN	O4-C4	3.57	1.51	1.43
8	A	406	LMN	CBS-CCM	3.36	1.61	1.53
8	A	406	LMN	O1-C1	-3.08	1.34	1.40
8	A	406	LMN	C4-C3	-2.86	1.45	1.52
9	A	408	GJ9	C34-N10	2.76	1.53	1.46
9	A	408	GJ9	C11-N10	2.54	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	408	GJ9	C32-N13	2.47	1.49	1.46
8	A	406	LMN	CBR-CBL	2.42	1.61	1.52
9	A	408	GJ9	C28-C29	2.38	1.56	1.50
7	A	401	CLR	C18-C13	-2.28	1.50	1.54
8	A	406	LMN	C4-C5	-2.22	1.48	1.53
8	A	406	LMN	OAN-CCH	2.20	1.48	1.43
7	A	404	CLR	C8-C14	-2.17	1.49	1.53
7	A	403	CLR	C18-C13	-2.14	1.50	1.54
8	A	406	LMN	O5-C5	2.09	1.49	1.44
8	A	406	LMN	CCQ-CCH	-2.09	1.47	1.52
7	A	403	CLR	C8-C14	-2.07	1.49	1.53
8	A	406	LMN	O1-CBS	2.07	1.48	1.42
7	A	402	CLR	C18-C13	-2.05	1.50	1.54
9	A	408	GJ9	C15-N16	2.05	1.39	1.37
9	A	408	GJ9	C04-N05	2.03	1.49	1.46
7	A	401	CLR	C7-C6	2.01	1.54	1.50

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	408	GJ9	C11-C12-N13	5.60	119.75	113.30
9	A	408	GJ9	C09-C08-C35	-5.26	121.70	129.62
9	A	408	GJ9	C20-C15-N16	-4.28	117.93	122.62
9	A	408	GJ9	C24-C14-C15	-3.55	117.43	120.76
7	A	404	CLR	C22-C20-C17	-3.35	103.37	110.28
7	A	404	CLR	C12-C13-C14	-3.06	102.53	107.27
7	A	401	CLR	C22-C20-C17	-3.05	103.98	110.28
7	A	407	CLR	C22-C20-C17	-3.00	104.09	110.28
7	A	403	CLR	C22-C20-C17	-2.94	104.20	110.28
7	A	402	CLR	C13-C17-C20	-2.90	114.95	119.49
7	A	405	CLR	C13-C17-C20	-2.85	115.02	119.49
7	A	405	CLR	C12-C13-C14	-2.83	102.88	107.27
9	A	408	GJ9	C21-C22-C24	2.71	120.81	117.84
7	A	407	CLR	C13-C17-C20	-2.65	115.33	119.49
7	A	407	CLR	C12-C13-C14	-2.60	103.24	107.27
7	A	403	CLR	C13-C17-C20	-2.56	115.47	119.49
7	A	404	CLR	C18-C13-C12	2.54	114.59	110.59
7	A	401	CLR	C13-C17-C20	-2.48	115.61	119.49
7	A	405	CLR	C22-C20-C17	-2.46	105.20	110.28
7	A	402	CLR	C21-C20-C22	-2.44	106.54	110.36
7	A	407	CLR	C18-C13-C12	2.37	114.34	110.59
7	A	402	CLR	C22-C20-C17	-2.36	105.41	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	403	CLR	C18-C13-C12	2.35	114.30	110.59
7	A	401	CLR	C18-C13-C12	2.33	114.26	110.59
7	A	403	CLR	C7-C8-C14	-2.31	107.56	110.91
7	A	407	CLR	C8-C7-C6	-2.30	109.43	112.73
7	A	405	CLR	C18-C13-C12	2.29	114.21	110.59
7	A	403	CLR	C12-C13-C14	-2.29	103.72	107.27
7	A	401	CLR	C12-C13-C14	-2.28	103.74	107.27
7	A	401	CLR	C7-C8-C14	-2.25	107.64	110.91
9	A	408	GJ9	C17-N16-C15	2.23	120.08	117.30
9	A	408	GJ9	C12-N13-C14	-2.23	111.77	119.32
9	A	408	GJ9	C14-C15-C20	2.22	120.63	118.66
7	A	402	CLR	C12-C13-C14	-2.17	103.91	107.27
7	A	404	CLR	C16-C17-C20	-2.17	108.79	112.15
9	A	408	GJ9	C33-C34-N10	-2.15	111.28	115.35
9	A	408	GJ9	C32-N13-C12	-2.14	113.64	117.47
7	A	402	CLR	C18-C13-C12	2.14	113.96	110.59
7	A	404	CLR	C13-C17-C20	-2.09	116.21	119.49
7	A	402	CLR	C7-C8-C14	-2.07	107.91	110.91
8	A	406	LMN	CBL-CBR-CCM	-2.06	110.53	117.16
7	A	405	CLR	C11-C12-C13	-2.06	109.25	112.78
7	A	407	CLR	C24-C23-C22	-2.04	103.85	113.24
9	A	408	GJ9	C34-N10-C11	-2.03	107.76	113.22
9	A	408	GJ9	C14-C15-N16	2.02	121.44	119.30
7	A	401	CLR	C24-C23-C22	-2.02	103.98	113.24

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	406	LMN	C2-C1-O1-CBS
8	A	406	LMN	O5-C1-O1-CBS
8	A	406	LMN	O1-CBS-CCM-CBQ
8	A	406	LMN	O1-CBS-CCM-CBR
8	A	406	LMN	OBV-CBT-CCM-CBQ
8	A	406	LMN	OBX-CCJ-OBV-CBT
9	A	408	GJ9	S36-C06-N05-C37
8	A	406	LMN	OAL-CBP-CCF-OBX
8	A	406	LMN	O1-CBS-CCM-CBT
7	A	407	CLR	C17-C20-C22-C23
8	A	406	LMN	OAL-CBP-CCF-CCQ
7	A	407	CLR	C21-C20-C22-C23
7	A	402	CLR	C17-C20-C22-C23

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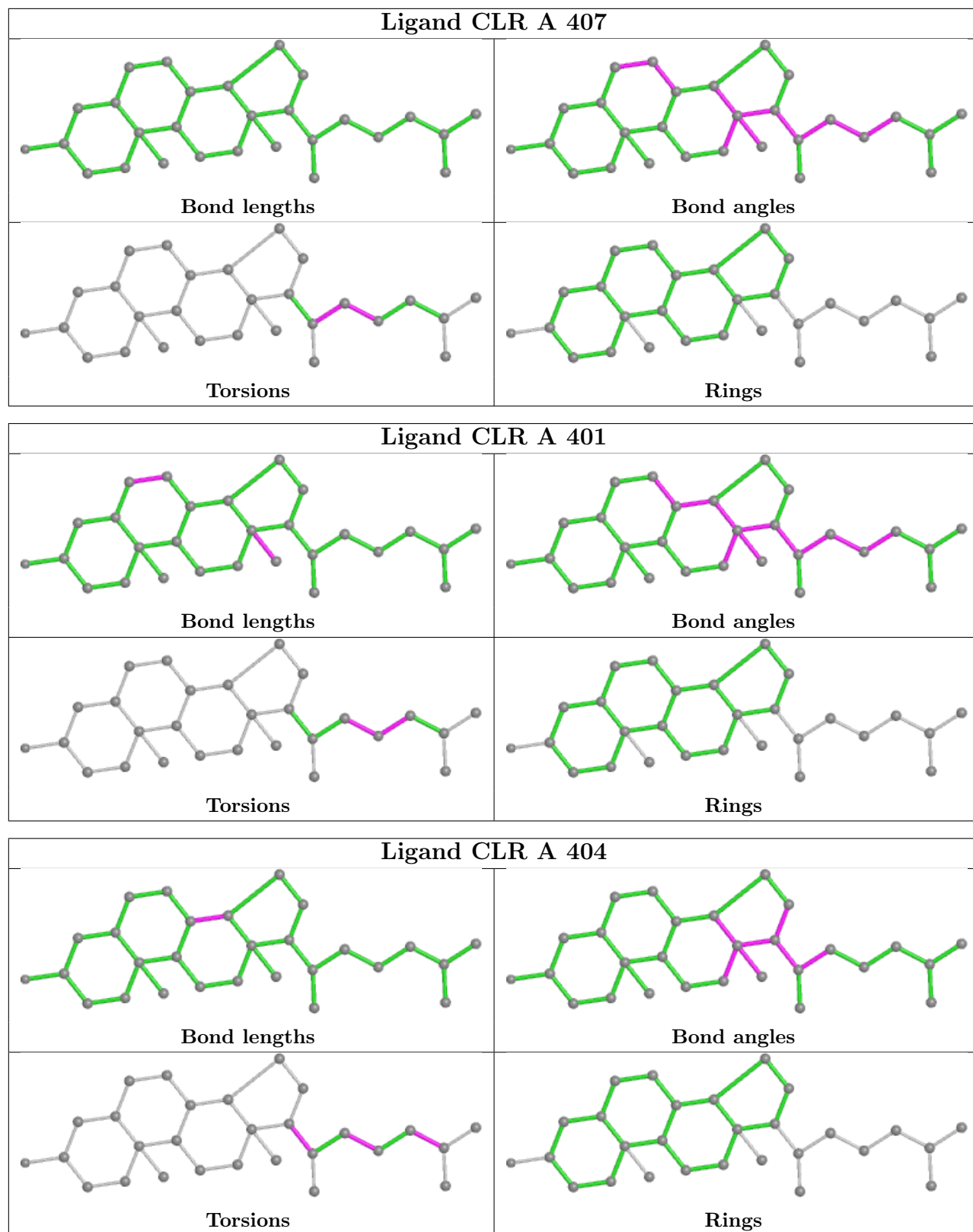
Mol	Chain	Res	Type	Atoms
7	A	402	CLR	C21-C20-C22-C23
9	A	408	GJ9	O25-C26-C27-C28
8	A	406	LMN	CBE-CBG-CBI-CBK
8	A	406	LMN	CAY-CBA-CBC-CBE
8	A	406	LMN	CBB-CBD-CBF-CBH
7	A	405	CLR	C20-C22-C23-C24
9	A	408	GJ9	C27-C26-O25-C24
7	A	407	CLR	C20-C22-C23-C24
8	A	406	LMN	OBV-CBT-CCM-CBS
7	A	401	CLR	C22-C23-C24-C25
8	A	406	LMN	OBV-CBT-CCM-CBR
8	A	406	LMN	CAX-CAZ-CBB-CBD
7	A	404	CLR	C16-C17-C20-C22
9	A	408	GJ9	C26-C27-C28-C29
7	A	404	CLR	C23-C24-C25-C27
7	A	401	CLR	C20-C22-C23-C24
8	A	406	LMN	CBG-CBI-CBK-CBQ
7	A	403	CLR	C20-C22-C23-C24
7	A	404	CLR	C20-C22-C23-C24
9	A	408	GJ9	C27-C28-C29-O30
9	A	408	GJ9	C24-C14-N13-C32

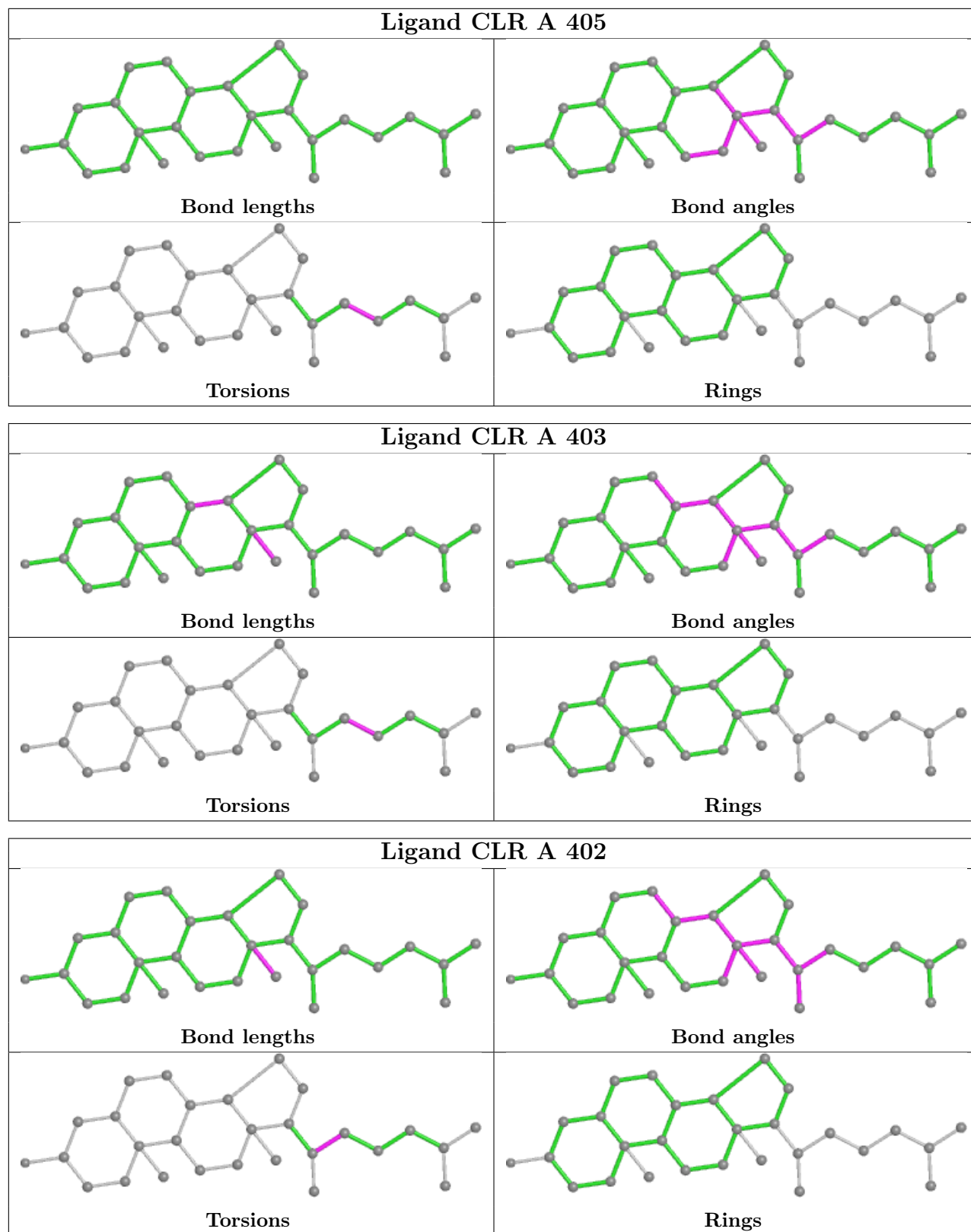
There are no ring outliers.

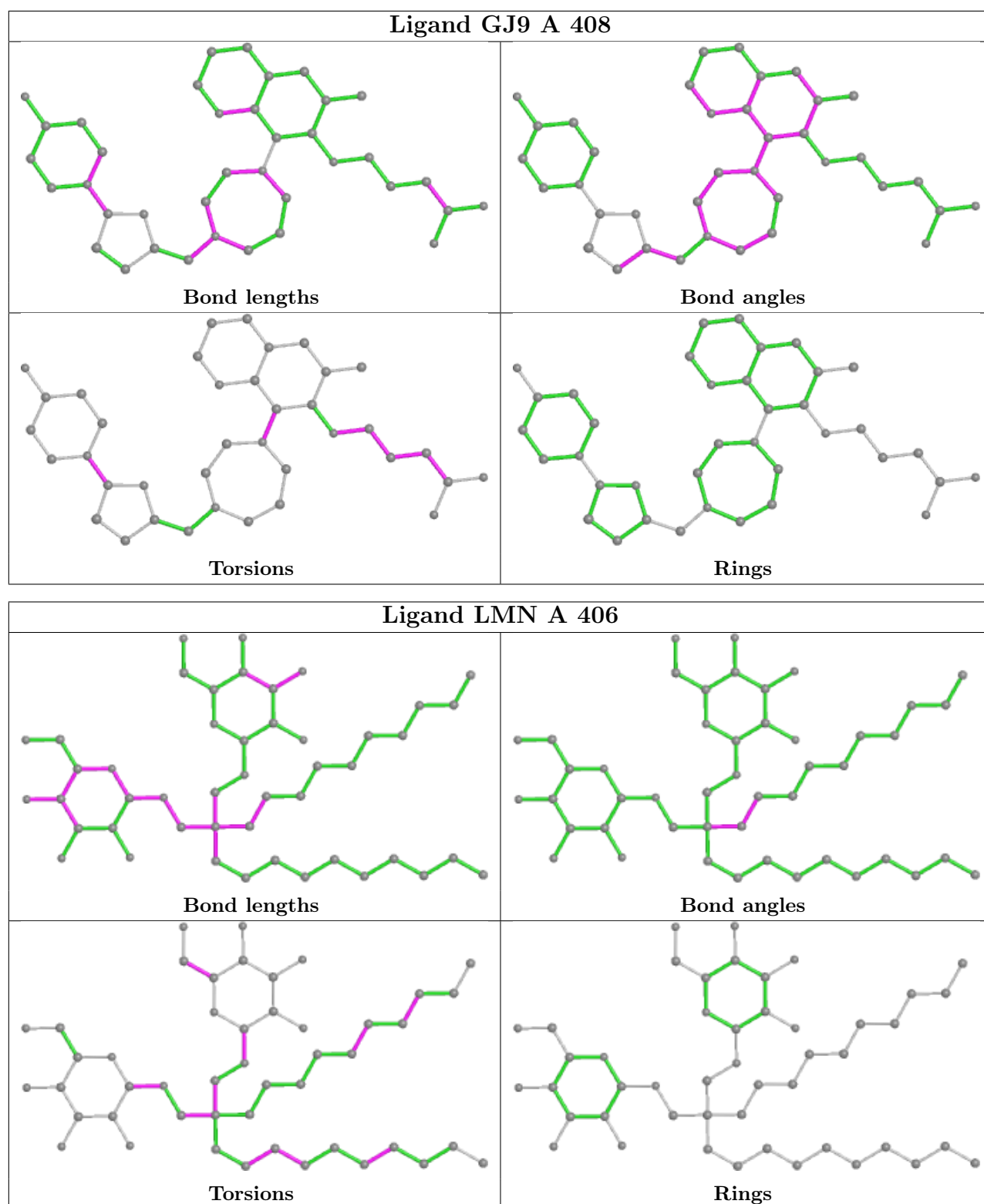
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	402	CLR	1	0

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







5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

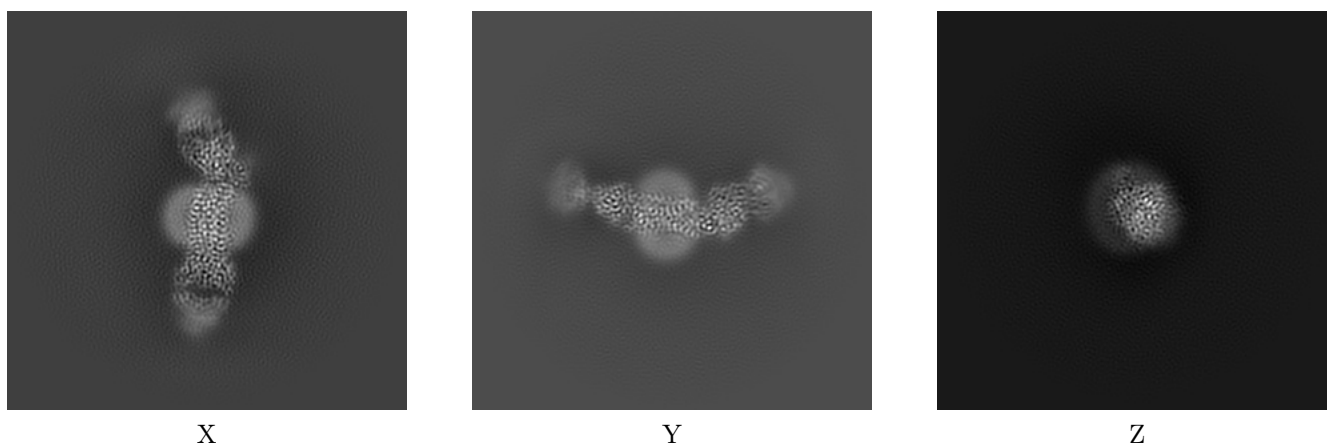
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25176. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

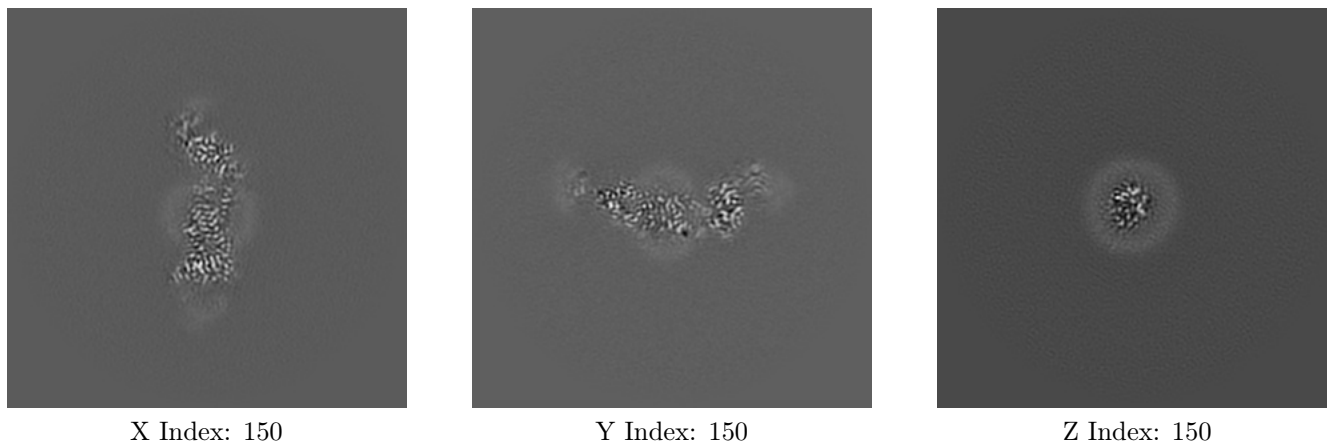
6.1.1 Primary map



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

6.2 Central slices [i](#)

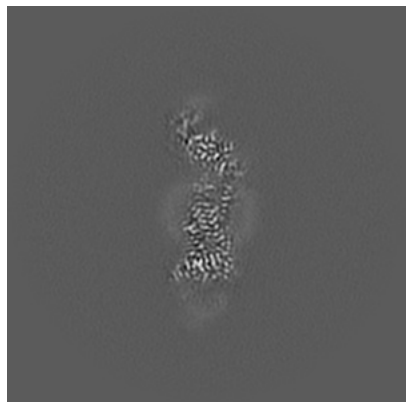
6.2.1 Primary map



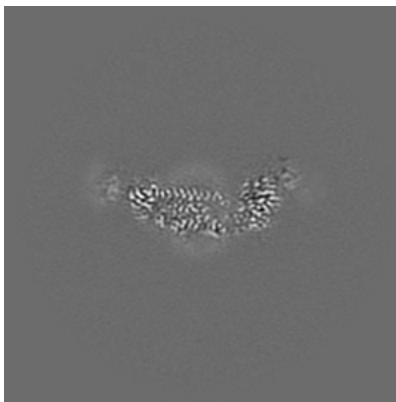
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

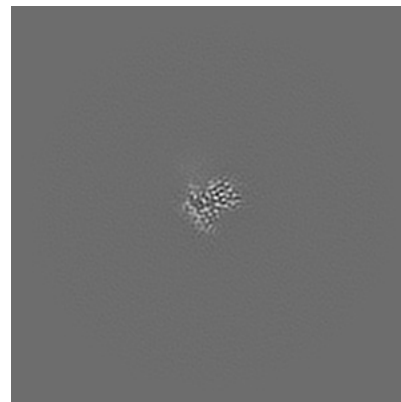
6.3.1 Primary map



X Index: 150



Y Index: 155



Z Index: 192

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

6.4 Orthogonal surface views [i](#)

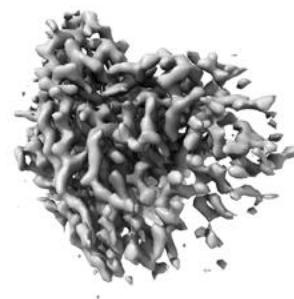
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.86. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

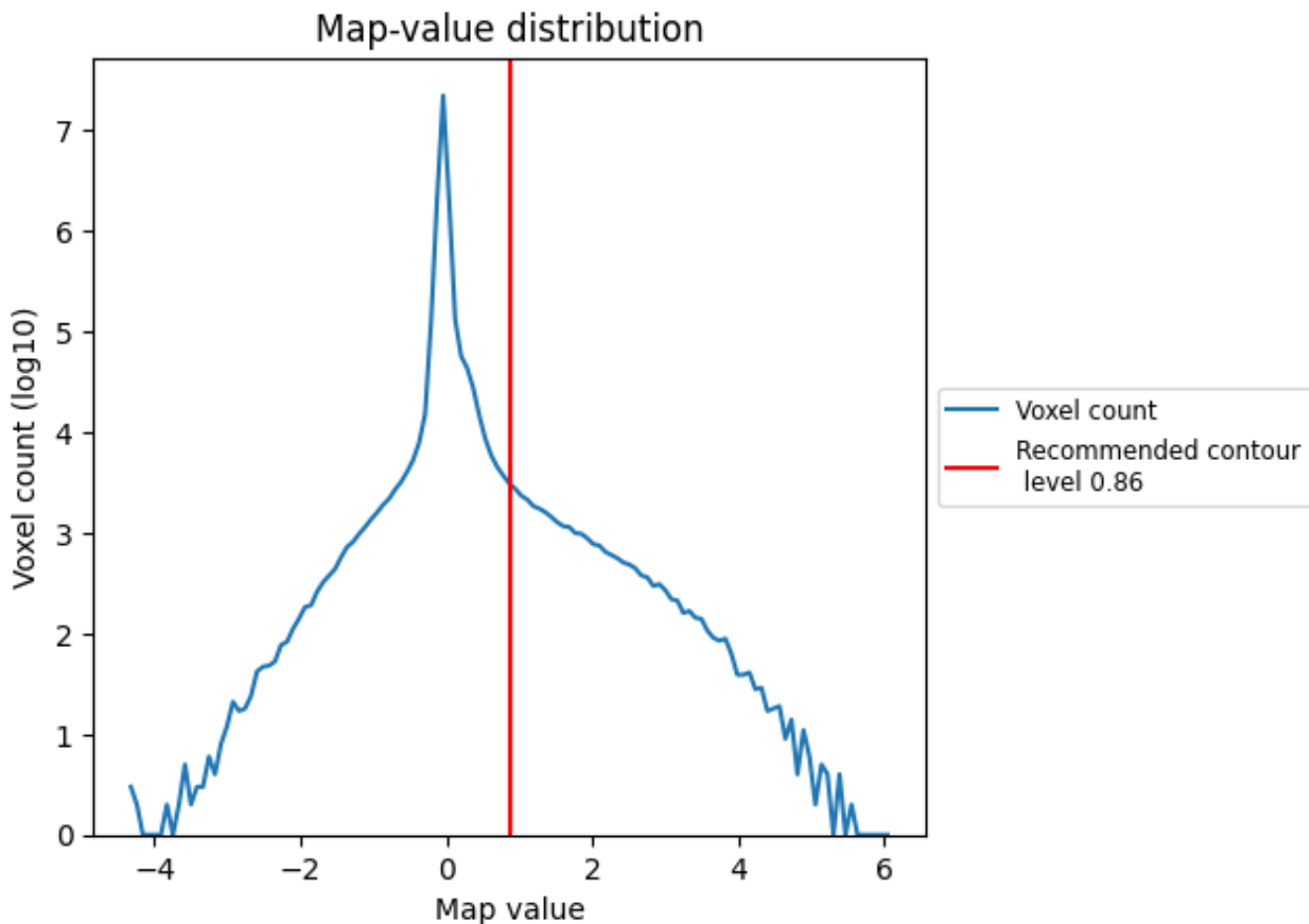
6.5 Mask visualisation

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

7 Map analysis [i](#)

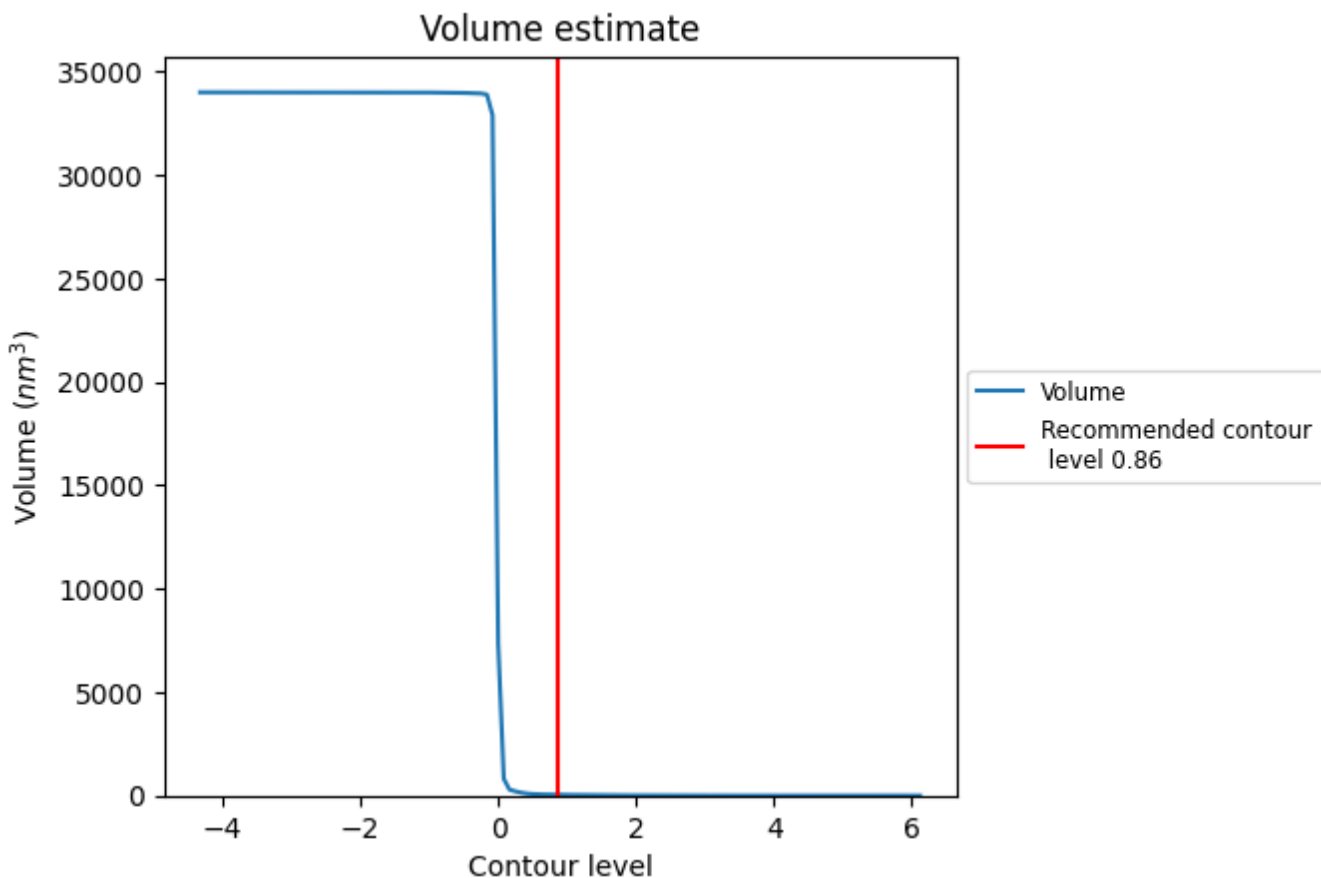
This section contains the results of statistical analysis of the map.

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.

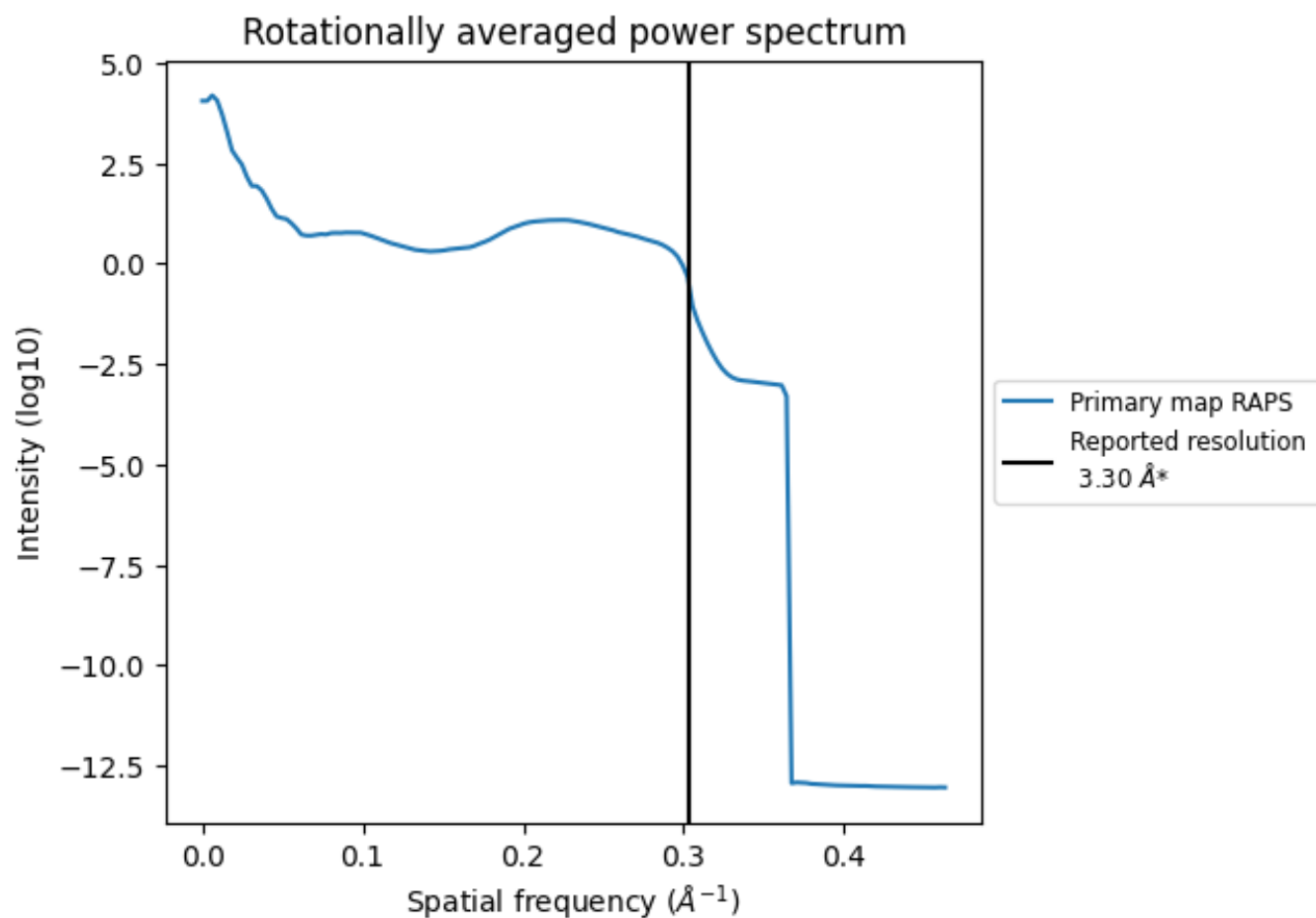
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 40 nm³; this corresponds to an approximate mass of 36 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 [i](#)

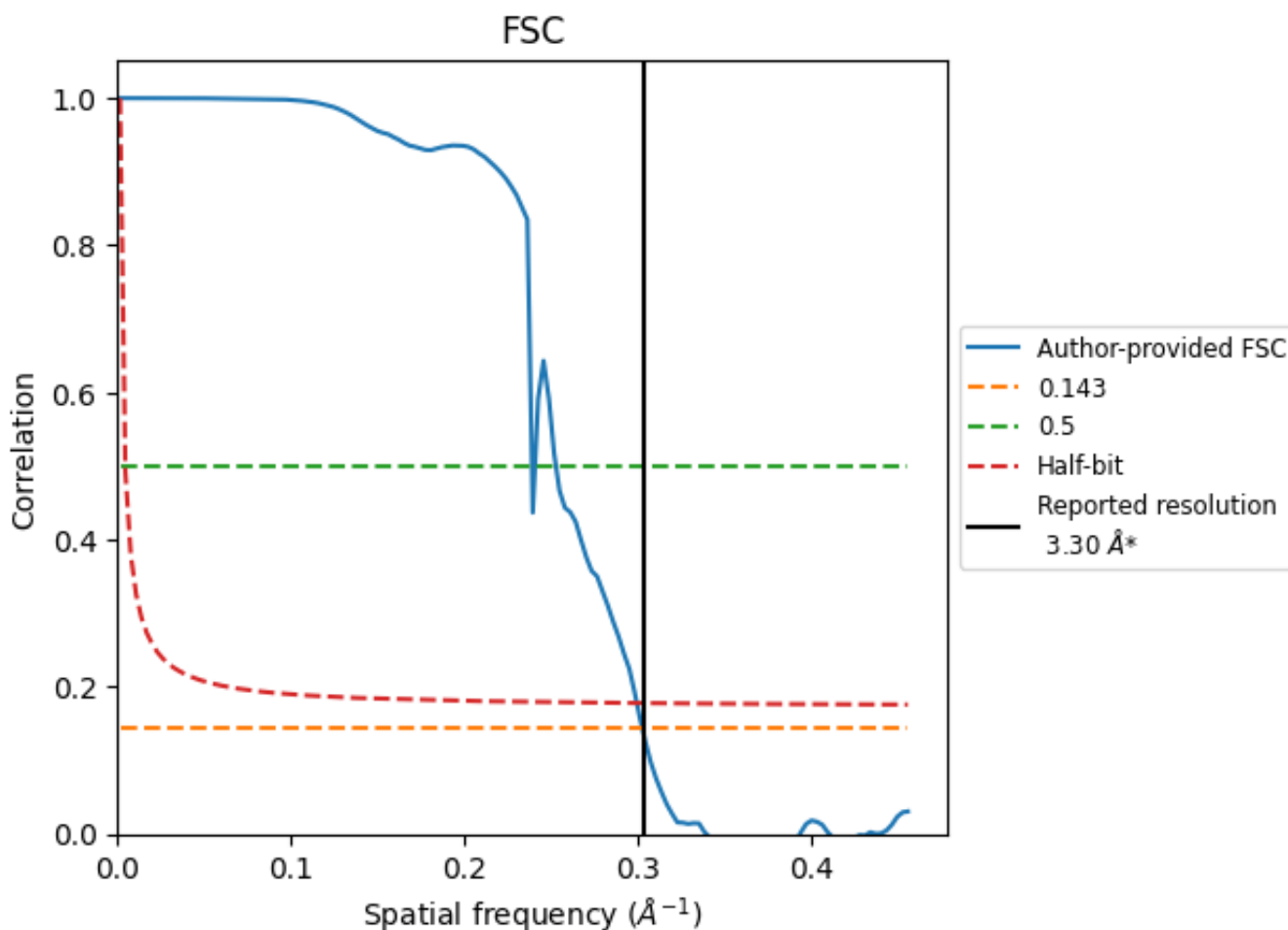


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

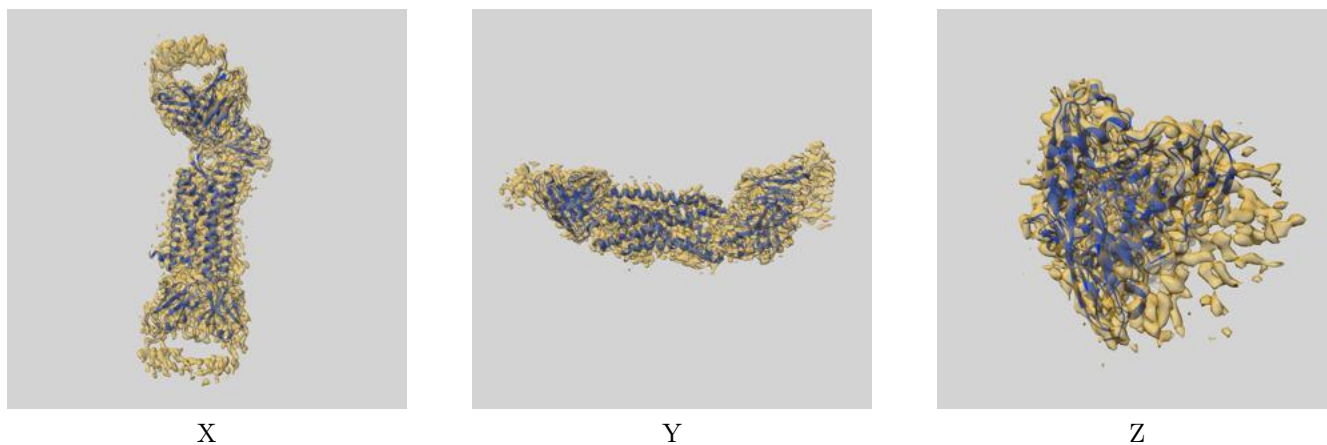
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.31	4.19	3.34
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

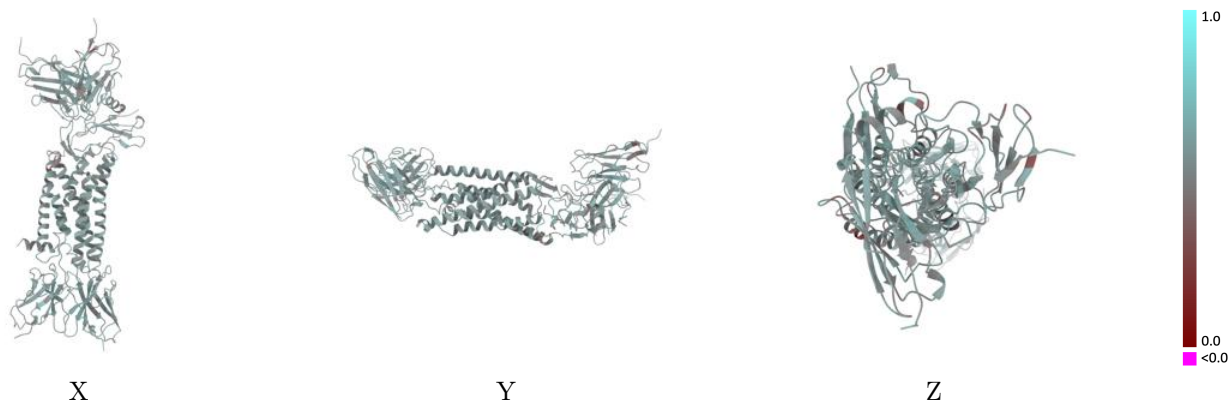
This section contains information regarding the fit between EMDB map EMD-25176 and PDB model 7SK8. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



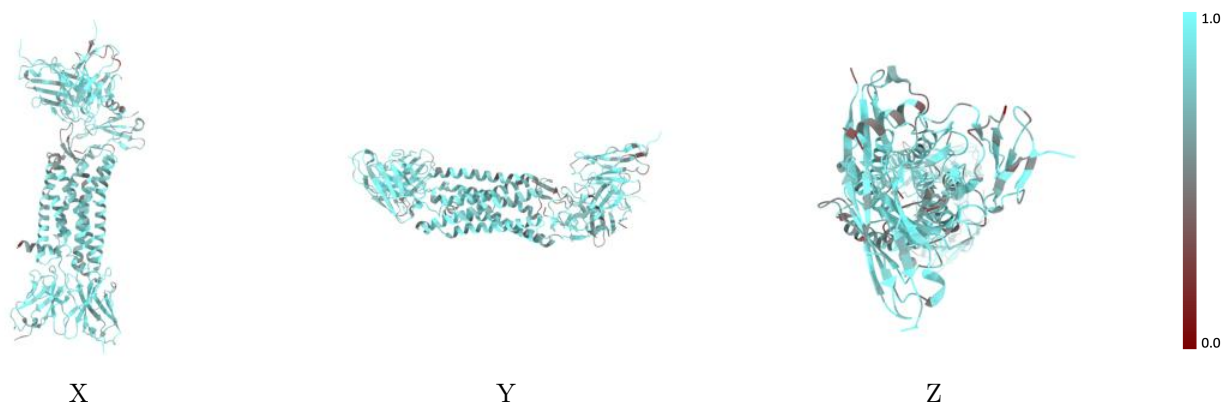
The images above show the 3D surface view of the map at the recommended contour level 0.86 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



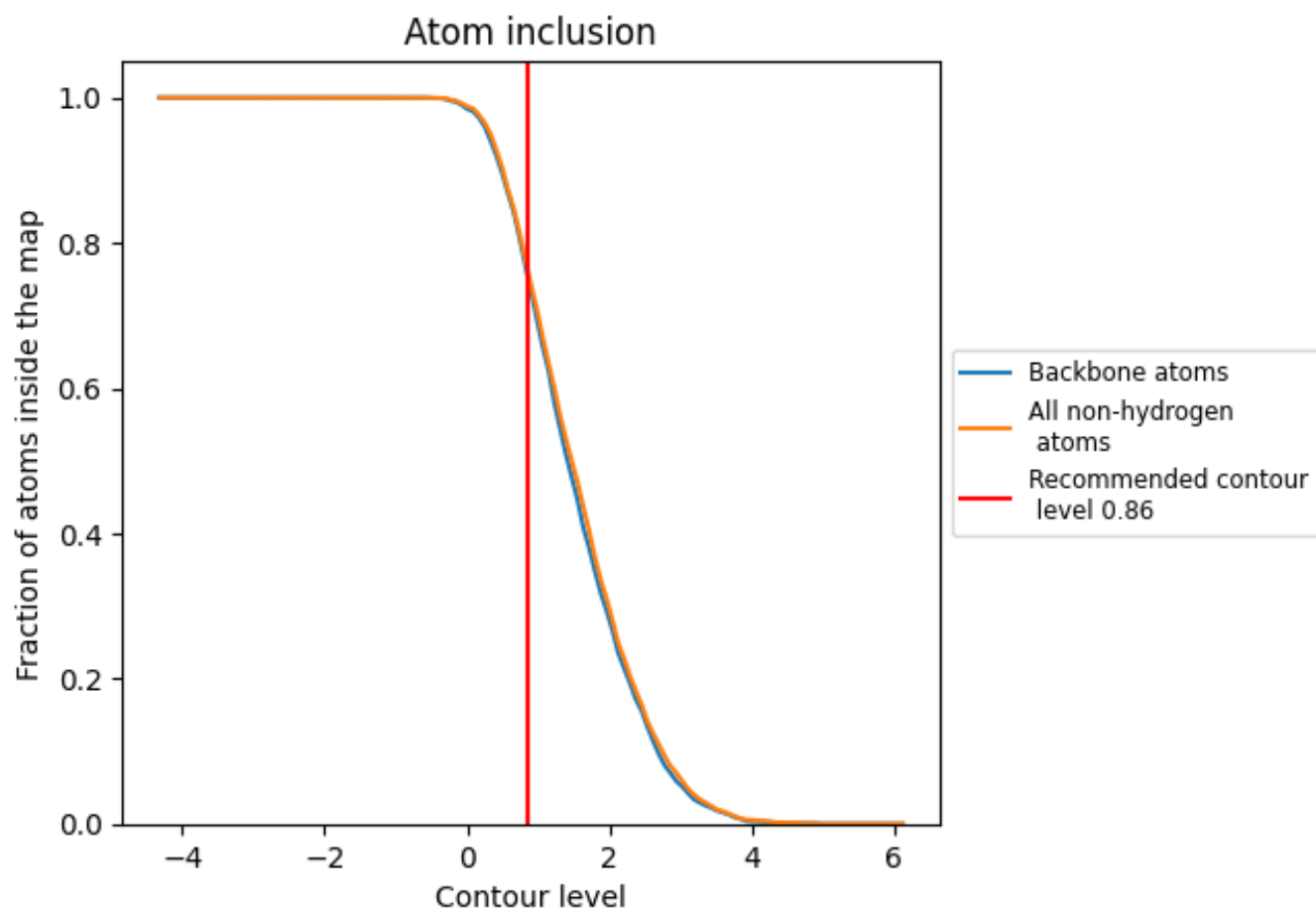
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.86).















9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.86) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7600	 0.5430
A	 0.7461	 0.5370
B	 0.7296	 0.5280
C	 0.7708	 0.5390
D	 0.8249	 0.5510
E	 0.8107	 0.5460
F	 0.8275	 0.5620

