



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 02:42 AM UTC

PDB ID : 8X94 / pdb_00008x94
EMDB ID : EMD-38161
Title : Structure of human TRPV1 in complex with antagonist –protein purified without CHS
Authors : Fan, J.; Lei, X.
Deposited on : 2023-11-29
Resolution : 2.55 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

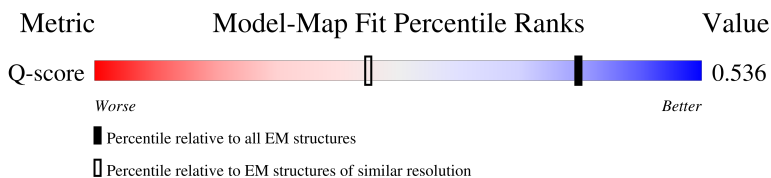
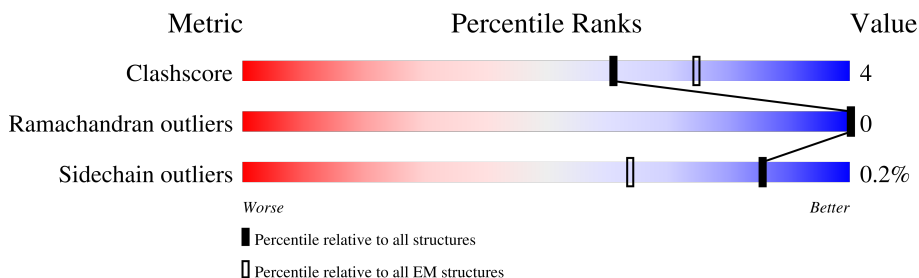
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.55 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	7475 (2.05 - 3.05)

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	1112	12% 43% 5% 52%
1	B	1112	12% 42% 5% 52%
1	C	1112	12% 44% . 52%
1	D	1112	12% 43% . 52%

2 Entry composition [i](#)

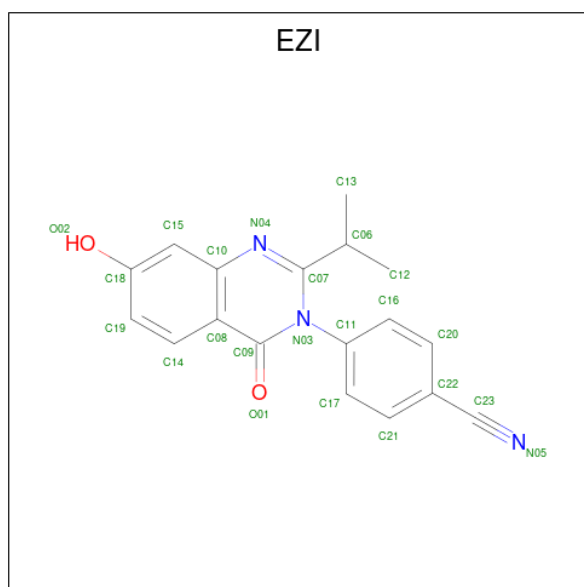
There are 3 unique types of molecules in this entry. The entry contains 17444 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transient receptor potential cation channel subfamily V member 1, Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	531	Total	C	N	O	S	0	0
			4310	2824	693	763	30		
1	B	531	Total	C	N	O	S	0	0
			4310	2824	693	763	30		
1	C	531	Total	C	N	O	S	0	0
			4310	2824	693	763	30		
1	D	531	Total	C	N	O	S	0	0
			4310	2824	693	763	30		

- Molecule 2 is 4-(7-Hydroxy-2-isopropyl-4-oxoquinazolin-3(4H)-yl)benzonitrile (CCD ID: EZI) (formula: $C_{18}H_{15}N_3O_2$) (labeled as "Ligand of Interest" by depositor).



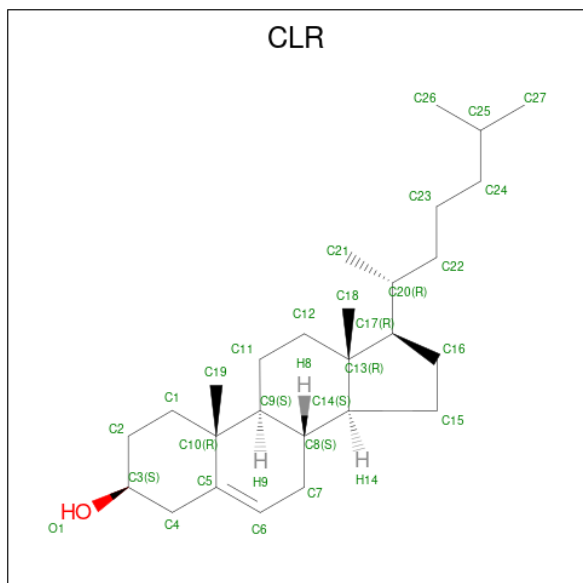
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			23	18	3	2	
2	B	1	Total	C	N	O	0
			23	18	3	2	

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Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	N	O	0
			23	18	3	2	
2	D	1	Total	C	N	O	0
			23	18	3	2	

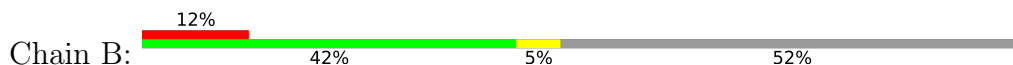
- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



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

GLY
SER
GLY
GLY
GLY
SER
GLY
GLY
SER
ALA
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

- Molecule 1: Transient receptor potential cation channel subfamily V member 1, Green fluorescent protein



ALA	VAL	ALA	ALA	GLN	ASN	ASN	CYS	GLN	LEU	LEU	SER	LEU	LEU	PHE	LEU	LEU	GLN	LYS	SER	LYS	LYS	HIS	LEU	THR	ASP	ASN	GLU	GLY	PHE	LYS	ASP	PRO	GLU	THR	THR	THR	TLE	PRO	LEU	LEU	LEU	LEU	GLU	ILE
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[illegible]

K241	G242	R243	T244	G245	F246	V247	F248	G249	E250	L251	P252	L255	A256	A257	G258	T259	M260	Q261	L262	G263	L264	V265	K266	F267	L268	L269	Q270	M271	S272	W273	Q274	T275	A276	D277	L278	S279	A280	R281	D282	S283	V284	T287	V288	T299	A300	D301	M302	V306	M309	E312	I313	L314	L315
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L316	G317	A318	K319	L320	H321	P322	T323	L324	K325	L326	E327	E328	K332	K333	G334	R356	Q359	E360	P361	E362	C363	L366	E372	Y375	G376	P377	V378	H379	L382	C391	E392	K393	F406	T407	N409	F417	F430	O443	L447	D459	M466	V475
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Category	Value	Color
E478	1.0	Green
S502	1.0	Red
T505	1.0	Green
D509	1.0	Red
S510	1.0	Green
T526	1.0	Green
M541	1.0	Green
A546	1.0	Green
T550	1.0	Green
M572	1.0	Green
D601	1.0	Green
GLY	1.0	Green
LYS	1.0	Green
ASN	1.0	Green
ASP	1.0	Green
SER	1.0	Green
LEU	1.0	Green
PRO	1.0	Green
SER	1.0	Green
GLU	1.0	Green
THR	1.0	Green
SER	1.0	Green
HIS	1.0	Green
ARG	1.0	Green
TRP	1.0	Green
ARG	1.0	Green
GLY	1.0	Green
PRO	1.0	Green
ALA	1.0	Green
CYS	1.0	Green
ARG	1.0	Green
PRO	1.0	Green
PRO	1.0	Green
ASP	1.0	Green
SER	1.0	Green
S627	1.0	Green
T642	1.0	Green
L676	1.0	Green
H677	1.0	Green
M678	1.0	Green
S712	1.0	Red
F713	1.0	Red
L714	1.0	Red
K715	1.0	Red
C716	1.0	Red
L717	1.0	Red

R718	K719	A720	F721	R722	L726	L727	Q728	W729	G730	Y731	T732	P733	D734	G736	T737	D738	Y739	E747	V748	N749	W750	T751	T752	W753	ASN	THR	ASN	ASN	VAL	GLY	ILE	ILE	ASN	ASN	GLU	ASP	PRO	GLY	ASN	CYS	GLY	GLY	GLY	VAL	LVS	ARG	THR	LEU	LEU	SER	PHE	SER	SER	ARG	VAL	VAL	SER	GLY
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ARG	HIS	TRP	LYS	ASN	PHE	ALA	LEU	VAL	PRO	LEU	ARG	GLU	ALA	ALA	ALA	ARG	ASP	ARG	GLN	GLU	GLU	VAL	TYR	LEU	ARG	GLN	PHE	SER	SER	GLY	SER	LEU	LYS	PRO	PRO	GLU	ASP	ALA	GLU	VAL	PHE	LYS	SER	SER	PRO	ALA	ALA	SER	GLY	GLU	LYS	VAL	GLU	ARG
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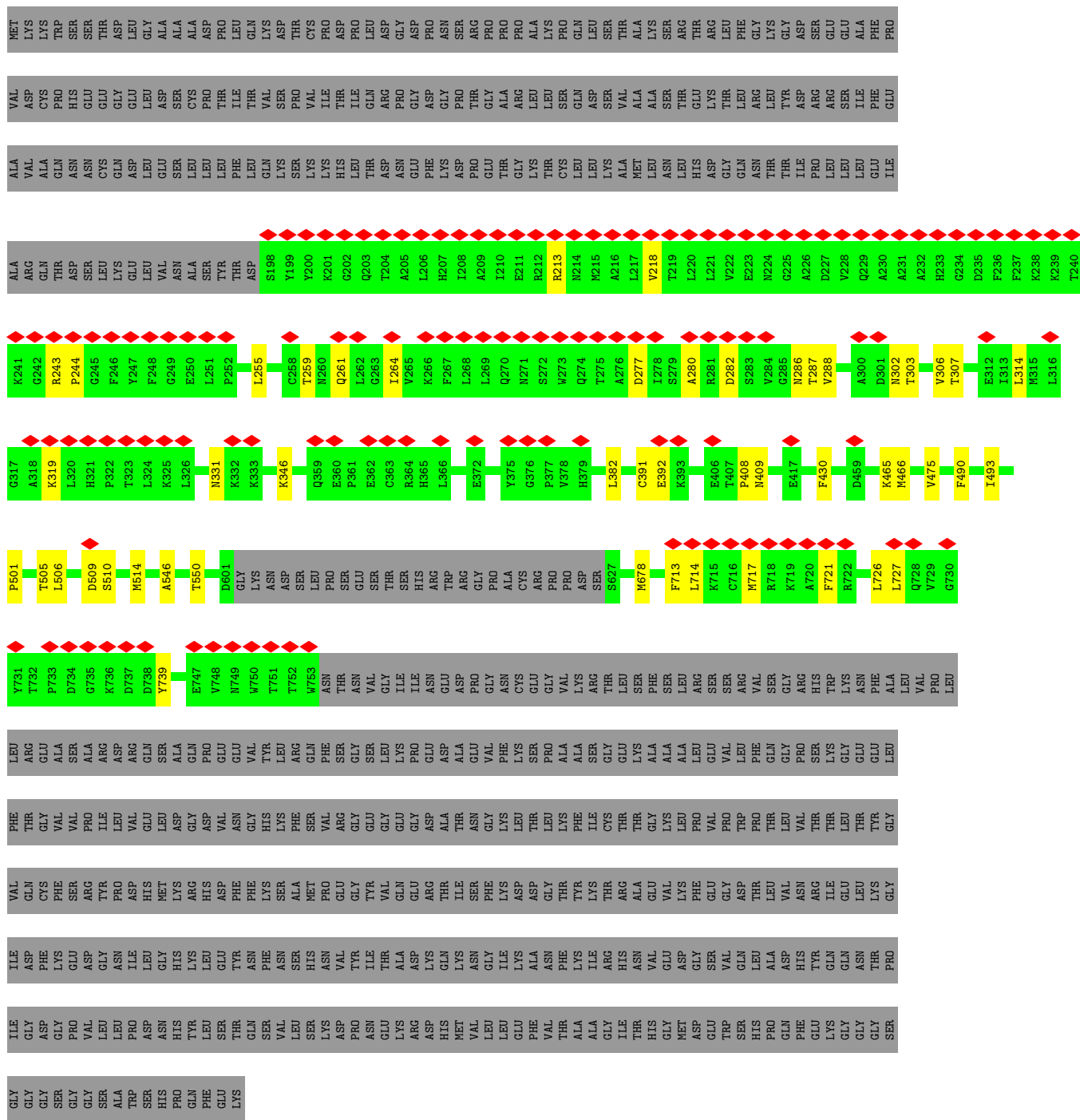
LEU	PHE	GLN	GLY	PRO	SER	LYS	GLY	GLU	LEU	PHE	THR	GLY	VAL	VAL	PRO	ILE	LEU	VAL	GLU	LEU	ASP	GLY	ASP	VAL	ASN	GLY	HIS	LYS	PHE	SER	VAL	ARG	VAL	GLY	GLY	GLY	GLY	GLY	ASP	ALA	ALA	THR	THR	ASN	GLY	LYS	LEU	LEU	THR	THR	GLY	LYS	LEU	PRO	VAL	PRO
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TRP	PRO	THR	THR	LEU	VAL	THR	THR	THR	LEU	THR	THR	TYR	GLY	VAL	GLN	CYS	PHE	SER	ARG	ARG	TYR	PRO	ASP	HIS	HIS	MET	MET	LYS	LYS	SER	ALA	ALA	MET	MET	GLU	GLU	GLY	TYR	VAL	VAL	GLN	GLU	ARG	THR	ARG	THR	THR	THR	LYS	LYS	ALA	ALA	GLU	VAL	VAL	LYS	PHE	PHE	GLY	GLY	GLY	GLY
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ASP	THR	LEU	VAL	ASN	ARG	ILE	GLU	LEU	LYS	GLY	ILE	ASP	PHE	LYS	GLU	ASP	GLY	ASN	ILE	LEU	HIS	LYS	LEU	GLU	TYR	ASN	PHE	SER	HIS	ASN	VAL	TYR	ILE	THR	ALA	ASP	LYS	GLN	LYS	ASN	GLY	ILE	LYS	ALA	ASN	PHE	ILE	LYS	ARG	HIS	ASN	VAL	GLU	ASP	GLY	SER	VAL
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GLN	LEU	ALA	ASP	HIS	TYR	GLN	GLN	ASN	THR	PRO	ILE	GLY	ASP	GLY	VAL	LEU	LEU	PRO	ASP	ASN	HIS	TYR	LEU	SER	THR	GLN	SER	VAL	LEU	SER	LYS	ASP	PRO	ASN	GLU	LYS	ARG	ASP	HIS	MET	VAL	LEU	LEU	GLU	PHE	VAL	THR	THR	HIS	GLY	GLY	MET	ASP	GLU	PRO
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- Molecule 1: Transient receptor potential cation channel subfamily V member 1, Green fluorescent protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	183350	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.866	Depositor
Minimum map value	-3.014	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.120	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	272.0, 272.0, 272.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EZI, 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	0.14	0/4413	0.33	0/5970
1	B	0.14	0/4413	0.35	0/5970
1	C	0.13	0/4413	0.33	0/5970
1	D	0.12	0/4413	0.32	0/5970
All	All	0.13	0/17652	0.33	0/23880

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4310	0	4344	34	0
1	B	4310	0	4344	38	0
1	C	4310	0	4344	26	0
1	D	4310	0	4344	31	0
2	A	23	0	0	0	0
2	B	23	0	0	0	0
2	C	23	0	0	0	0
2	D	23	0	0	0	0
3	A	28	0	46	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	46	11	0
3	C	28	0	46	10	0
3	D	28	0	46	9	0
All	All	17444	0	17560	155	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 4.

All (155) 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:D:1202:CLR:H212	3:D:1202:CLR:H183	1.55	0.89
3:C:1202:CLR:H212	3:C:1202:CLR:H183	1.55	0.89
3:B:1202:CLR:H183	3:B:1202:CLR:H212	1.55	0.88
3:A:1202:CLR:H183	3:A:1202:CLR:H212	1.55	0.87
3:B:1202:CLR:H212	3:B:1202:CLR:H121	1.63	0.79
3:A:1202:CLR:H212	3:A:1202:CLR:H121	1.63	0.79
1:D:550:THR:HG21	3:D:1202:CLR:H161	1.63	0.79
1:C:550:THR:HG21	3:C:1202:CLR:H161	1.64	0.79
3:D:1202:CLR:H212	3:D:1202:CLR:H121	1.63	0.79
3:C:1202:CLR:H212	3:C:1202:CLR:H121	1.63	0.77
1:B:550:THR:HG21	3:B:1202:CLR:H161	1.71	0.71
1:A:550:THR:HG21	3:A:1202:CLR:H161	1.71	0.71
1:D:465:LYS:HA	1:D:465:LYS:HE2	1.74	0.70
1:A:382:LEU:HD21	1:A:727:LEU:HD23	1.74	0.68
1:D:382:LEU:HD21	1:D:727:LEU:HD23	1.75	0.68
3:D:1202:CLR:H183	3:D:1202:CLR:C21	2.19	0.66
1:B:382:LEU:HD21	1:B:727:LEU:HD23	1.76	0.65
3:A:1202:CLR:H121	3:A:1202:CLR:C21	2.27	0.65
3:C:1202:CLR:H121	3:C:1202:CLR:C21	2.27	0.65
3:C:1202:CLR:H183	3:C:1202:CLR:C21	2.19	0.64
1:C:382:LEU:HD21	1:C:727:LEU:HD23	1.79	0.64
3:B:1202:CLR:H121	3:B:1202:CLR:C21	2.27	0.64
1:C:726:LEU:HD22	1:C:739:TYR:HB3	1.80	0.62
3:D:1202:CLR:H121	3:D:1202:CLR:C21	2.27	0.62
1:D:243:ARG:HG2	1:D:244:PRO:HD2	1.80	0.62
1:A:692:GLN:H	1:A:692:GLN:CD	2.07	0.61
1:A:726:LEU:HD22	1:A:739:TYR:HB3	1.82	0.61
3:A:1202:CLR:H183	3:A:1202:CLR:C21	2.19	0.61
1:D:726:LEU:HD22	1:D:739:TYR:HB3	1.83	0.61
1:D:550:THR:CG2	3:D:1202:CLR:H161	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1202:CLR:H183	3:B:1202:CLR:C21	2.18	0.59
1:C:391:CYS:SG	1:C:392:GLU:N	2.76	0.59
1:C:550:THR:CG2	3:C:1202:CLR:H161	2.32	0.58
1:B:726:LEU:HD22	1:B:739:TYR:HB3	1.85	0.57
1:B:391:CYS:SG	1:B:392:GLU:N	2.77	0.57
1:B:257:ALA:HA	1:B:309:MET:HE2	1.86	0.57
1:D:213:ARG:NH1	1:D:259:THR:O	2.38	0.57
1:A:277:ASP:HB3	1:A:280:ALA:HB2	1.87	0.56
1:D:713:PHE:HD2	1:D:714:LEU:HD22	1.71	0.56
1:C:277:ASP:HB3	1:C:280:ALA:HB2	1.87	0.55
3:C:1202:CLR:C21	3:C:1202:CLR:C12	2.85	0.55
1:B:199:TYR:OH	1:B:243:ARG:NH1	2.40	0.55
1:B:713:PHE:HD2	1:B:714:LEU:HD22	1.72	0.55
1:A:717:MET:SD	1:A:717:MET:N	2.81	0.54
1:A:550:THR:CG2	3:A:1202:CLR:H161	2.38	0.54
1:C:717:MET:SD	1:C:717:MET:N	2.81	0.54
1:D:717:MET:SD	1:D:717:MET:N	2.80	0.54
1:A:713:PHE:HD2	1:A:714:LEU:HD22	1.73	0.53
3:A:1202:CLR:C21	3:A:1202:CLR:C12	2.85	0.53
1:D:303:THR:O	1:D:307:THR:HG23	2.09	0.53
3:B:1202:CLR:C21	3:B:1202:CLR:C12	2.85	0.53
1:C:199:TYR:OH	1:C:243:ARG:NH1	2.42	0.53
1:A:391:CYS:SG	1:A:392:GLU:N	2.82	0.53
1:B:277:ASP:HB3	1:B:280:ALA:HB2	1.89	0.53
1:D:391:CYS:SG	1:D:392:GLU:N	2.82	0.52
1:A:243:ARG:HG2	1:A:244:PRO:HD2	1.90	0.52
1:B:550:THR:CG2	3:B:1202:CLR:H161	2.38	0.52
1:B:717:MET:CE	1:B:719:LYS:H	2.22	0.52
1:B:213:ARG:NH1	1:B:259:THR:O	2.43	0.52
1:B:430:PHE:CZ	1:B:721:PHE:HB2	2.45	0.52
1:C:243:ARG:HG2	1:C:244:PRO:HD2	1.92	0.51
3:D:1202:CLR:C21	3:D:1202:CLR:C12	2.85	0.51
1:C:713:PHE:HD2	1:C:714:LEU:HD22	1.75	0.51
3:C:1202:CLR:H212	3:C:1202:CLR:C18	2.25	0.51
3:A:1202:CLR:H212	3:A:1202:CLR:C12	2.32	0.51
1:D:255:LEU:O	1:D:259:THR:OG1	2.23	0.50
1:C:509:ASP:OD2	1:C:510:SER:N	2.44	0.50
1:A:213:ARG:NH1	1:A:259:THR:O	2.45	0.49
1:B:327:GLU:OE2	1:B:356:ARG:NH2	2.39	0.49
1:A:443:CYS:O	1:A:447:ILE:HG13	2.13	0.49
1:C:430:PHE:CZ	1:C:721:PHE:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:GLU:N	1:A:328:GLU:OE1	2.46	0.49
1:B:408:PRO:HB2	1:B:409:ASN:OD1	2.13	0.49
1:B:443:CYS:O	1:B:447:ILE:HG13	2.12	0.49
1:C:213:ARG:NH1	1:C:259:THR:O	2.46	0.49
1:C:328:GLU:N	1:C:328:GLU:OE1	2.45	0.49
1:A:199:TYR:OH	1:A:243:ARG:NH1	2.46	0.48
3:B:1202:CLR:H212	3:B:1202:CLR:C12	2.32	0.48
1:C:443:CYS:O	1:C:447:ILE:HG13	2.13	0.48
1:B:328:GLU:N	1:B:328:GLU:OE1	2.46	0.48
1:D:501:PRO:HG2	1:D:506:LEU:HD12	1.94	0.48
1:B:572:MET:HE2	1:D:678:MET:HE3	1.94	0.48
1:B:287:THR:HG22	1:B:288:VAL:H	1.79	0.48
1:A:430:PHE:CZ	1:A:721:PHE:HB2	2.48	0.48
1:B:546:ALA:HB3	3:B:1202:CLR:H263	1.96	0.48
1:D:287:THR:HG22	1:D:288:VAL:H	1.79	0.47
1:A:287:THR:HG22	1:A:288:VAL:H	1.79	0.47
1:C:490:PHE:HD2	1:C:493:ILE:HD11	1.79	0.47
1:D:277:ASP:HB3	1:D:280:ALA:HB2	1.96	0.47
1:A:546:ALA:HB3	3:A:1202:CLR:H263	1.95	0.47
1:B:642:THR:HG23	1:B:676:LEU:HD11	1.96	0.47
1:A:490:PHE:HD2	1:A:493:ILE:HD11	1.79	0.47
1:B:243:ARG:HG2	1:B:244:PRO:HD2	1.96	0.46
3:B:1202:CLR:H212	3:B:1202:CLR:C18	2.25	0.46
1:A:408:PRO:HB2	1:A:409:ASN:OD1	2.15	0.46
1:C:642:THR:HG23	1:C:676:LEU:HD11	1.97	0.46
1:B:261:GLN:HB3	1:B:264:ILE:HD13	1.98	0.46
1:C:261:GLN:HB3	1:C:264:ILE:HD13	1.96	0.46
1:D:505:THR:O	1:D:505:THR:OG1	2.33	0.46
1:B:526:THR:HG21	1:B:541:MET:HB2	1.98	0.46
1:C:287:THR:HG22	1:C:288:VAL:H	1.81	0.46
3:D:1202:CLR:H212	3:D:1202:CLR:C18	2.25	0.46
1:A:568:MET:O	1:A:572:MET:HG2	2.16	0.45
1:B:255:LEU:O	1:B:259:THR:OG1	2.24	0.45
1:C:546:ALA:HB3	3:C:1202:CLR:H263	1.98	0.45
1:B:302:ASN:O	1:B:306:VAL:HG23	2.16	0.45
1:D:490:PHE:HD2	1:D:493:ILE:HD11	1.81	0.45
1:D:261:GLN:HB3	1:D:264:ILE:HD13	1.99	0.45
1:B:466:MET:SD	1:B:475:VAL:HG21	2.57	0.45
1:C:466:MET:SD	1:C:475:VAL:HG21	2.57	0.45
1:A:572:MET:HG3	1:B:678:MET:HE3	1.99	0.44
1:D:466:MET:SD	1:D:475:VAL:HG21	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:GLN:HB3	1:A:264:ILE:HD13	1.99	0.44
1:B:325:LYS:HB3	1:B:328:GLU:OE1	2.17	0.44
1:D:546:ALA:HB3	3:D:1202:CLR:H263	1.99	0.44
1:A:325:LYS:HB3	1:A:328:GLU:OE1	2.18	0.44
1:D:408:PRO:HB2	1:D:409:ASN:OD1	2.18	0.44
1:A:302:ASN:O	1:A:306:VAL:HG23	2.18	0.43
1:C:302:ASN:O	1:C:306:VAL:HG23	2.18	0.43
3:C:1202:CLR:H211	3:C:1202:CLR:H232	1.89	0.43
1:D:302:ASN:O	1:D:306:VAL:HG23	2.18	0.43
1:A:372:GLU:CD	1:A:744:ARG:HH21	2.26	0.43
1:B:466:MET:HE3	1:B:466:MET:HB3	1.83	0.43
1:D:286:ASN:OD1	1:D:331:ASN:ND2	2.43	0.43
1:B:379:HIS:CE1	1:B:747:GLU:HB2	2.54	0.42
1:A:471:ASP:N	1:A:471:ASP:OD1	2.52	0.42
1:B:478:GLU:H	1:B:478:GLU:HG2	1.73	0.42
1:A:417:GLU:OE2	1:A:421:ARG:NH1	2.53	0.42
1:A:526:THR:HG21	1:A:541:MET:HB2	2.02	0.42
1:D:430:PHE:CZ	1:D:721:PHE:HB2	2.55	0.42
1:A:505:THR:O	1:A:505:THR:OG1	2.34	0.41
1:B:269:LEU:HD13	1:B:316:LEU:HD22	2.02	0.41
1:D:346:LYS:HA	1:D:346:LYS:HD3	1.71	0.41
1:B:738:ASP:OD1	1:B:738:ASP:N	2.50	0.41
3:A:1202:CLR:H211	3:A:1202:CLR:H232	1.89	0.41
1:C:325:LYS:HB3	1:C:328:GLU:OE1	2.20	0.41
1:A:361:PRO:C	1:A:363:CYS:H	2.28	0.41
1:B:361:PRO:C	1:B:363:CYS:H	2.28	0.41
1:A:309:MET:O	1:A:313:ILE:HG22	2.21	0.41
1:B:509:ASP:OD1	1:B:510:SER:N	2.54	0.41
1:A:246:PHE:CE2	1:A:248:PHE:HB3	2.56	0.41
1:D:314:LEU:HD23	1:D:314:LEU:HA	1.89	0.41
3:B:1202:CLR:H232	3:B:1202:CLR:H211	1.89	0.41
1:C:379:HIS:CE1	1:C:747:GLU:HB2	2.56	0.41
1:D:282:ASP:OD1	1:D:286:ASN:N	2.54	0.41
1:B:218:VAL:HG11	1:B:264:ILE:HG12	2.02	0.40
1:C:255:LEU:O	1:C:259:THR:OG1	2.25	0.40
1:D:218:VAL:HG11	1:D:264:ILE:HG12	2.03	0.40
1:B:299:THR:HG22	1:B:302:ASN:HB2	2.03	0.40
1:B:314:LEU:HD23	1:B:314:LEU:HA	1.96	0.40
1:A:319:LYS:HE3	1:A:319:LYS:HB3	1.87	0.40
1:C:361:PRO:C	1:C:363:CYS:H	2.29	0.40
1:D:319:LYS:HE3	1:D:319:LYS:HB3	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:THR:HG22	1:A:302:ASN:HB2	2.02	0.40
1:D:509:ASP:OD1	1:D:510:SER:N	2.55	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	527/1112 (47%)	504 (96%)	23 (4%)	0	100	100
1	B	527/1112 (47%)	500 (95%)	27 (5%)	0	100	100
1	C	527/1112 (47%)	502 (95%)	25 (5%)	0	100	100
1	D	527/1112 (47%)	499 (95%)	28 (5%)	0	100	100
All	All	2108/4448 (47%)	2005 (95%)	103 (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	467/965 (48%)	467 (100%)	0	100	100
1	B	467/965 (48%)	466 (100%)	1 (0%)	87	93
1	C	467/965 (48%)	466 (100%)	1 (0%)	87	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	467/965 (48%)	466 (100%)	1 (0%)	87	93
All	All	1868/3860 (48%)	1865 (100%)	3 (0%)	85	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	505	THR
1	C	600	GLU
1	D	514	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	ASN
1	A	394	ASN
1	A	749	ASN
1	B	224	ASN
1	C	224	ASN
1	C	311	ASN
1	C	749	ASN
1	D	270	GLN
1	D	494	GLN
1	D	749	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
3	CLR	B	1202	-	31,31,31	0.53	0	48,48,48	1.77	9 (18%)
2	EZI	B	1201	-	25,25,25	2.41	7 (28%)	33,36,36	1.57	6 (18%)
3	CLR	D	1202	-	31,31,31	0.53	0	48,48,48	1.77	9 (18%)
2	EZI	C	1201	-	25,25,25	2.42	8 (32%)	33,36,36	1.57	6 (18%)
2	EZI	A	1201	-	25,25,25	2.41	7 (28%)	33,36,36	1.57	6 (18%)
3	CLR	C	1202	-	31,31,31	0.53	0	48,48,48	1.78	9 (18%)
2	EZI	D	1201	-	25,25,25	2.41	8 (32%)	33,36,36	1.56	6 (18%)
3	CLR	A	1202	-	31,31,31	0.53	0	48,48,48	1.78	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	B	1202	-	-	2/10/68/68	0/4/4/4
2	EZI	B	1201	-	-	0/10/10/10	0/3/3/3
3	CLR	D	1202	-	-	2/10/68/68	0/4/4/4
2	EZI	C	1201	-	-	0/10/10/10	0/3/3/3
2	EZI	A	1201	-	-	0/10/10/10	0/3/3/3
3	CLR	C	1202	-	-	2/10/68/68	0/4/4/4
2	EZI	D	1201	-	-	0/10/10/10	0/3/3/3
3	CLR	A	1202	-	-	2/10/68/68	0/4/4/4

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1201	EZI	C08-C09	-6.16	1.35	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	EZI	C08-C09	-6.10	1.35	1.47
2	B	1201	EZI	C08-C09	-6.10	1.35	1.47
2	C	1201	EZI	C08-C09	-6.10	1.35	1.47
2	C	1201	EZI	C07-N04	6.06	1.35	1.29
2	A	1201	EZI	C07-N04	5.97	1.35	1.29
2	B	1201	EZI	C07-N04	5.97	1.35	1.29
2	D	1201	EZI	C07-N04	5.94	1.35	1.29
2	A	1201	EZI	C09-N03	-4.24	1.32	1.40
2	C	1201	EZI	C09-N03	-4.24	1.32	1.40
2	B	1201	EZI	C09-N03	-4.22	1.32	1.40
2	D	1201	EZI	C09-N03	-4.16	1.32	1.40
2	B	1201	EZI	C10-N04	-4.05	1.32	1.39
2	A	1201	EZI	C10-N04	-4.03	1.32	1.39
2	C	1201	EZI	C10-N04	-4.03	1.32	1.39
2	D	1201	EZI	C10-N04	-4.03	1.32	1.39
2	A	1201	EZI	C22-C23	3.87	1.52	1.44
2	B	1201	EZI	C22-C23	3.86	1.52	1.44
2	C	1201	EZI	C22-C23	3.86	1.52	1.44
2	D	1201	EZI	C22-C23	3.86	1.52	1.44
2	B	1201	EZI	C08-C10	-3.18	1.36	1.40
2	A	1201	EZI	C08-C10	-3.12	1.36	1.40
2	C	1201	EZI	C08-C10	-3.12	1.36	1.40
2	D	1201	EZI	C08-C10	-3.12	1.36	1.40
2	D	1201	EZI	C07-N03	-2.03	1.36	1.39
2	A	1201	EZI	O01-C09	-2.03	1.18	1.22
2	B	1201	EZI	O01-C09	-2.03	1.18	1.22
2	C	1201	EZI	O01-C09	-2.03	1.18	1.22
2	C	1201	EZI	C07-N03	-2.01	1.36	1.39
2	D	1201	EZI	O01-C09	-2.00	1.18	1.22

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1202	CLR	C13-C17-C20	-7.12	108.50	119.50
3	B	1202	CLR	C13-C17-C20	-7.12	108.50	119.50
3	A	1202	CLR	C13-C17-C20	-7.11	108.52	119.50
3	D	1202	CLR	C13-C17-C20	-7.08	108.57	119.50
2	A	1201	EZI	N03-C07-N04	-5.05	119.83	124.21
2	C	1201	EZI	N03-C07-N04	-5.04	119.85	124.21
2	B	1201	EZI	N03-C07-N04	-5.03	119.86	124.21
2	D	1201	EZI	N03-C07-N04	-4.95	119.93	124.21
2	A	1201	EZI	C08-C09-N03	4.23	120.47	114.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1201	EZI	C08-C09-N03	4.20	120.44	114.69
2	B	1201	EZI	C08-C09-N03	4.20	120.44	114.69
2	C	1201	EZI	C08-C09-N03	4.20	120.43	114.69
3	A	1202	CLR	C16-C17-C13	-4.14	98.97	103.84
3	D	1202	CLR	C16-C17-C13	-4.10	99.01	103.84
3	C	1202	CLR	C16-C17-C13	-4.10	99.01	103.84
3	B	1202	CLR	C16-C17-C13	-4.08	99.05	103.84
3	A	1202	CLR	C22-C20-C17	3.54	117.66	110.33
3	C	1202	CLR	C22-C20-C17	3.53	117.64	110.33
3	D	1202	CLR	C22-C20-C17	3.52	117.63	110.33
3	B	1202	CLR	C22-C20-C17	3.51	117.61	110.33
3	D	1202	CLR	C18-C13-C17	-3.49	105.34	111.68
3	B	1202	CLR	C18-C13-C17	-3.47	105.39	111.68
3	C	1202	CLR	C18-C13-C17	-3.46	105.41	111.68
3	A	1202	CLR	C18-C13-C17	-3.45	105.42	111.68
2	C	1201	EZI	C16-C11-N03	3.20	123.48	119.65
2	B	1201	EZI	C16-C11-N03	3.18	123.46	119.65
2	D	1201	EZI	C16-C11-N03	3.13	123.40	119.65
2	A	1201	EZI	C16-C11-N03	3.11	123.38	119.65
3	D	1202	CLR	O1-C3-C4	2.67	115.72	109.71
3	B	1202	CLR	O1-C3-C4	2.66	115.71	109.71
3	C	1202	CLR	O1-C3-C4	2.65	115.68	109.71
3	A	1202	CLR	O1-C3-C4	2.63	115.63	109.71
2	A	1201	EZI	C08-C10-N04	-2.59	119.81	122.41
2	C	1201	EZI	C08-C10-N04	-2.59	119.81	122.41
2	D	1201	EZI	C08-C10-N04	-2.59	119.81	122.41
2	B	1201	EZI	C08-C10-N04	-2.59	119.81	122.41
3	A	1202	CLR	C17-C13-C14	2.47	102.94	100.10
3	D	1202	CLR	C17-C13-C14	2.46	102.93	100.10
3	C	1202	CLR	C17-C13-C14	2.46	102.92	100.10
3	B	1202	CLR	C17-C13-C14	2.43	102.88	100.10
3	D	1202	CLR	C15-C16-C17	2.39	109.83	105.14
3	A	1202	CLR	C15-C16-C17	2.39	109.82	105.14
3	B	1202	CLR	C15-C16-C17	2.38	109.80	105.14
3	C	1202	CLR	C15-C16-C17	2.37	109.78	105.14
2	B	1201	EZI	C17-C11-N03	-2.28	116.93	119.65
2	C	1201	EZI	C17-C11-N03	-2.26	116.94	119.65
2	D	1201	EZI	C17-C11-N03	-2.24	116.97	119.65
2	A	1201	EZI	C17-C11-N03	-2.23	116.99	119.65
2	A	1201	EZI	C10-N04-C07	2.19	120.49	117.46
2	B	1201	EZI	C10-N04-C07	2.19	120.49	117.46
3	A	1202	CLR	C21-C20-C17	-2.19	109.60	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1202	CLR	C21-C20-C17	-2.19	109.60	112.88
3	B	1202	CLR	C21-C20-C17	-2.18	109.61	112.88
3	C	1202	CLR	C21-C20-C17	-2.17	109.63	112.88
2	C	1201	EZI	C10-N04-C07	2.16	120.45	117.46
2	D	1201	EZI	C10-N04-C07	2.15	120.44	117.46
3	A	1202	CLR	C3-C4-C5	-2.12	108.67	112.05
3	C	1202	CLR	C3-C4-C5	-2.09	108.72	112.05
3	B	1202	CLR	C3-C4-C5	-2.09	108.73	112.05
3	D	1202	CLR	C3-C4-C5	-2.06	108.76	112.05

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1202	CLR	C22-C23-C24-C25
3	B	1202	CLR	C22-C23-C24-C25
3	C	1202	CLR	C22-C23-C24-C25
3	D	1202	CLR	C22-C23-C24-C25
3	A	1202	CLR	C16-C17-C20-C21
3	B	1202	CLR	C16-C17-C20-C21
3	C	1202	CLR	C16-C17-C20-C21
3	D	1202	CLR	C16-C17-C20-C21

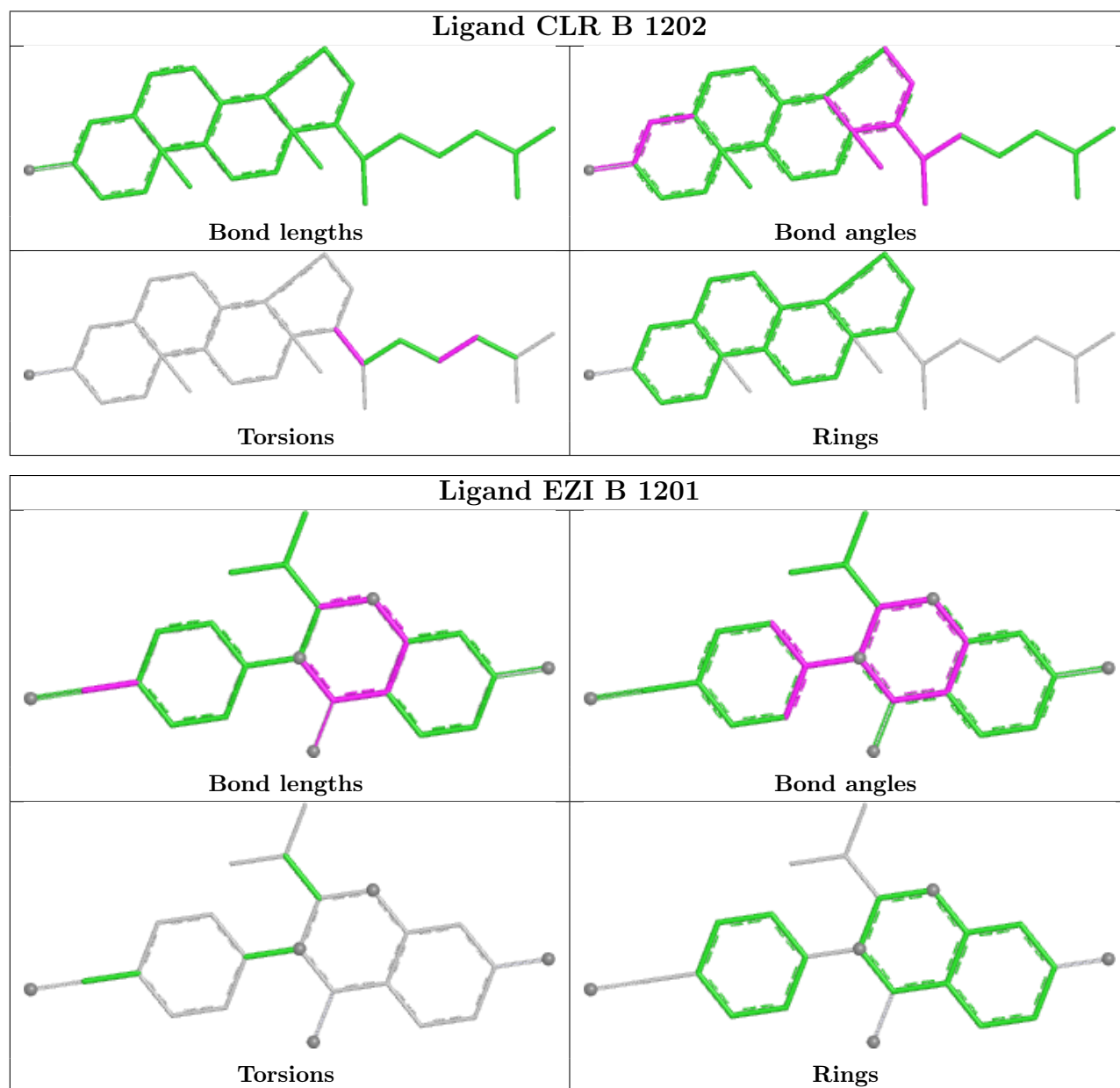
There are no ring outliers.

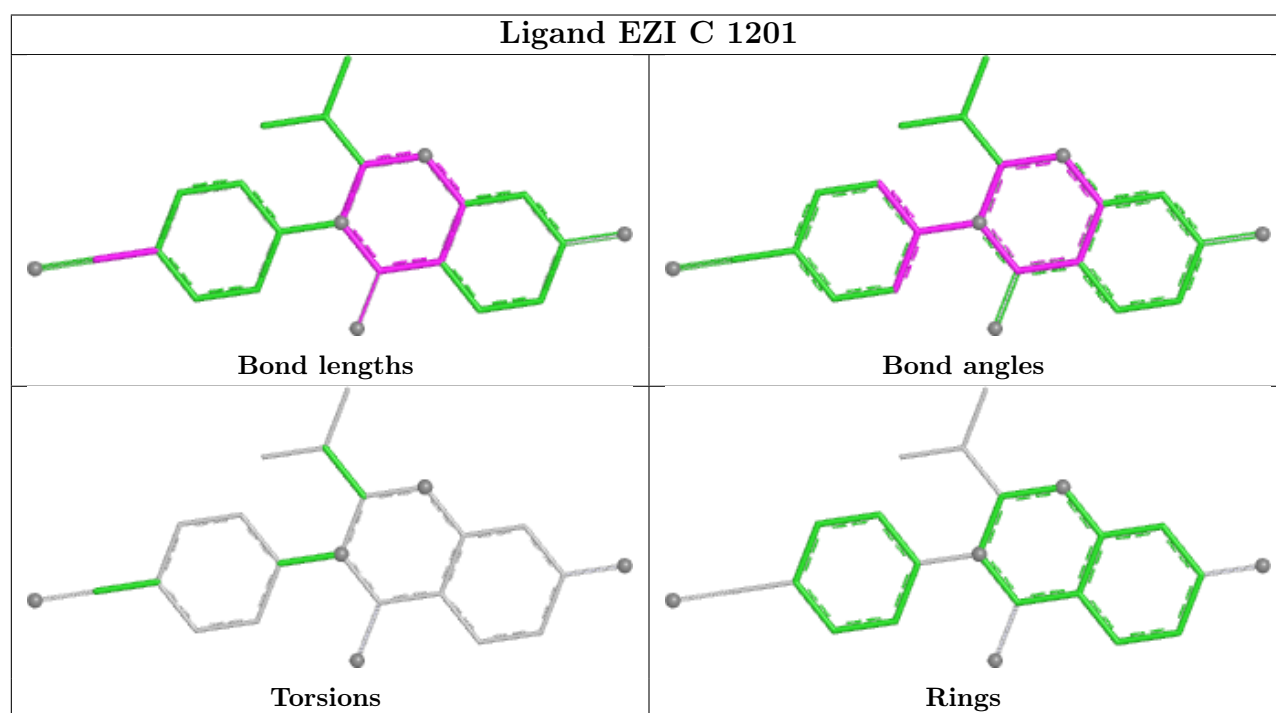
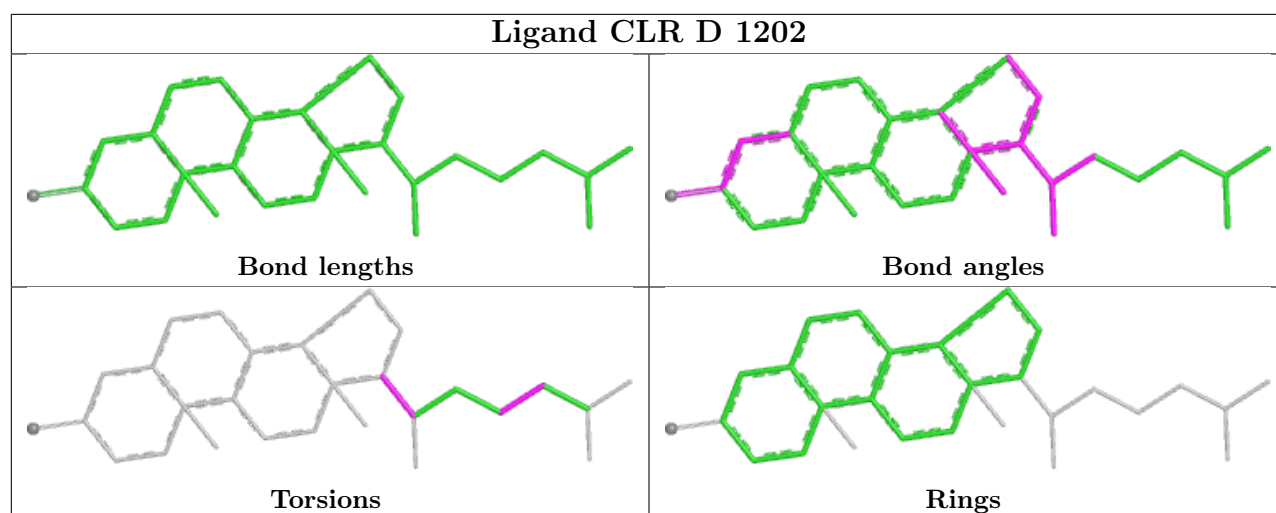
4 monomers are involved in 40 short contacts:

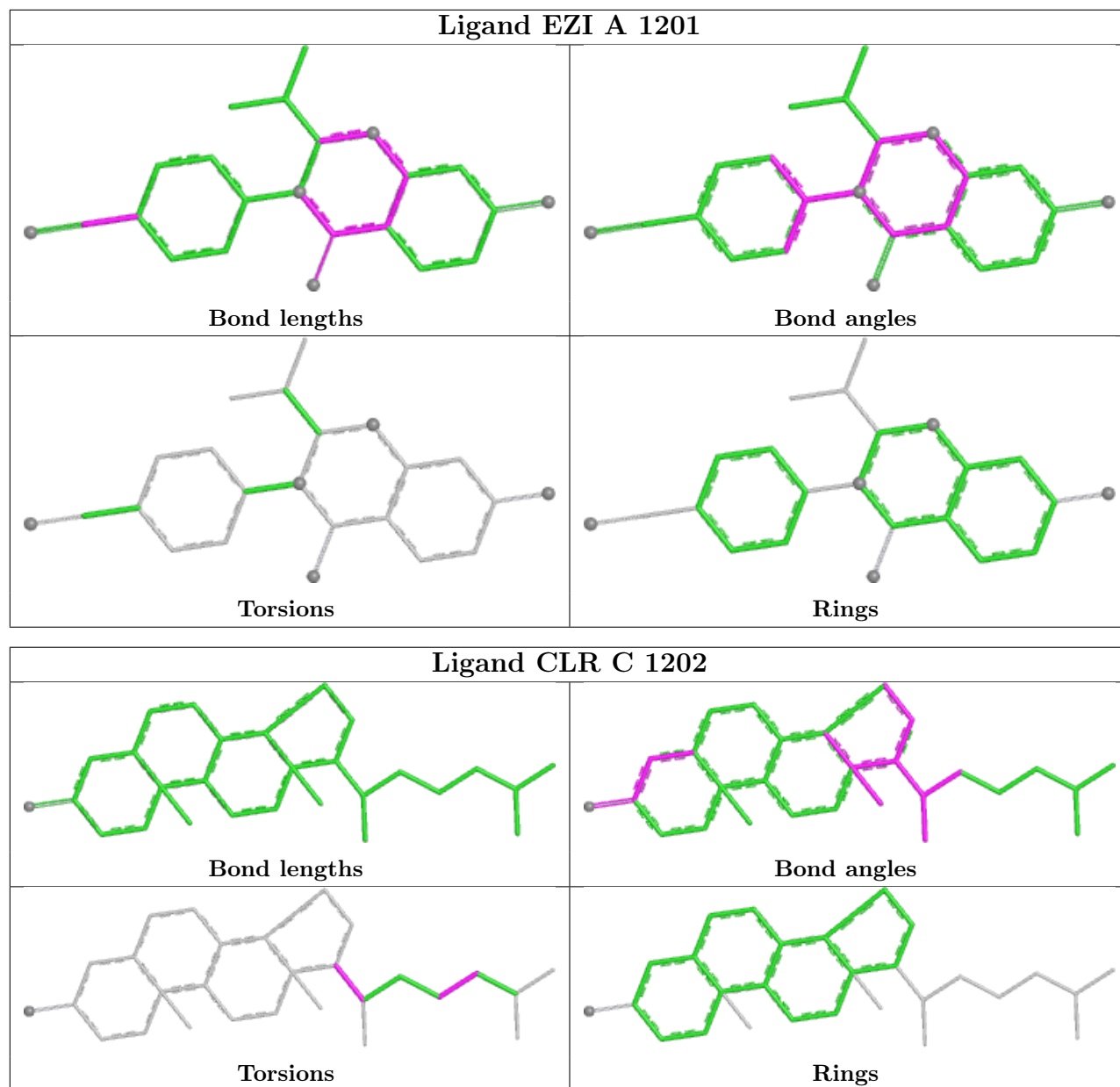
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1202	CLR	11	0
3	D	1202	CLR	9	0
3	C	1202	CLR	10	0
3	A	1202	CLR	10	0

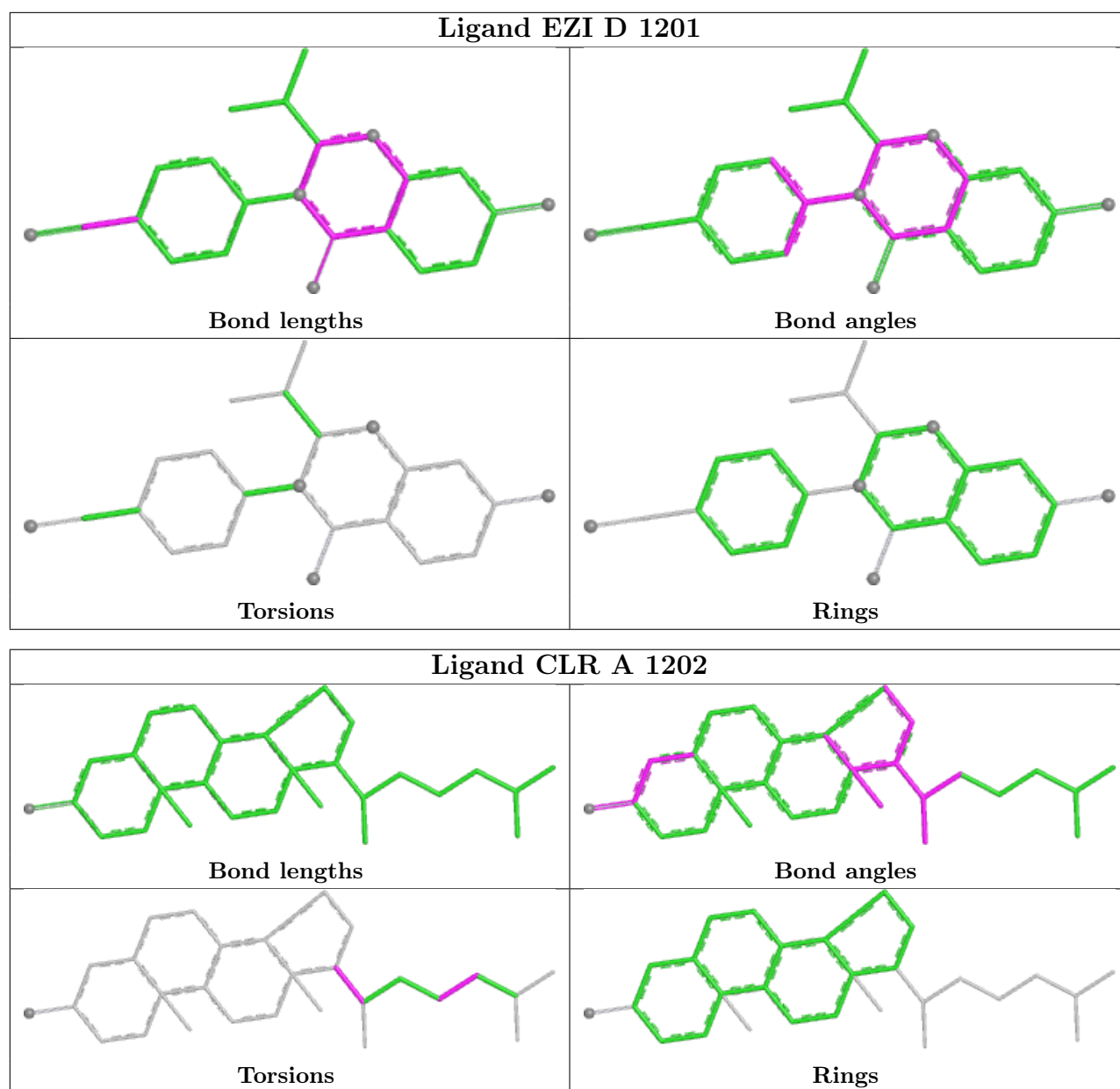
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









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.

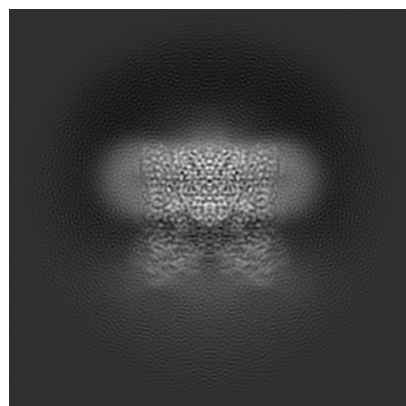
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38161. These allow visual inspection of the internal detail of the map and identification of artifacts.

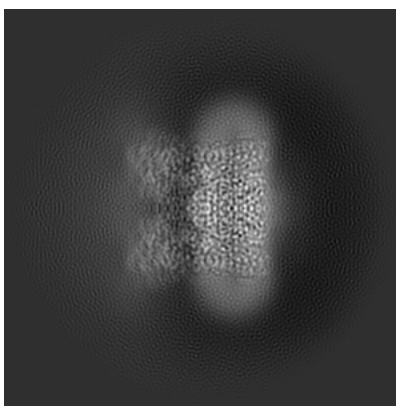
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

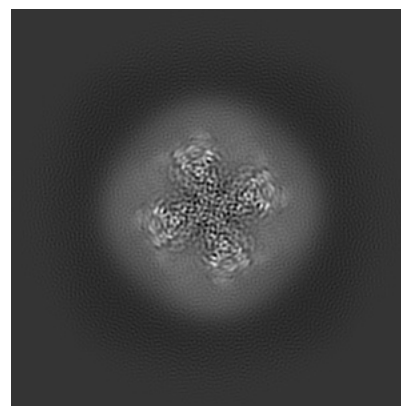
6.1.1 Primary map



X

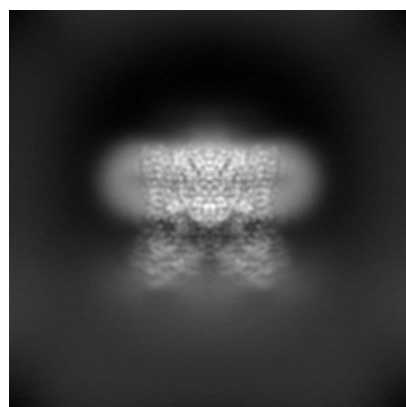


Y

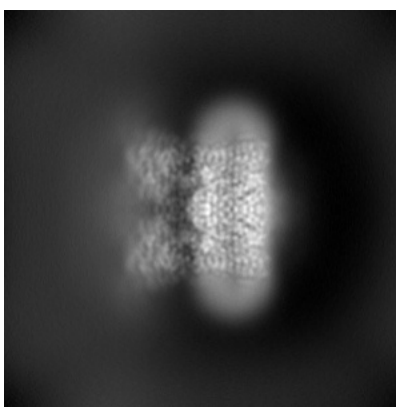


Z

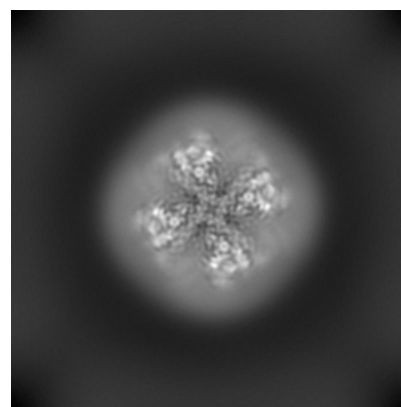
6.1.2 Raw map



X



Y

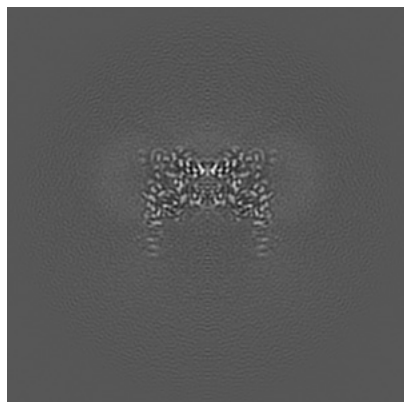


Z

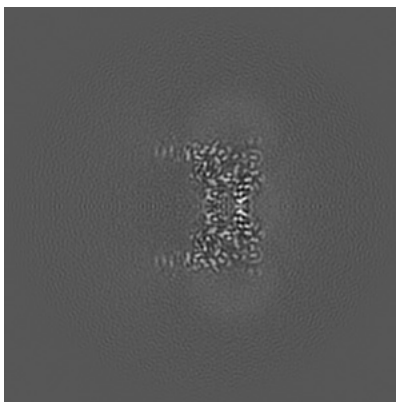
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

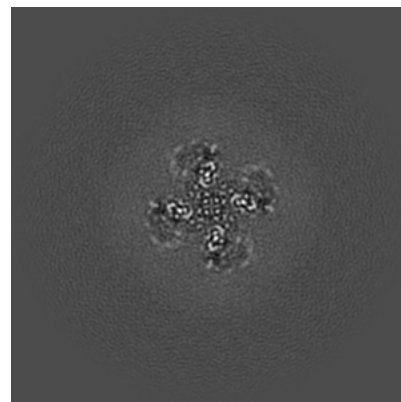
6.2.1 Primary map



X Index: 160

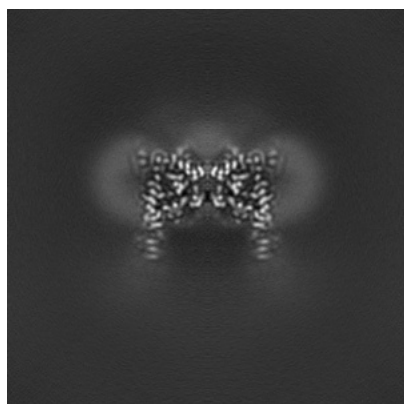


Y Index: 160

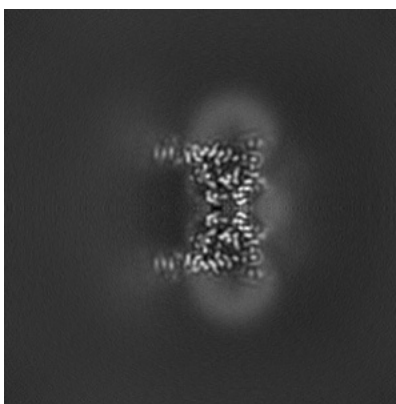


Z Index: 160

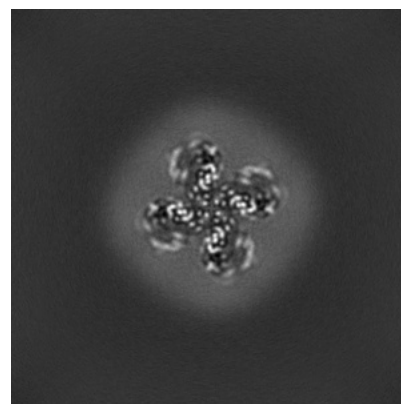
6.2.2 Raw map



X Index: 160



Y Index: 160

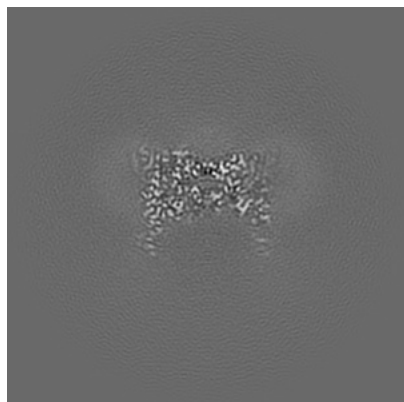


Z Index: 160

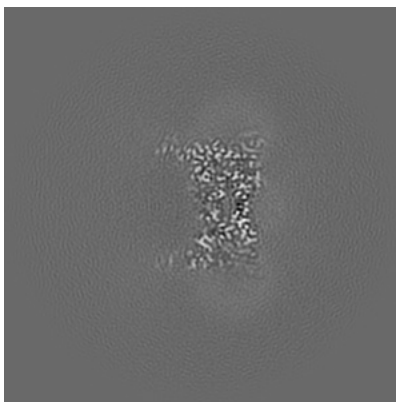
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

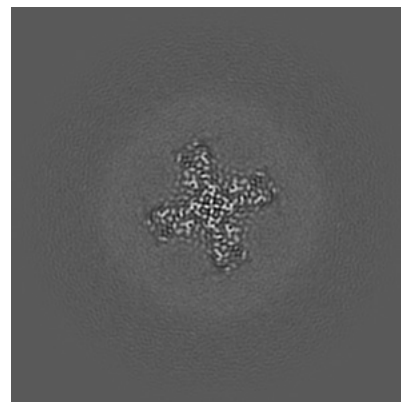
6.3.1 Primary map



X Index: 162

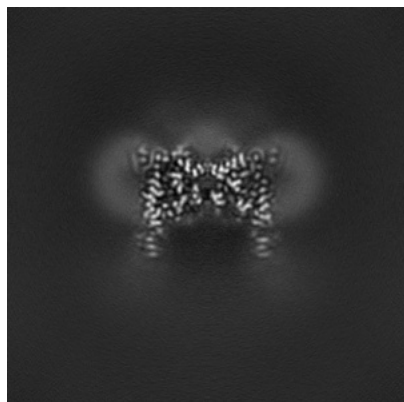


Y Index: 162

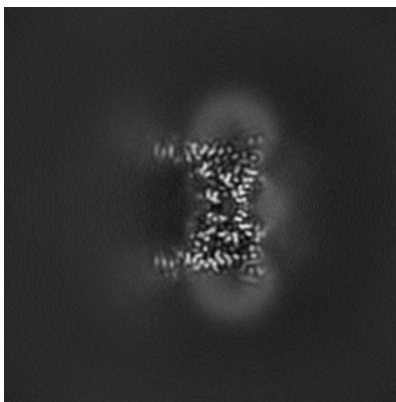


Z Index: 189

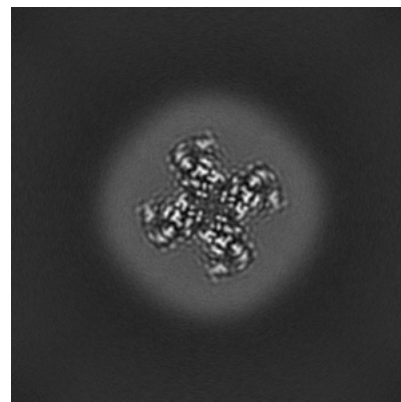
6.3.2 Raw map



X Index: 161



Y Index: 159

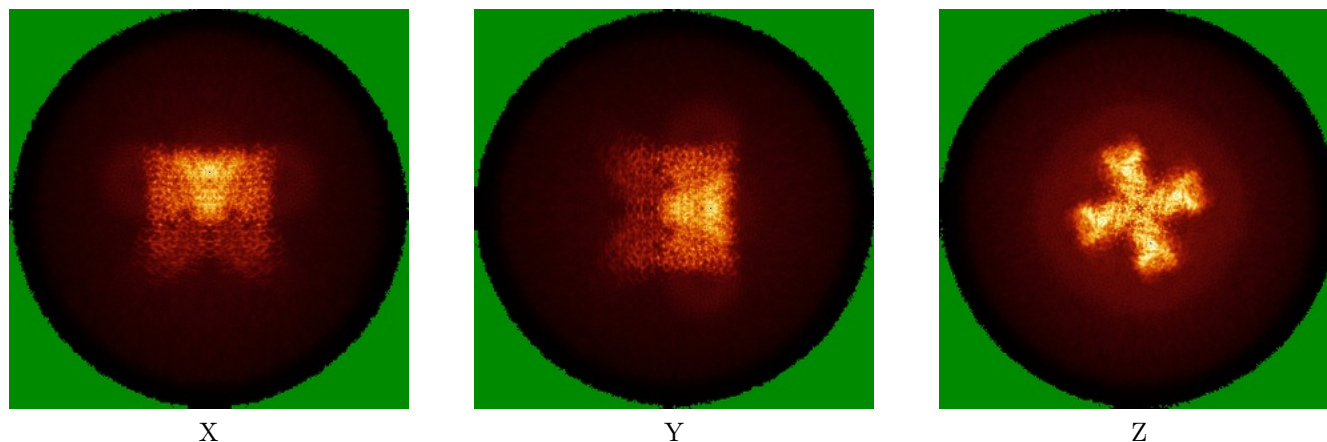


Z Index: 197

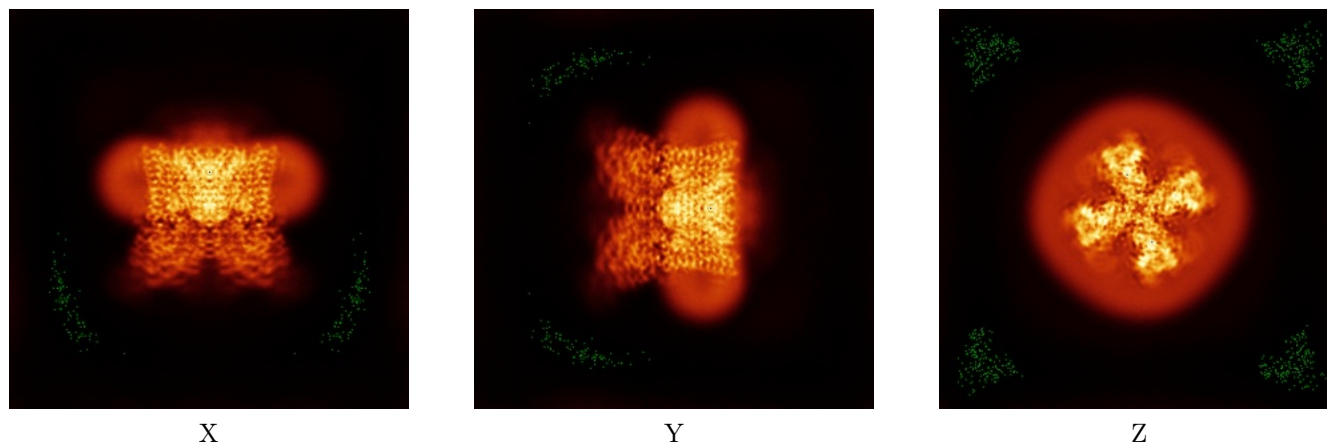
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map



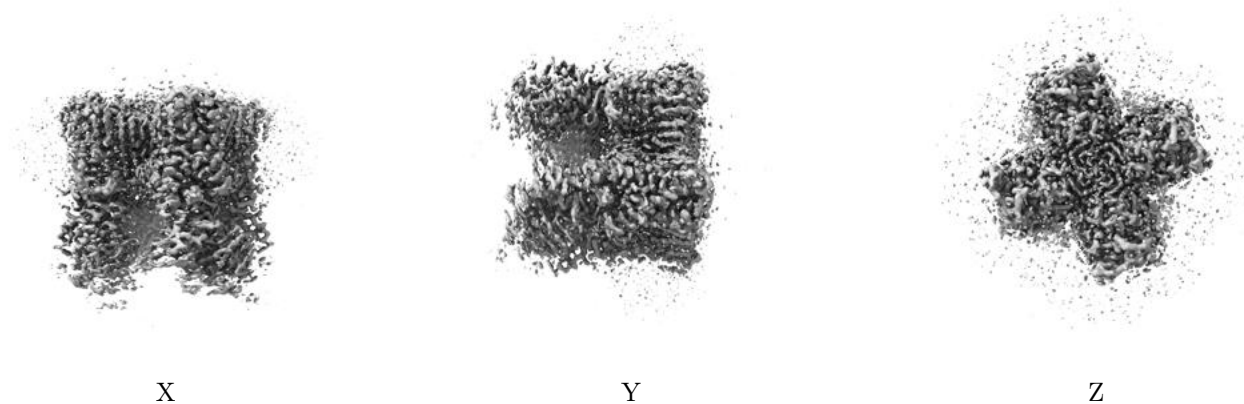
6.4.2 Raw map



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.

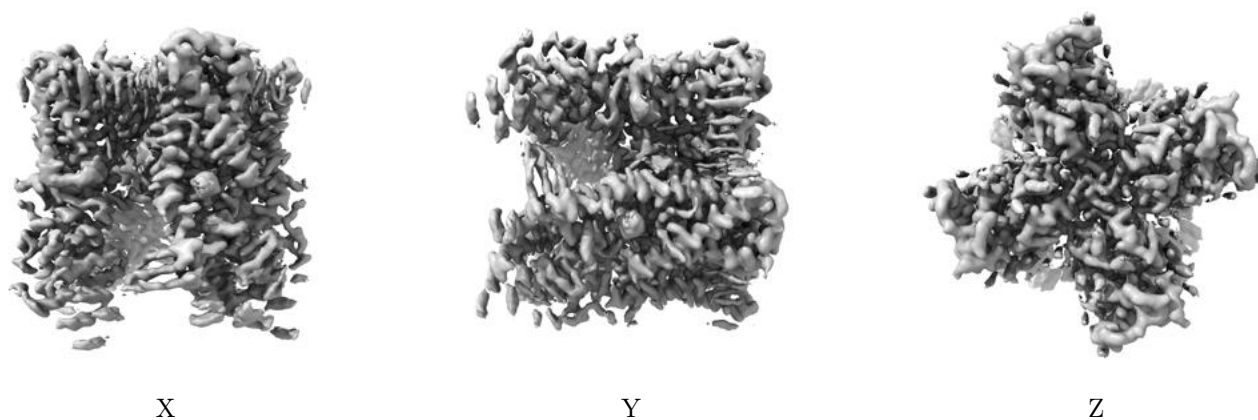
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

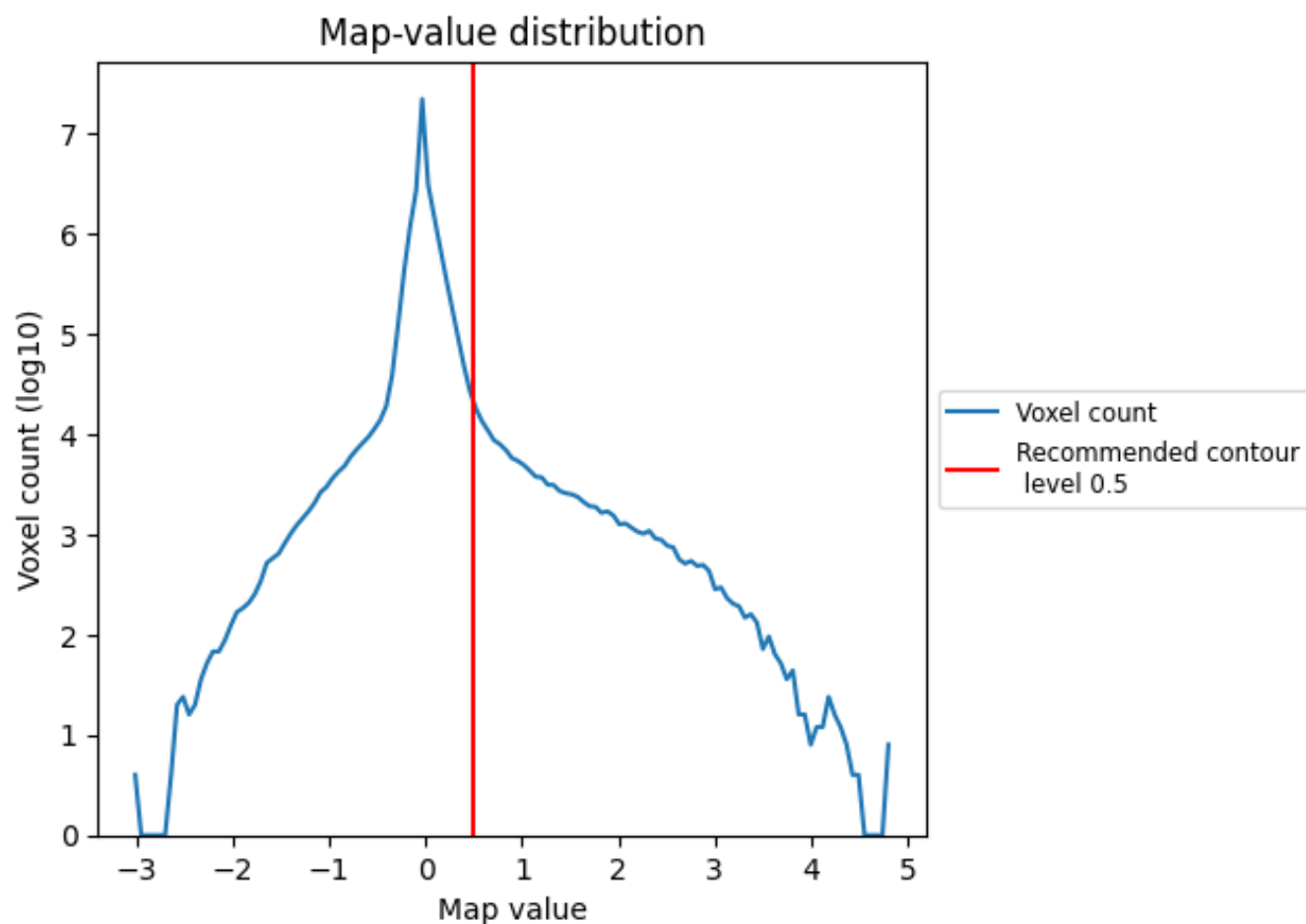
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

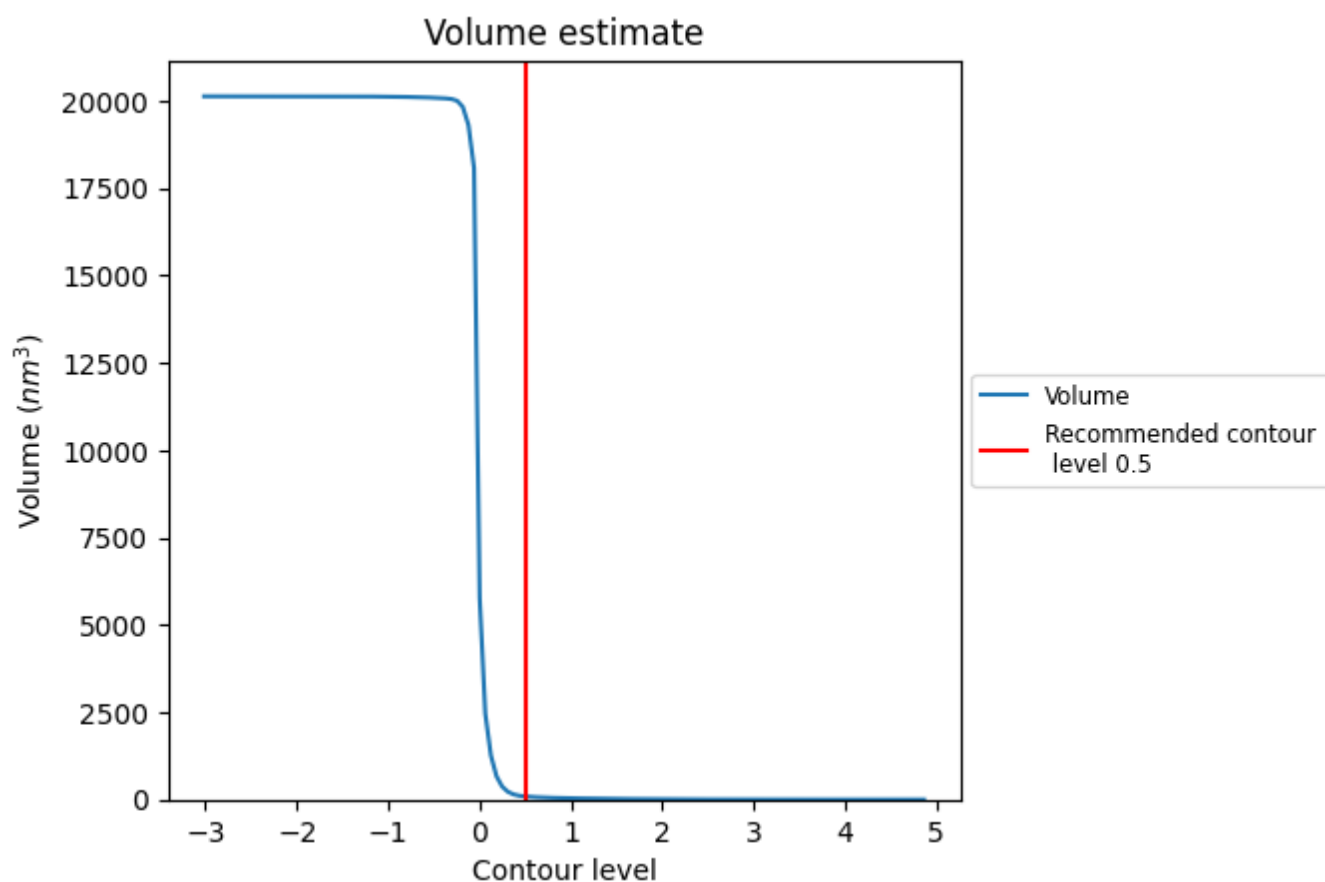
This section contains the results of statistical analysis of the map.

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.

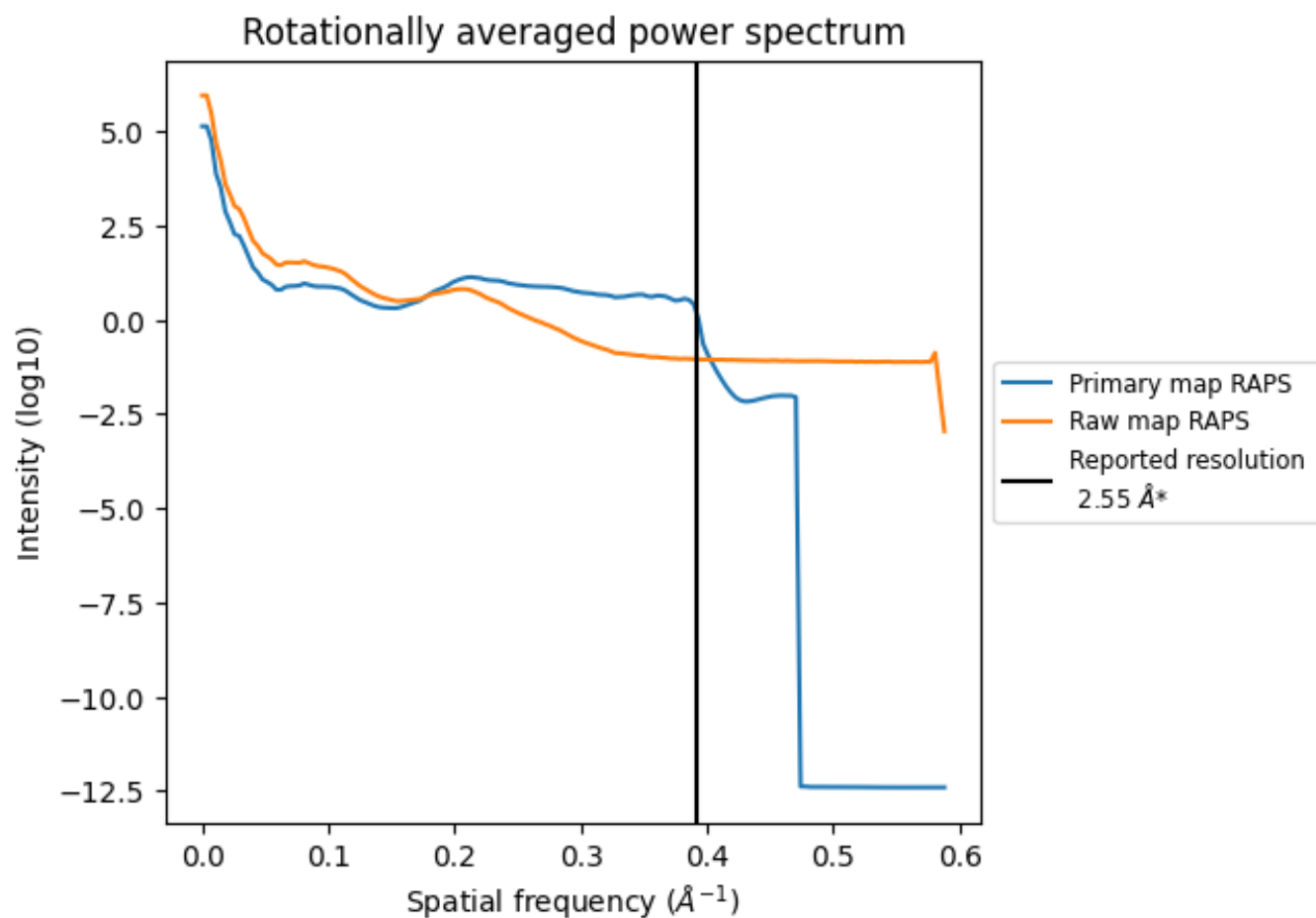
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 89 nm³; this corresponds to an approximate mass of 80 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 ⓘ

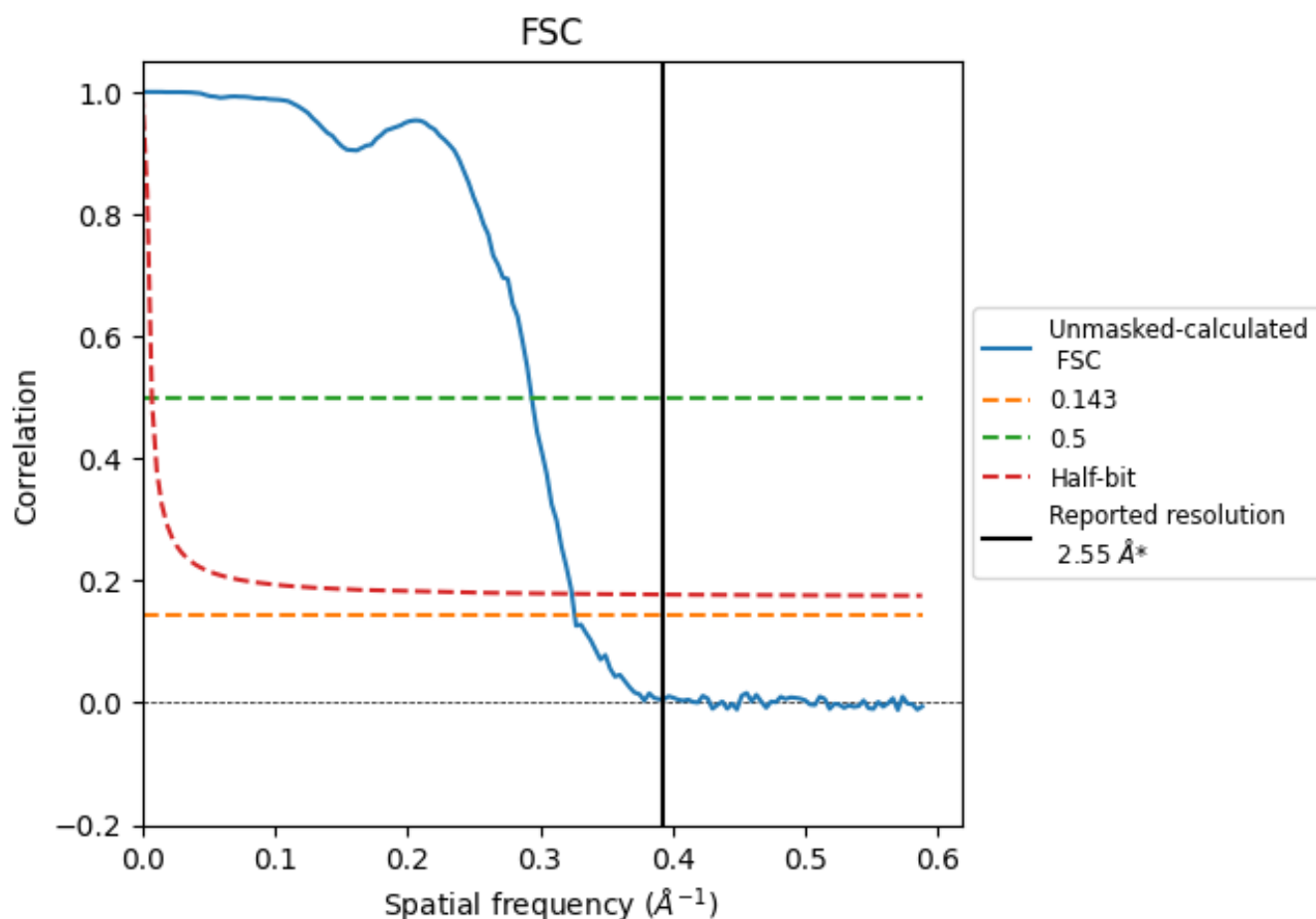


*Reported resolution corresponds to spatial frequency of 0.392 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.392 Å⁻¹

8.2 Resolution estimates [i](#)

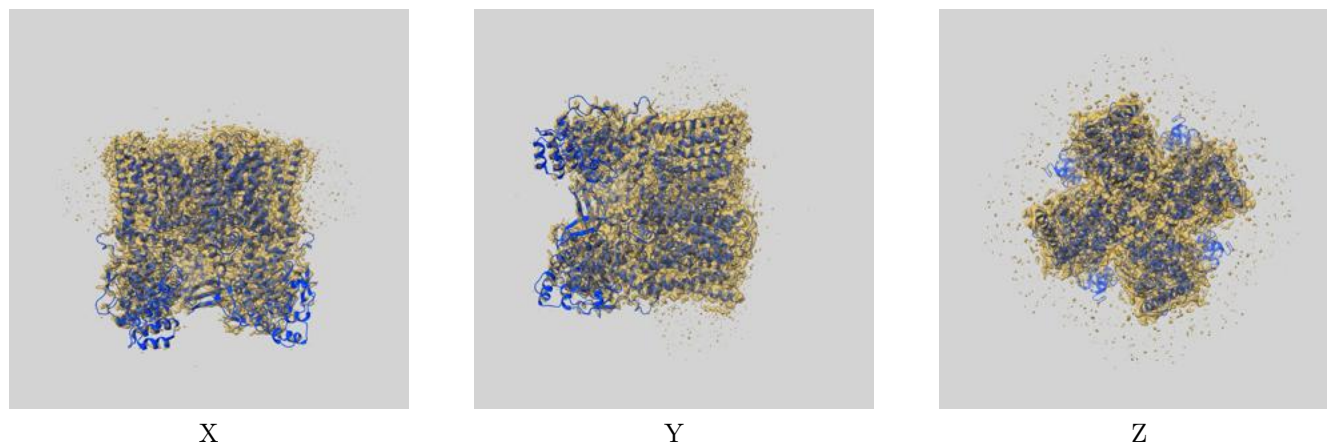
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.55	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.07	3.40	3.09

*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 3.07 differs from the reported value 2.55 by more than 10 %

9 Map-model fit [i](#)

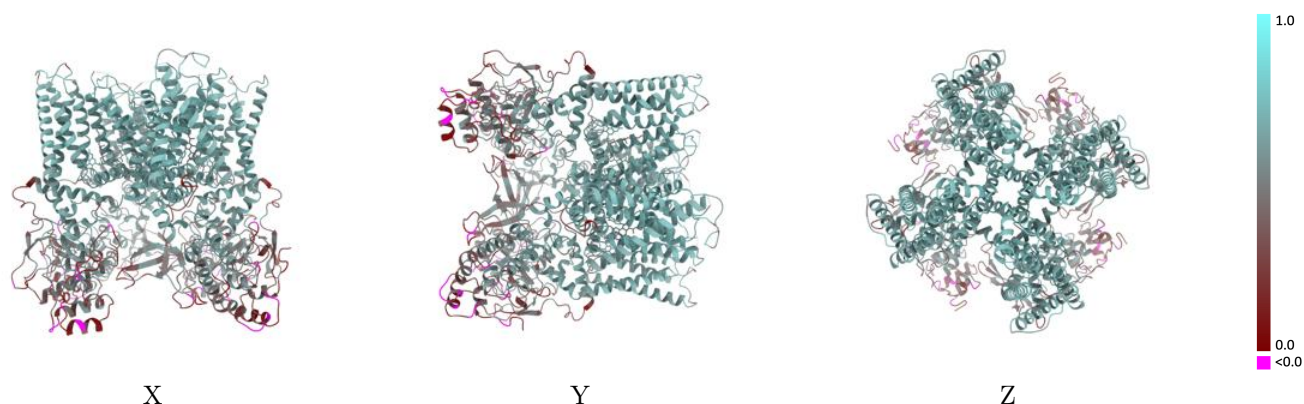
This section contains information regarding the fit between EMDB map EMD-38161 and PDB model 8X94. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



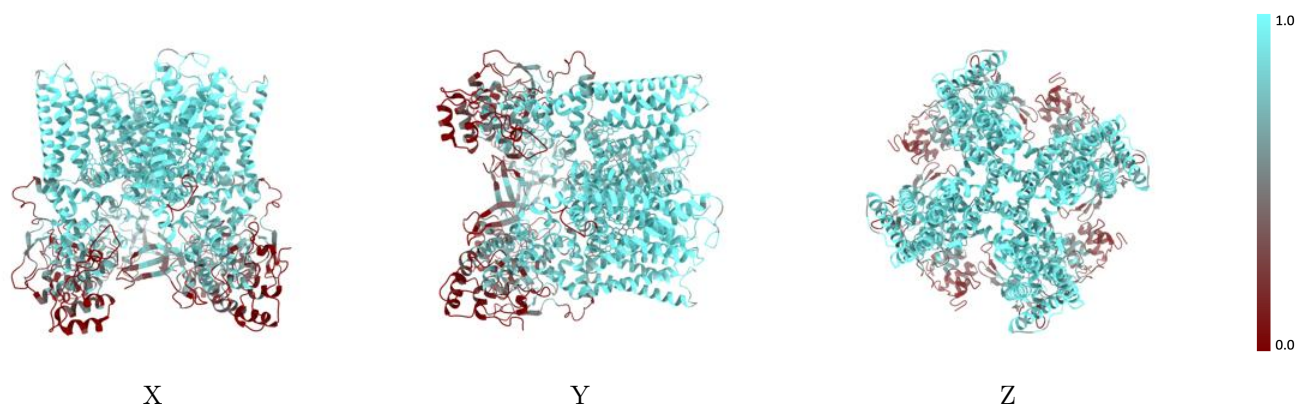
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



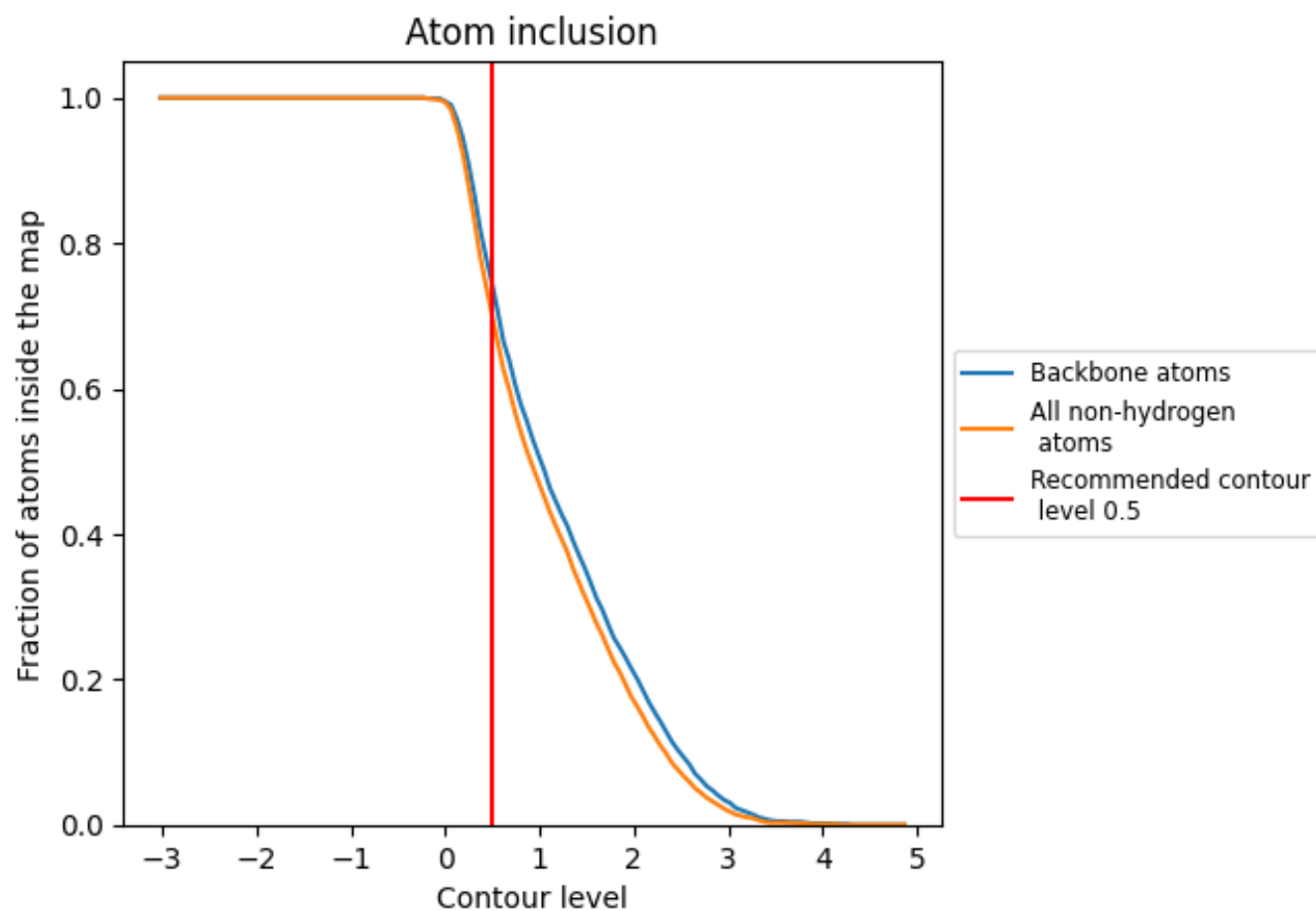
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 70% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6990	0.5360
A	0.7000	0.5350
B	0.6970	0.5330
C	0.7000	0.5380
D	0.6980	0.5390

