



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 12:15 AM UTC

PDB ID : 8JQR / pdb_00008jqr
EMDB ID : EMD-36577
Title : Structure of human TRPV1 in complex with antagonist
Authors : Fan, J.; Lei, X.
Deposited on : 2023-06-14
Resolution : 2.75 Å(reported)

This is a wwPDB EM Validation Summary 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

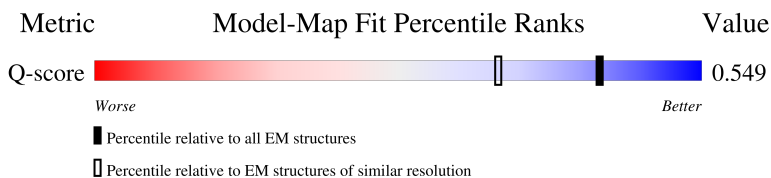
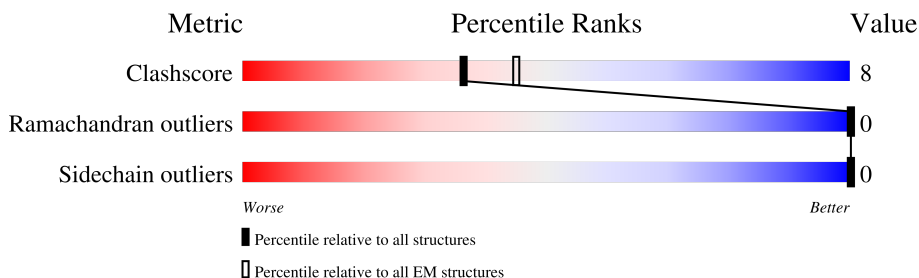
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.75 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	10570 (2.25 - 3.25)

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	10% 38% 10% 52%
1	B	1112	10% 38% 10% 52%
1	C	1112	9% 39% 9% 52%
1	D	1112	10% 39% 9% 52%

2 Entry composition

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.

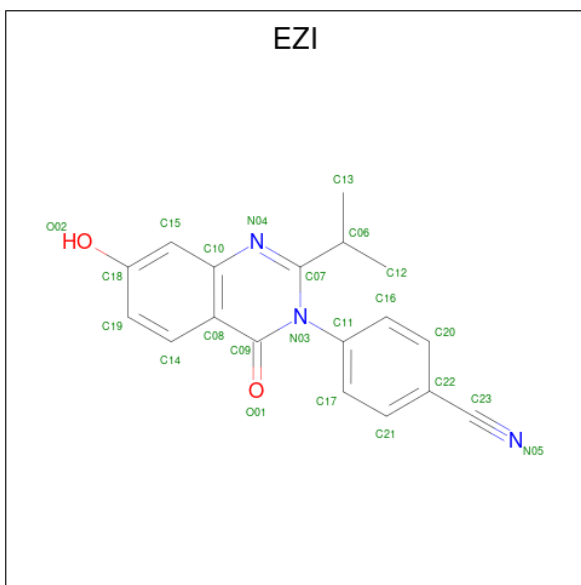
- Molecule 1 is a protein called Transient receptor potential cation channel subfamily V member 1, PreScission Site, Green fluorescent protein.

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		

There are 12 discrepancies between the modelled and reference sequences:

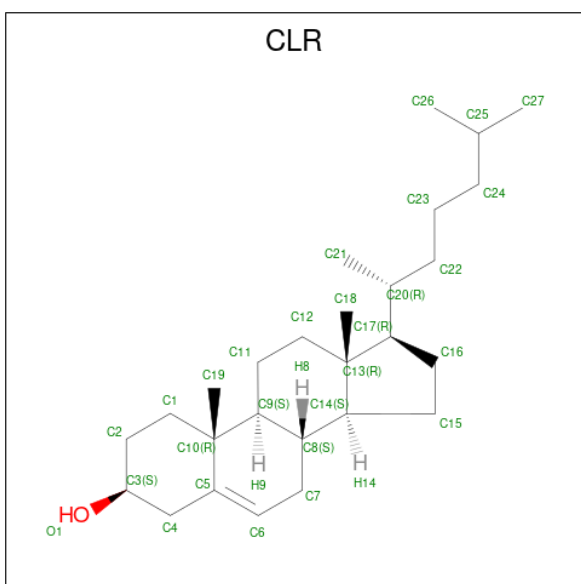
Chain	Residue	Modelled	Actual	Comment	Reference
A	840	ALA	-	linker	UNP Q8NER1
A	841	ALA	-	linker	UNP Q8NER1
A	842	ALA	-	linker	UNP Q8NER1
B	840	ALA	-	linker	UNP Q8NER1
B	841	ALA	-	linker	UNP Q8NER1
B	842	ALA	-	linker	UNP Q8NER1
C	840	ALA	-	linker	UNP Q8NER1
C	841	ALA	-	linker	UNP Q8NER1
C	842	ALA	-	linker	UNP Q8NER1
D	840	ALA	-	linker	UNP Q8NER1
D	841	ALA	-	linker	UNP Q8NER1
D	842	ALA	-	linker	UNP Q8NER1

- Molecule 2 is 4-(7-Hydroxy-2-isopropyl-4-oxoquinazolin-3(4H)-yl)benzonitrile (CCD ID: EZI) (formula: C₁₈H₁₅N₃O₂) (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	
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).

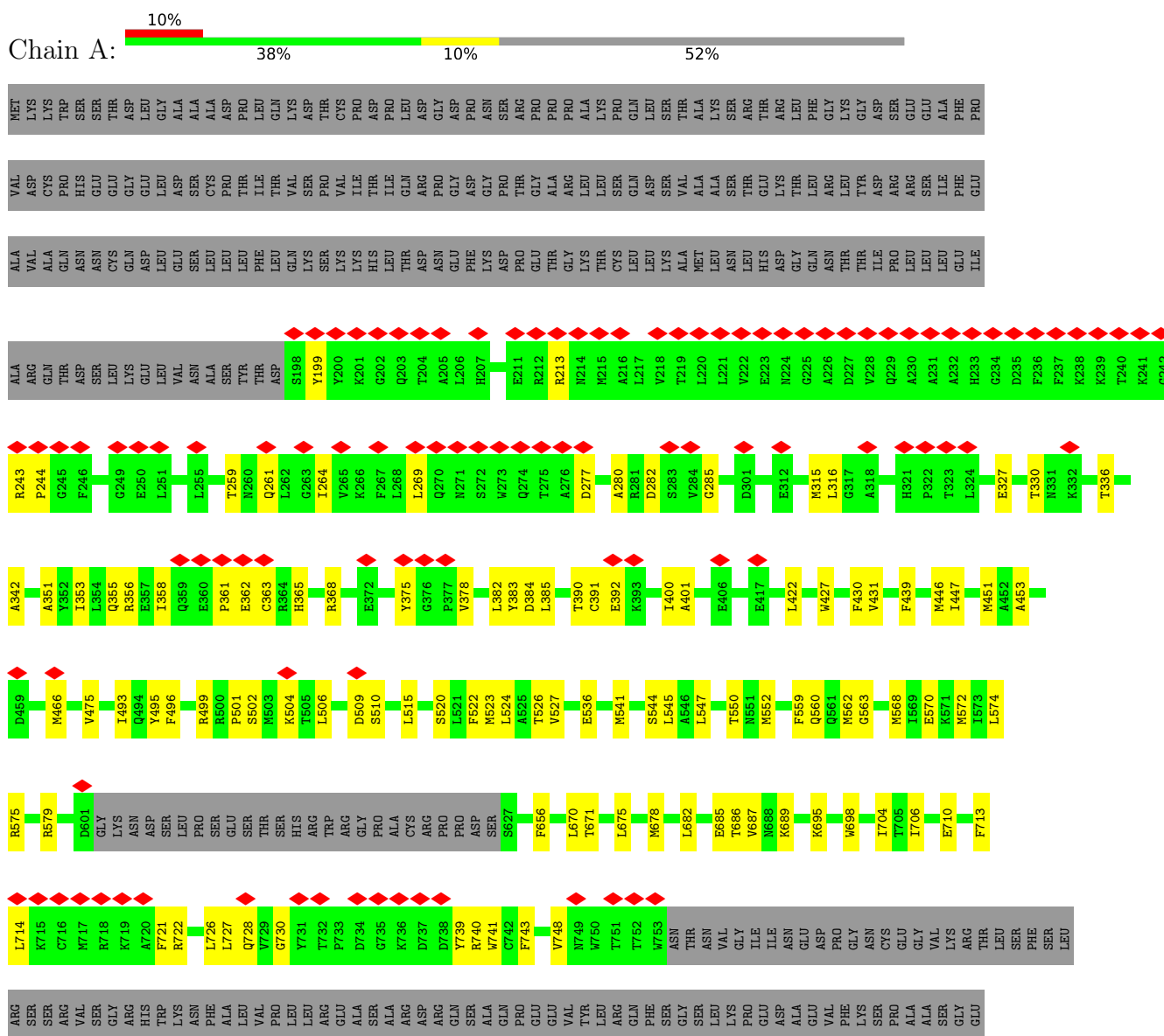


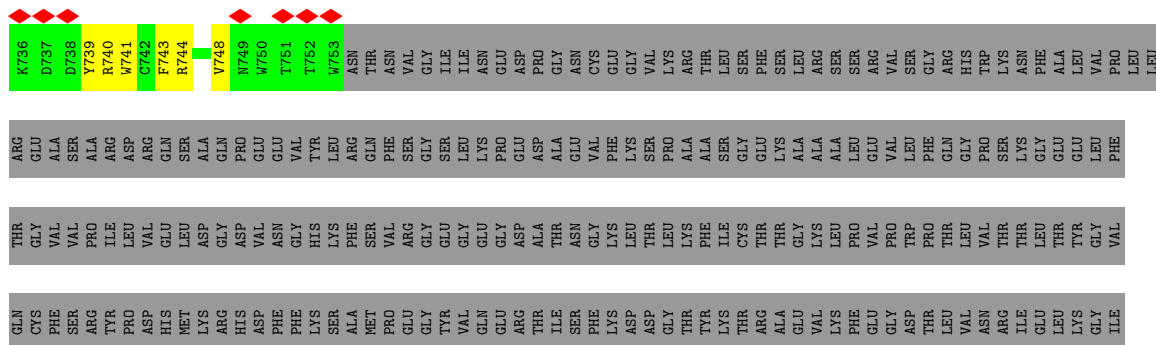
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total 28	C 27	O 1	0
3	B	1	Total 28	C 27	O 1	0
3	C	1	Total 28	C 27	O 1	0
3	D	1	Total 28	C 27	O 1	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

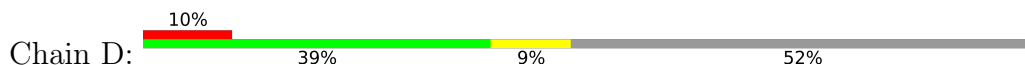
- Molecule 1: Transient receptor potential cation channel subfamily V member 1, PreScission Site, Green fluorescent protein





[illegible]

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



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

R243	P244	G245	G246	G249	F250	L251	L255	T259	M260	G261	L262	G263	L264	V265	G266	F267	L268	L269	G270	Z271	N271	S272	G273	Q274	T275	A276	D277	A280	E281	D282	G283	V284	G285	D301	M311	E312	M315	L316	G317	A318	H321	P322	T323	L324	E327	K332	A342	A351
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Year	Country	Value	Change
Y352			
I353			
L354			
Q355			
R356			
F357			
I358			
Q359			
E360			
P361			
E362			
C363			
R364			
R368			
E372			
Y375			
G376			
P377			
V378			
L382			
Y383			
D384			
L385			
S386			
C387			
I388			
D389			
T390			
C391			
E392			
K393			
T400			
A401			
E406			
E417			
L422			
W427			
F430			
V431			
F439			
I447			
M451			
R456			
D459			

Category	Value	Color
M466	1493	Red
I493	1496	Green
F496	1499	Green
R499	1500	Red
S501	1502	Green
S602	1503	Red
M503	1504	Green
K504	1505	Green
T505	1506	Green
L506	1509	Red
D509	1510	Green
S510	1515	Green
L515	1541	Green
M541	1547	Green
L547	1550	Green
T550	1551	Green
M551	1552	Green
M552	1559	Green
F559	1560	Green
Q560	1561	Green
Q561	1562	Green
M562	1563	Green
G563	1568	Green
M568	1572	Green
M572	1573	Green
T573	1574	Green
L574	1575	Green
R575	1579	Green
R579	1597	Green
T597	1601	Red
D601	GLY	Grey
LYS	GLY	Grey
ASN	ASN	Grey
ASP	ASP	Grey
SER	SER	Grey
LEU	LEU	Grey
PRO	PRO	Grey
THR	THR	Grey
SER	SER	Grey
HIS	HIS	Grey
ARG	ARG	Grey

[illegible]

Y739	E740	W741	F742	F743	W748	N749	W750	T751	T752	W753	ASN	THR	THR	ASN	ASN	VAL	GLY	ILE	ILE	ASN	ASN	ASN	CYS	GLU	GLY	VAL	LYS	ARG	THR	LEU	SER	PHE	SER	SER	SER	ARG	VAL	SER	GLY	ARG	HIS	TRP	LYS	ASN	PHE	ALA	LEU	VAL	PRO	LEU	ARG	GLU	ALA	SER
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ALA	ARG	ASP	ARG	GLN	SER	ALA	GLN	PRO	GLU	GLU	VAL	TYR	LEU	ARG	GLN	PHE	SER	GLY	SER	LEU	LYS	PRO	GLU	ASP	ALA	GLU	VAL	PHE	LYS	SER	PRO	ALA	ALA	SER	GLY	GLU	LYS	VAL	LEU	GLU	VAL	GLN	PRO	GLY	GLY	GLU	LEU	PHE	THR	GLY	VAL	VAL
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PRO	ILE	LEU	LEU	VAL	GLU	LEU	ASP	GLY	ASP	ASN	ASN	GLY	GLY	HIS	LYS	PHE	SER	VAL	VAL	ARG	GLY	GLU	GLY	GLU	GLY	ASP	ALA	THR	ASN	GLY	LYS	PHE	CYS	THR	THR	GLY	GLY	LEU	LEU	PRO	VAL	PRO	PRO	TRP	PRO	THR	THR	THR	LEU	VAL	THR	THR	GLY	VAL	GLN	CYS	PHE	PHE
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ARG	TTR	PRO	ASP	HIS	MET	LYS	ARG	ARG	HIS	ASP	PHE	PHI	LYS	SER	ALA	ALA	MET	PRO	GLU	GLY	TTR	VAL	GLN	GLU	ARG	THR	SER	SER	PHE	ASP	ASP	GLY	GLY	TTR	TTR	LYS	LYS	THR	THR	ARG	ALA	GLU	GLU	VAL	VAL	LYS	PHE	PHI	GLU	GLY	ASP	ASP	THR	THR	LEU	VAL	ASN	ARG	ILE	ILE	GLU	LYS	LEU	LYS	GLY	ILE	GLY	ASP	PHE	LYS	THR	THR
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ASP	GLY	ASN	ASN	LEU	GLY	HIS	LYS	LEU	GLU	TYR	ASN	PHE	ASN	HIS	ASN	ASN	VAL	TYR	LYS	GLN	LYS	ASN	ASN	PHE	LEU	LEU	ARG	HIS	ASN	VAL	GLN	LEU	ASP	GLY	GLY	SER	VAL	GLN	LEU	ALA	ASP	HIS	TYR	GLN	ASN	THR	PRO	ILE	GLY	ASP	GLY	PRO
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	239934	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 K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	8.094	Depositor
Minimum map value	-5.269	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.133	Depositor
Recommended contour level	0.7	Depositor
Map size ($\text{\AA}$)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	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: CLR, EZI

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	0.15	0/4413	0.33	0/5970
1	B	0.15	0/4413	0.33	0/5970
1	C	0.14	0/4413	0.32	0/5970
1	D	0.14	0/4413	0.32	0/5970
All	All	0.14	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	73	0
1	B	4310	0	4344	74	0
1	C	4310	0	4344	62	0
1	D	4310	0	4344	63	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	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	46	3	0
3	C	28	0	46	7	0
3	D	28	0	46	6	0
All	All	17444	0	17560	269	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 8.

The worst 5 of 269 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:579:ARG:HA	1:D:562:MET:HE1	1.69	0.75
3:C:1202:CLR:H211	3:C:1202:CLR:H242	1.72	0.72
3:D:1202:CLR:H242	3:D:1202:CLR:H211	1.72	0.72
3:A:1202:CLR:H211	3:A:1202:CLR:H242	1.72	0.72
1:B:382:LEU:HD21	1:B:727:LEU:HD23	1.76	0.67

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%)	494 (94%)	33 (6%)	0	100	100
1	B	527/1112 (47%)	497 (94%)	30 (6%)	0	100	100
1	C	527/1112 (47%)	498 (94%)	29 (6%)	0	100	100
1	D	527/1112 (47%)	493 (94%)	34 (6%)	0	100	100
All	All	2108/4448 (47%)	1982 (94%)	126 (6%)	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%)	467 (100%)	0	100	100
1	C	467/965 (48%)	467 (100%)	0	100	100
1	D	467/965 (48%)	467 (100%)	0	100	100
All	All	1868/3860 (48%)	1868 (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. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	311	ASN
1	D	420	ASN
1	D	498	GLN
1	B	420	ASN
1	B	494	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	0.35	0	48,48,48	0.52	0
3	CLR	A	1202	-	31,31,31	0.37	0	48,48,48	0.58	0
3	CLR	D	1202	-	31,31,31	0.38	0	48,48,48	0.62	0
3	CLR	C	1202	-	31,31,31	0.38	0	48,48,48	0.57	0
2	EZI	B	1201	-	25,25,25	2.44	7 (28%)	33,36,36	1.55	6 (18%)
2	EZI	D	1201	-	25,25,25	2.42	7 (28%)	33,36,36	1.55	6 (18%)
2	EZI	C	1201	-	25,25,25	2.42	7 (28%)	33,36,36	1.55	6 (18%)
2	EZI	A	1201	-	25,25,25	2.42	7 (28%)	33,36,36	1.55	6 (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
3	CLR	A	1202	-	-	2/10/68/68	0/4/4/4
3	CLR	D	1202	-	-	2/10/68/68	0/4/4/4
3	CLR	C	1202	-	-	2/10/68/68	0/4/4/4
2	EZI	B	1201	-	-	0/10/10/10	0/3/3/3
2	EZI	D	1201	-	-	0/10/10/10	0/3/3/3
2	EZI	C	1201	-	-	0/10/10/10	0/3/3/3
2	EZI	A	1201	-	-	0/10/10/10	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	EZI	C08-C09	-6.10	1.35	1.47
2	B	1201	EZI	C07-N04	6.10	1.35	1.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1201	EZI	C08-C09	-6.07	1.35	1.47
2	C	1201	EZI	C08-C09	-6.04	1.35	1.47
2	A	1201	EZI	C08-C09	-6.04	1.35	1.47

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	EZI	N03-C07-N04	-4.91	119.96	124.21
2	B	1201	EZI	N03-C07-N04	-4.89	119.97	124.21
2	D	1201	EZI	N03-C07-N04	-4.87	120.00	124.21
2	C	1201	EZI	N03-C07-N04	-4.84	120.02	124.21
2	C	1201	EZI	C08-C09-N03	4.26	120.52	114.69

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1202	CLR	C20-C22-C23-C24
3	C	1202	CLR	C23-C24-C25-C27
3	D	1202	CLR	C23-C24-C25-C27
3	A	1202	CLR	C23-C24-C25-C27
3	C	1202	CLR	C23-C24-C25-C26

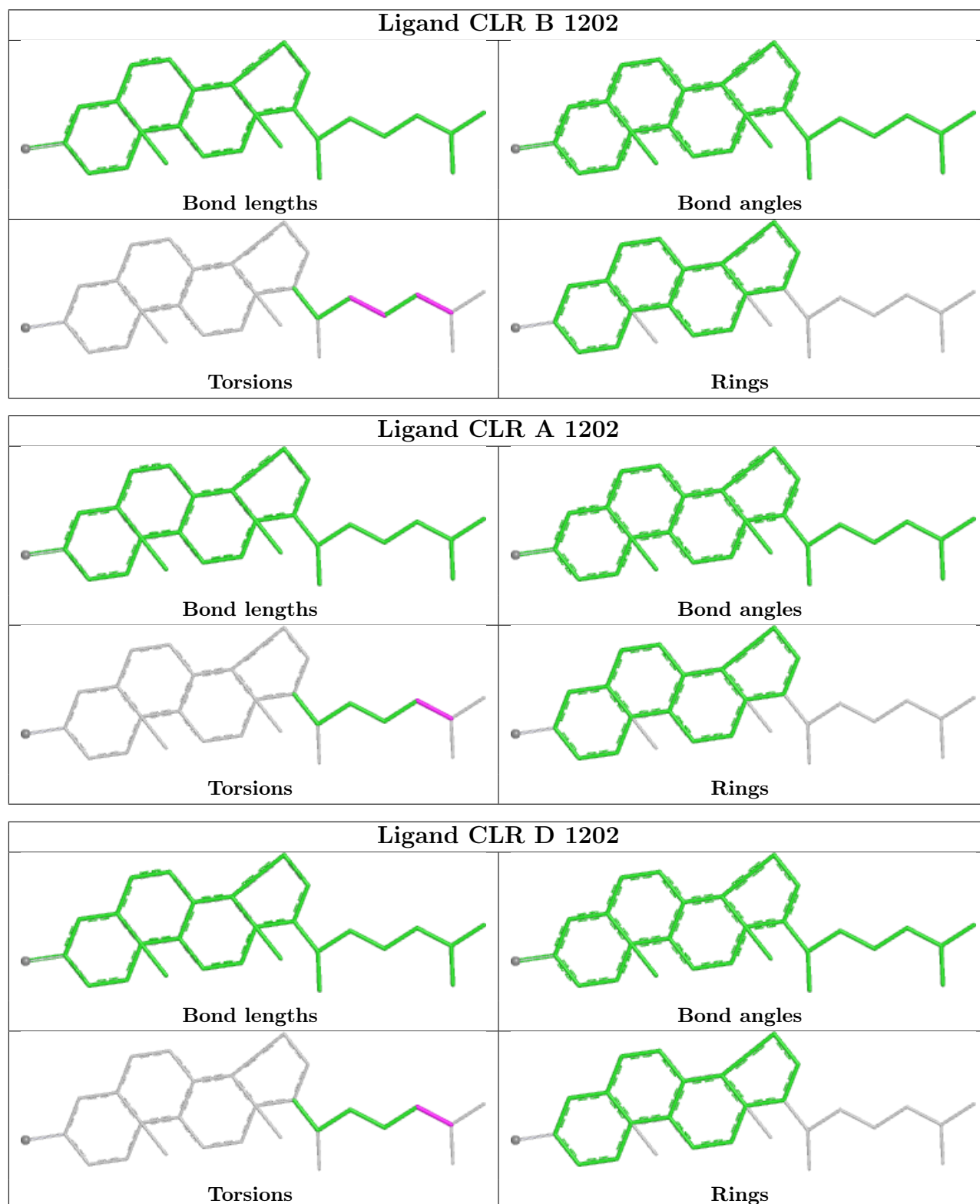
There are no ring outliers.

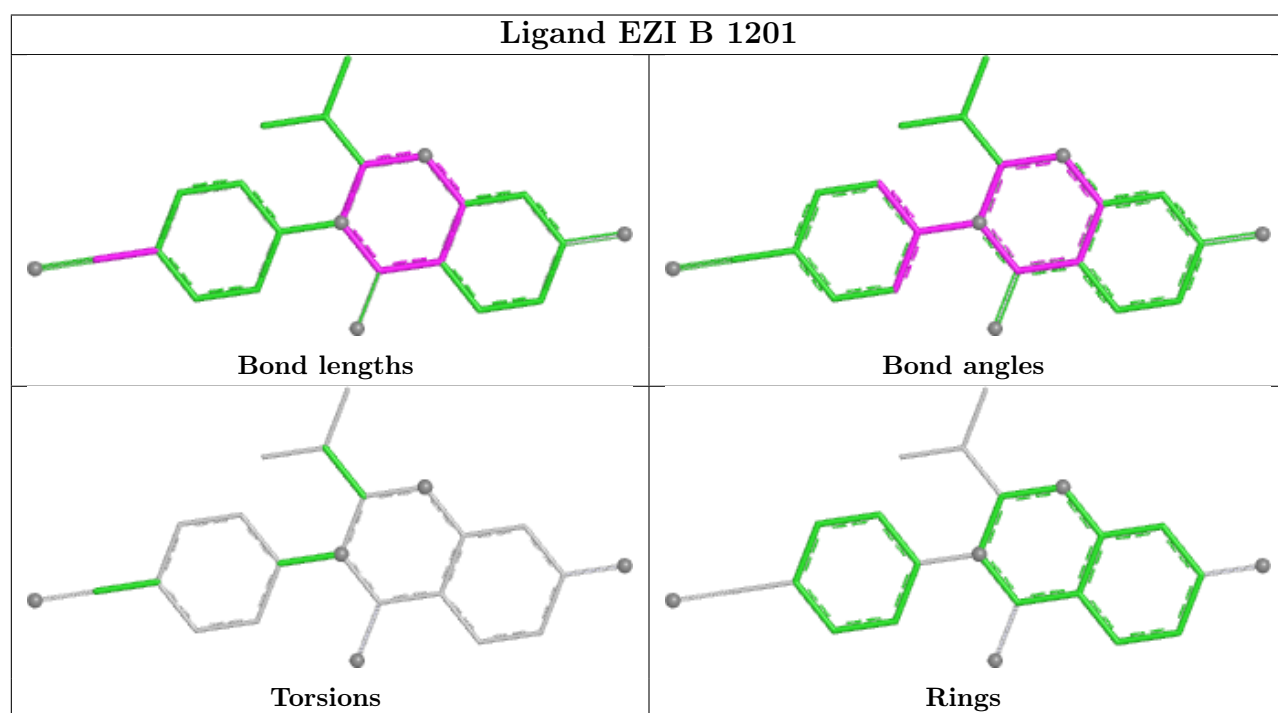
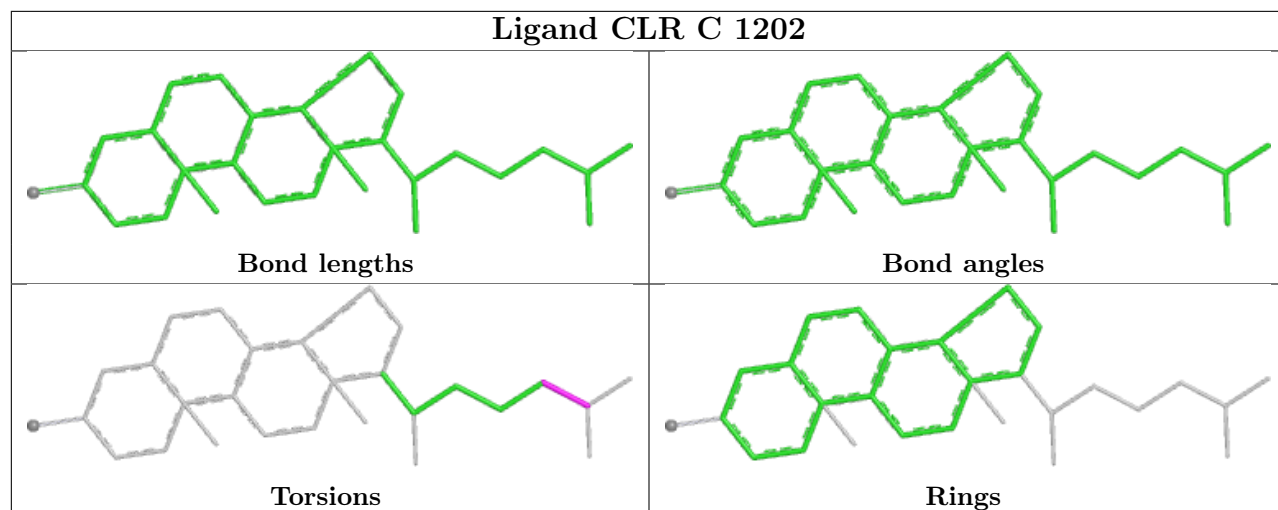
4 monomers are involved in 21 short contacts:

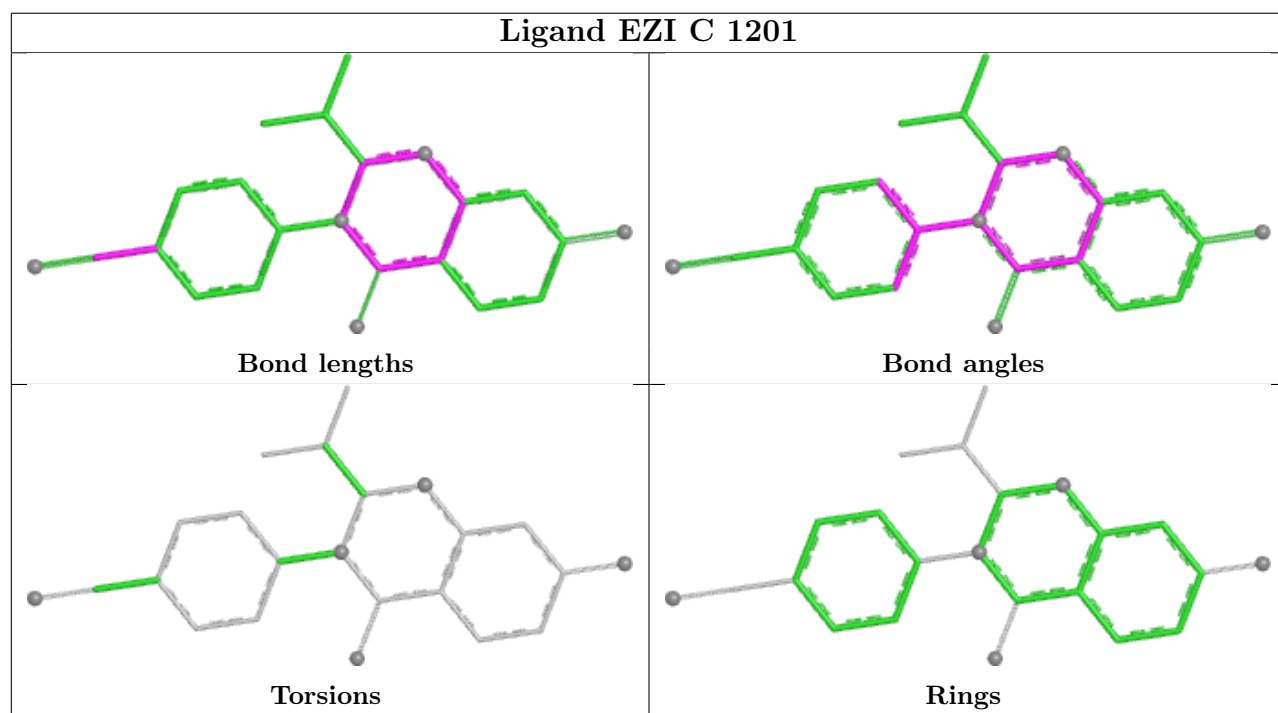
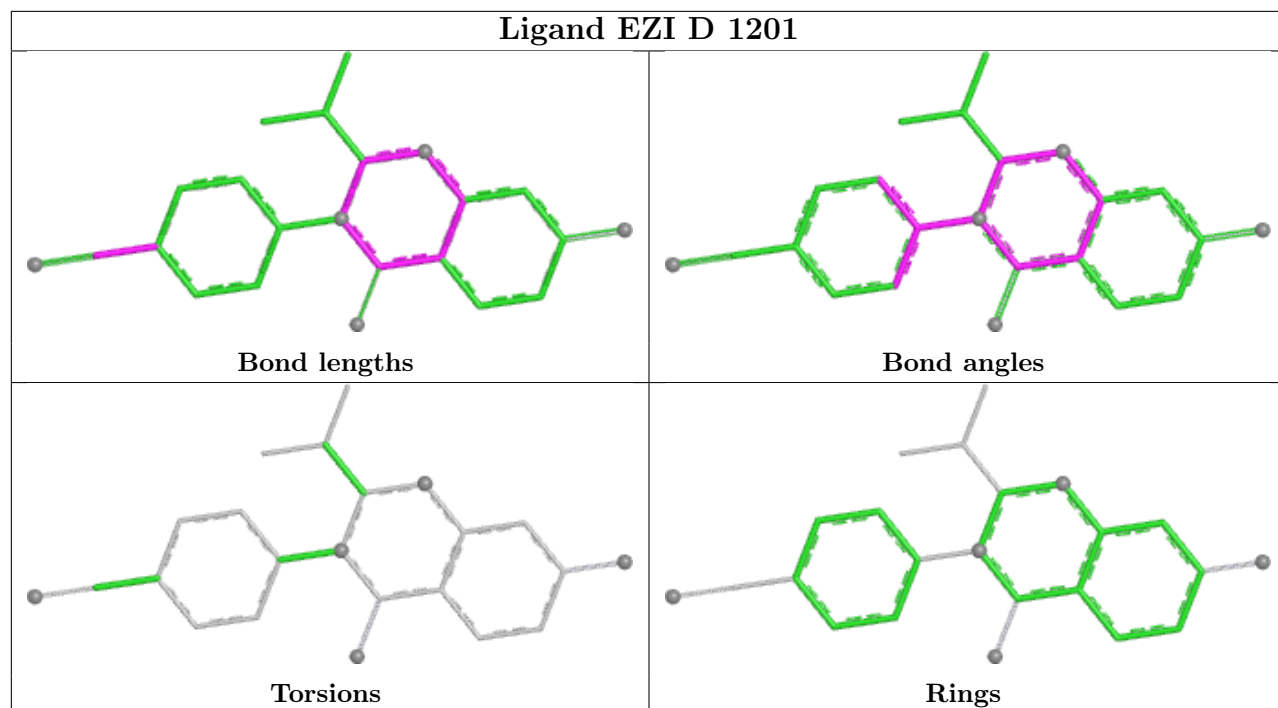
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1202	CLR	3	0
3	A	1202	CLR	5	0
3	D	1202	CLR	6	0
3	C	1202	CLR	7	0

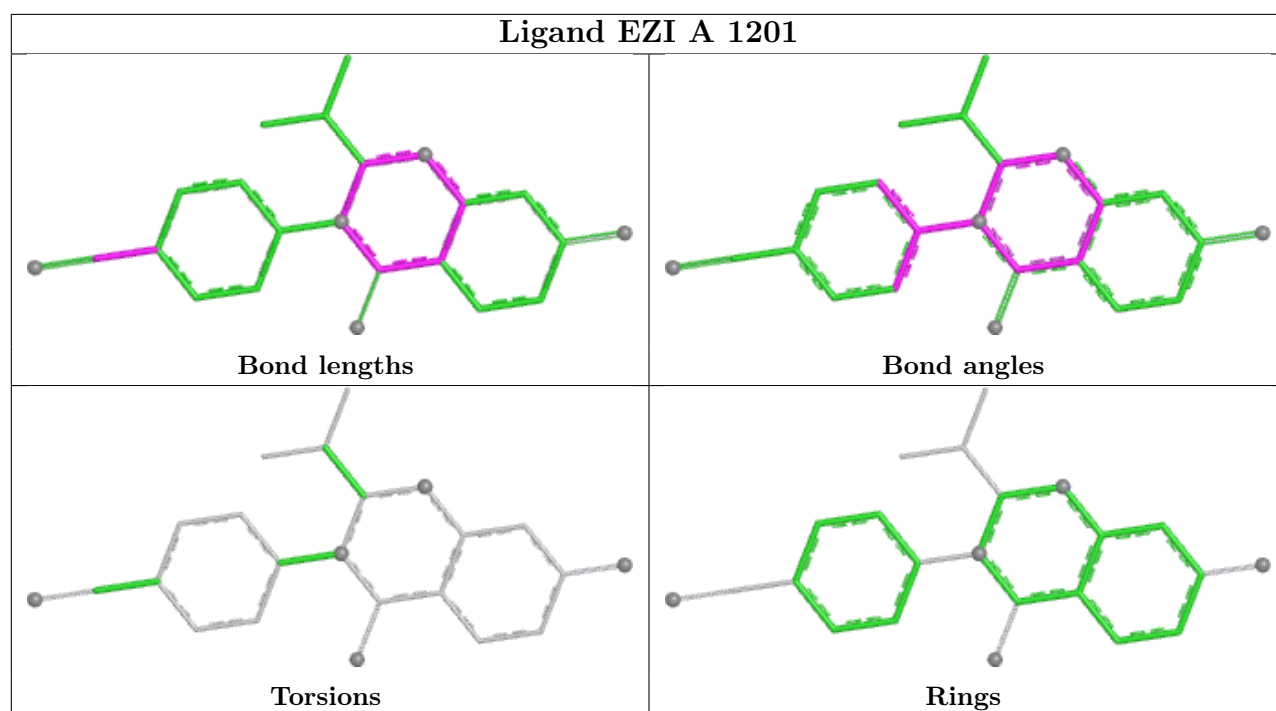
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

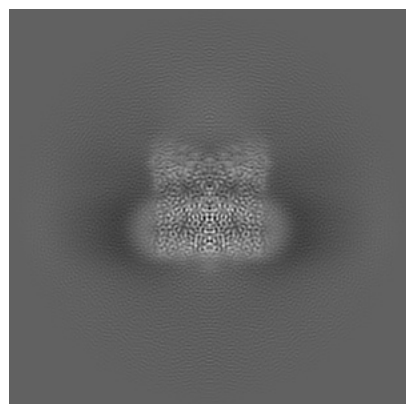
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36577. These allow visual inspection of the internal detail of the map and identification of artifacts.

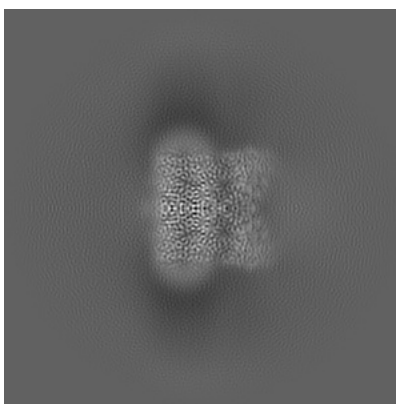
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

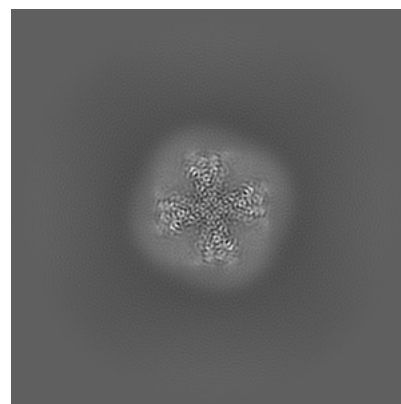
6.1.1 Primary map



X

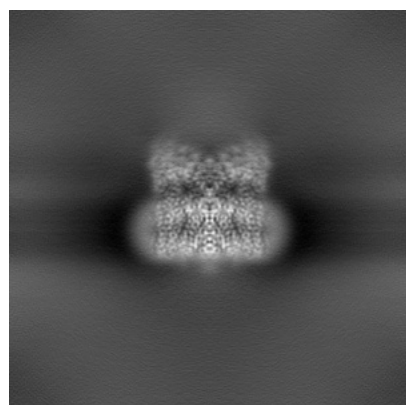


Y

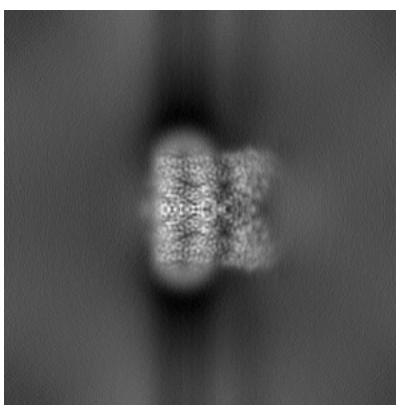


Z

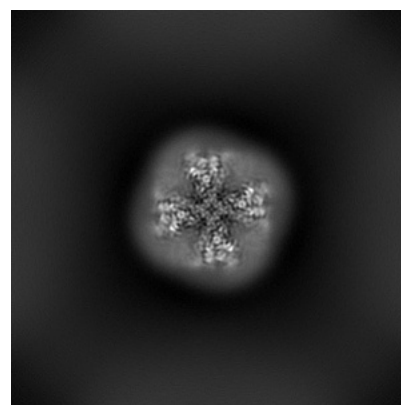
6.1.2 Raw map



X



Y

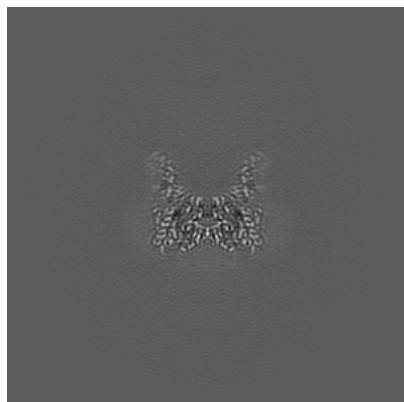


Z

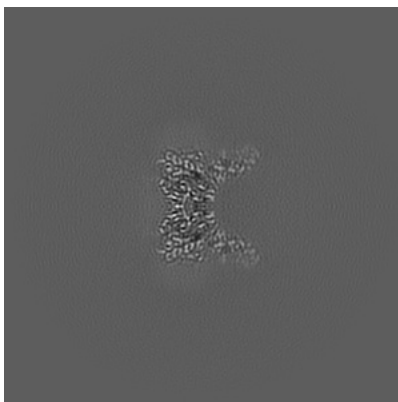
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

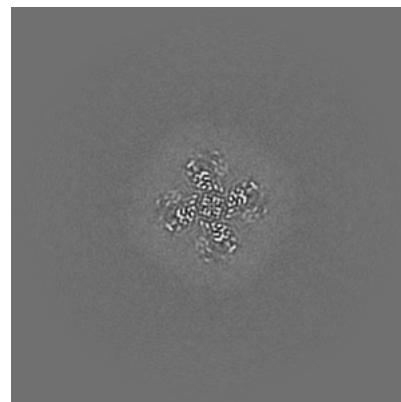
6.2.1 Primary map



X Index: 160

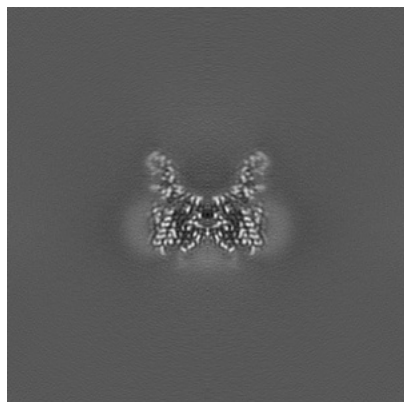


Y Index: 160

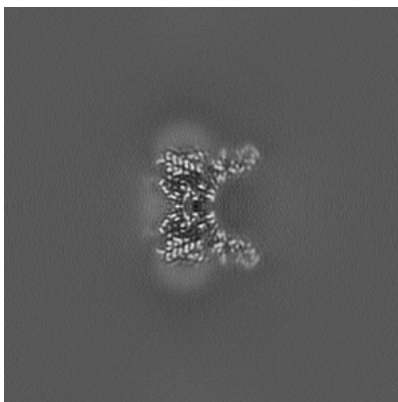


Z Index: 160

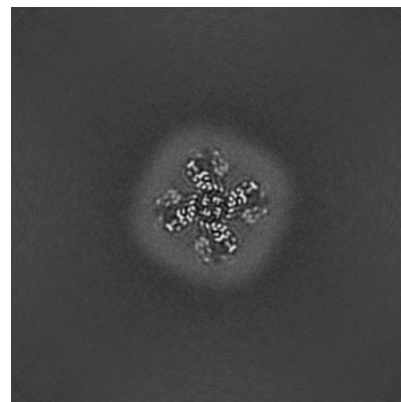
6.2.2 Raw map



X Index: 160



Y Index: 160

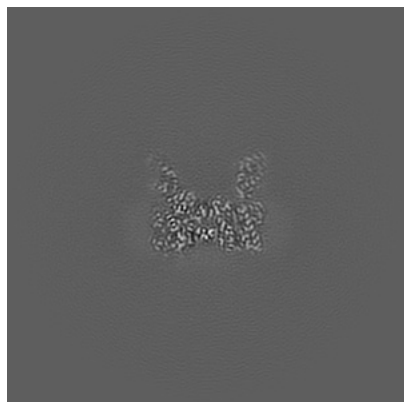


Z Index: 160

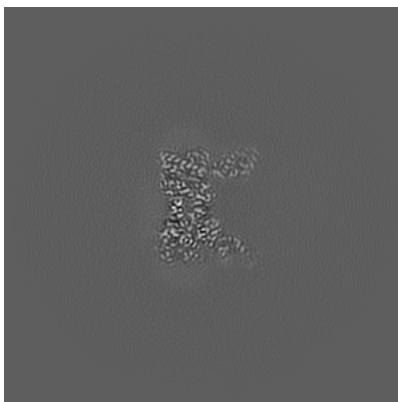
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

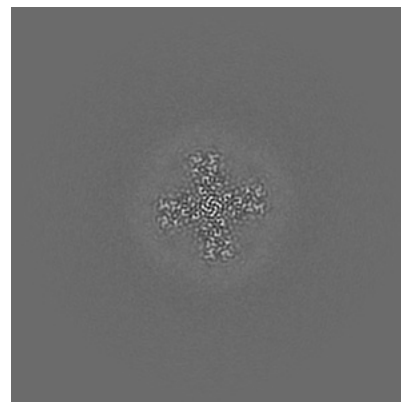
6.3.1 Primary map



X Index: 163

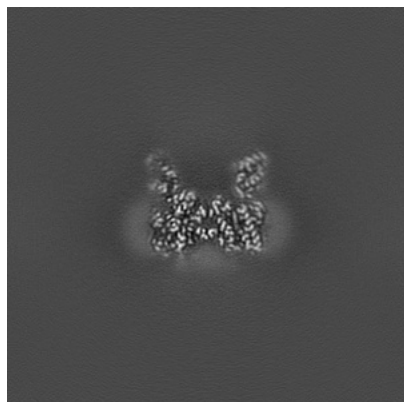


Y Index: 157

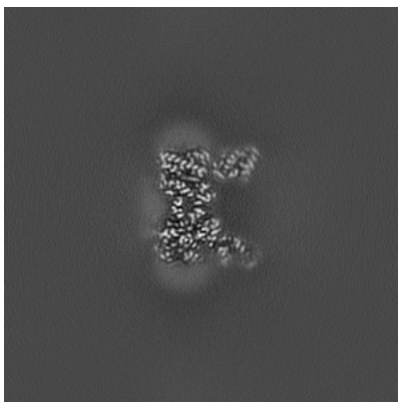


Z Index: 136

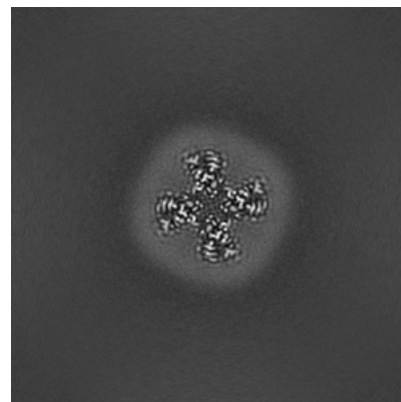
6.3.2 Raw map



X Index: 163



Y Index: 157

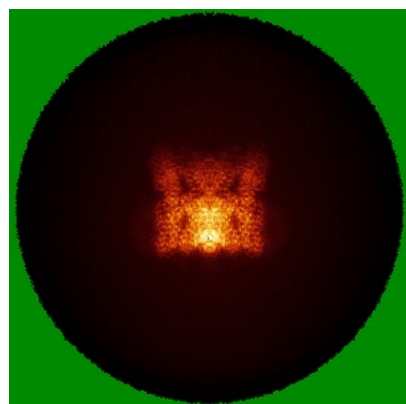


Z Index: 132

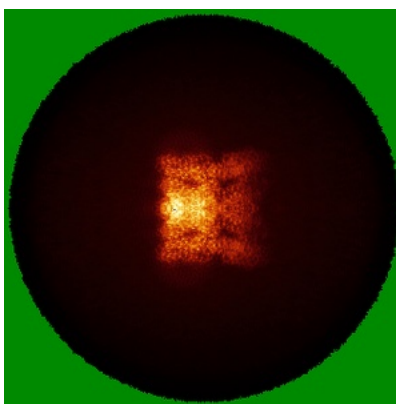
The images above show the largest variance slices of the map in three orthogonal directions.

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

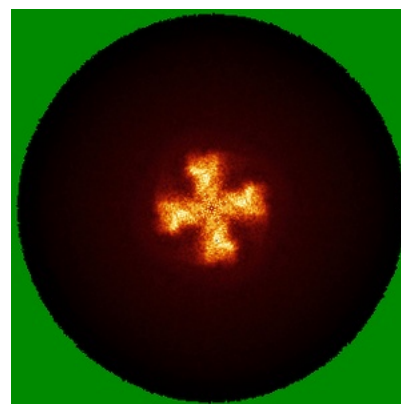
6.4.1 Primary map



X

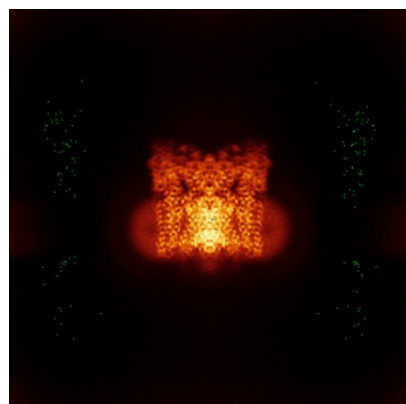


Y

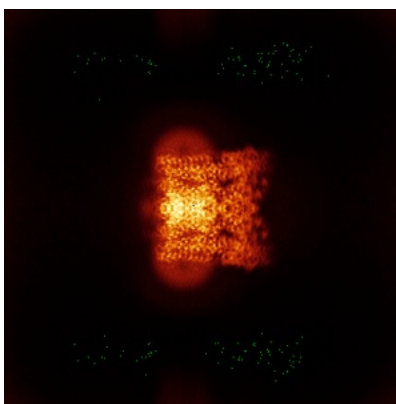


Z

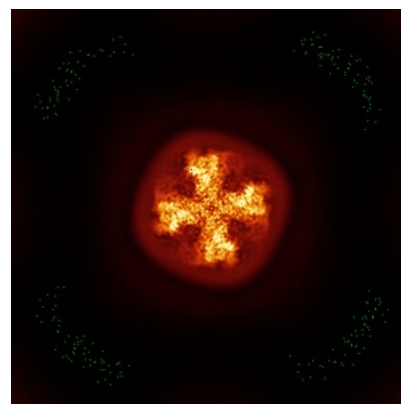
6.4.2 Raw map



X



Y

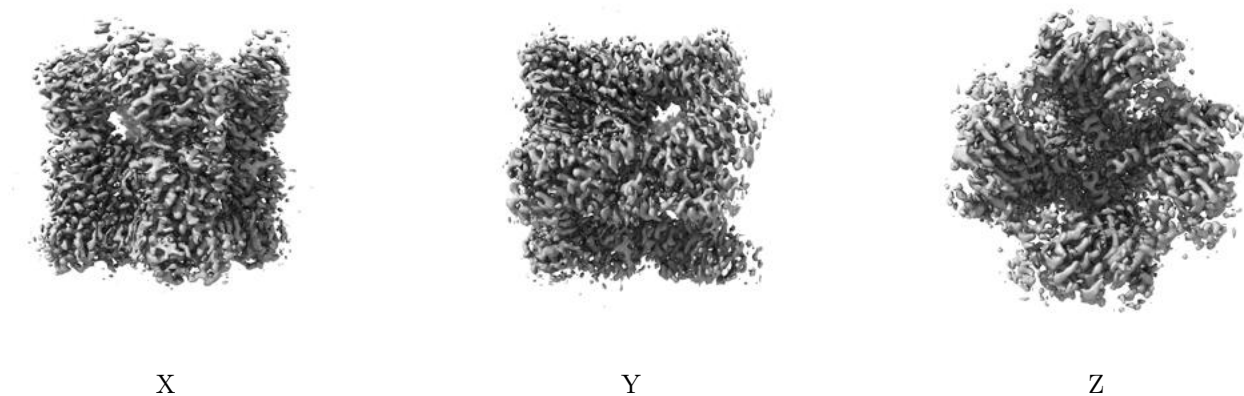


Z

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.

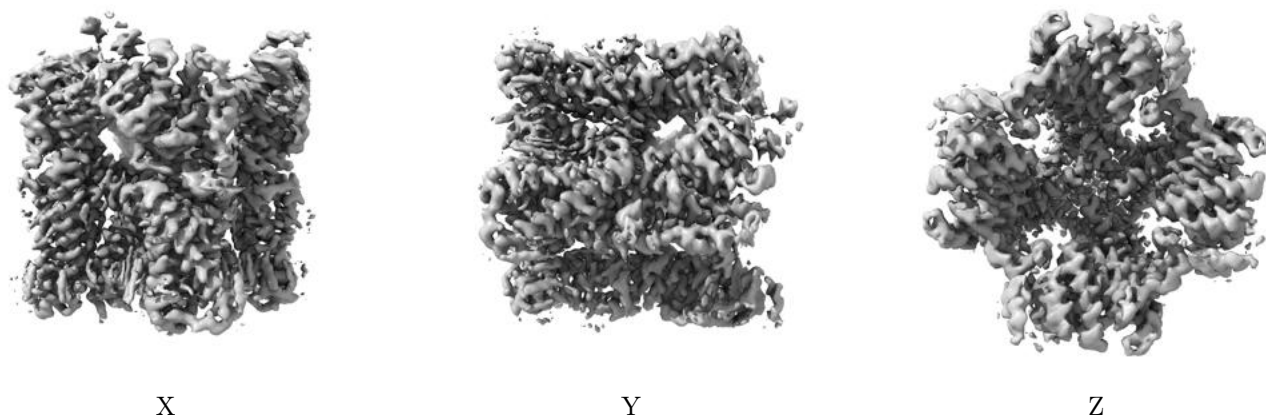
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. 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.

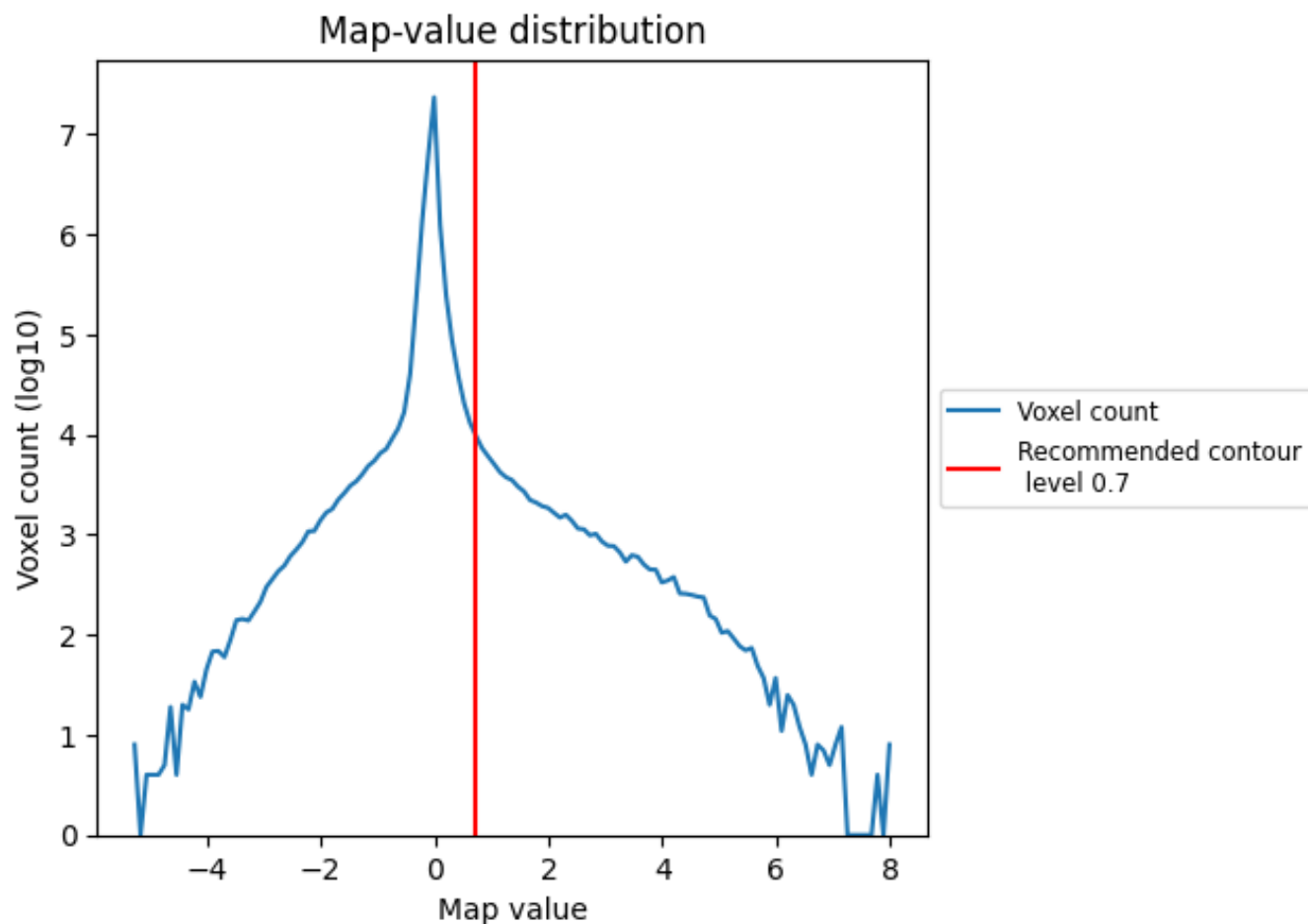
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

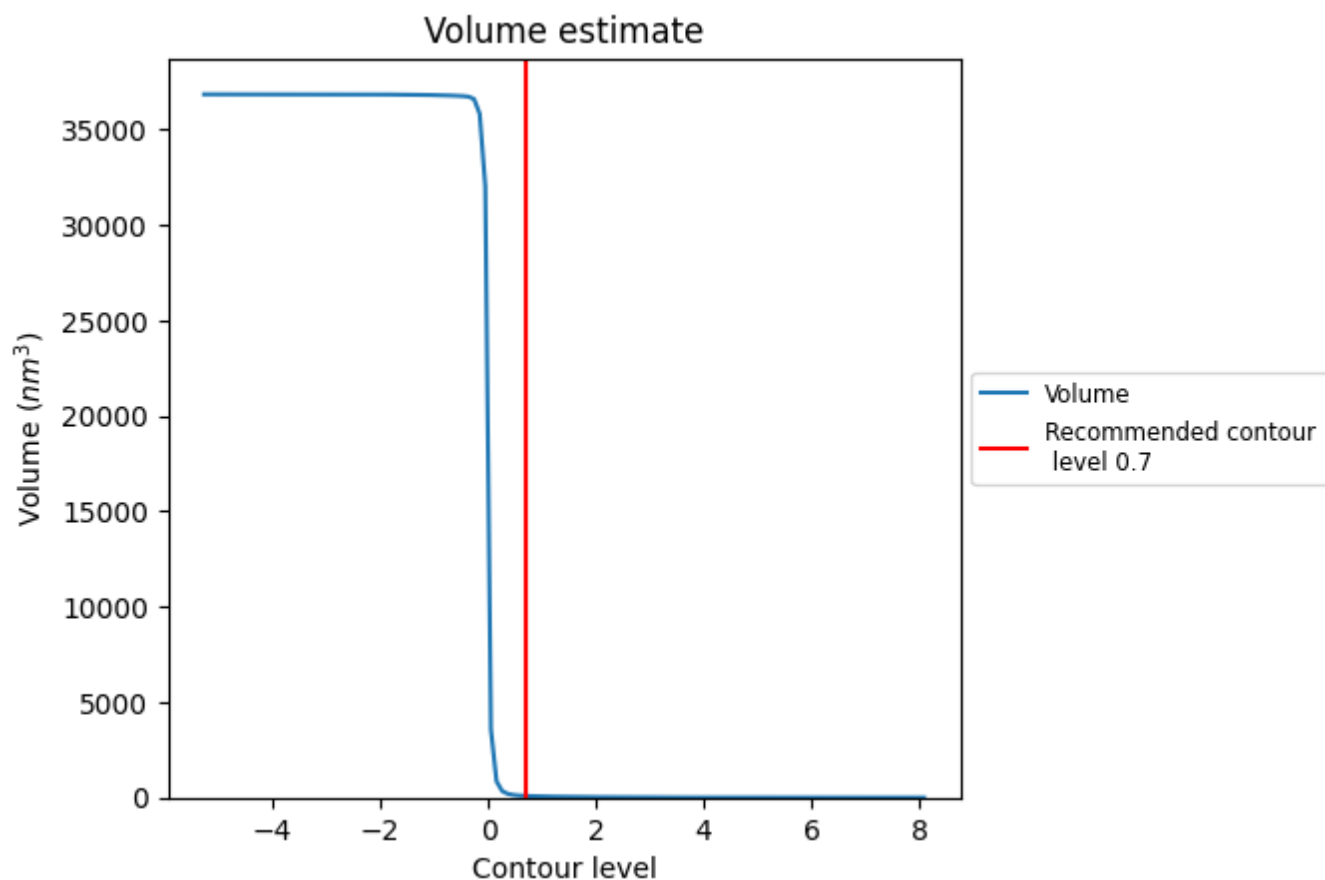
This section contains the results of statistical analysis of the map.

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.

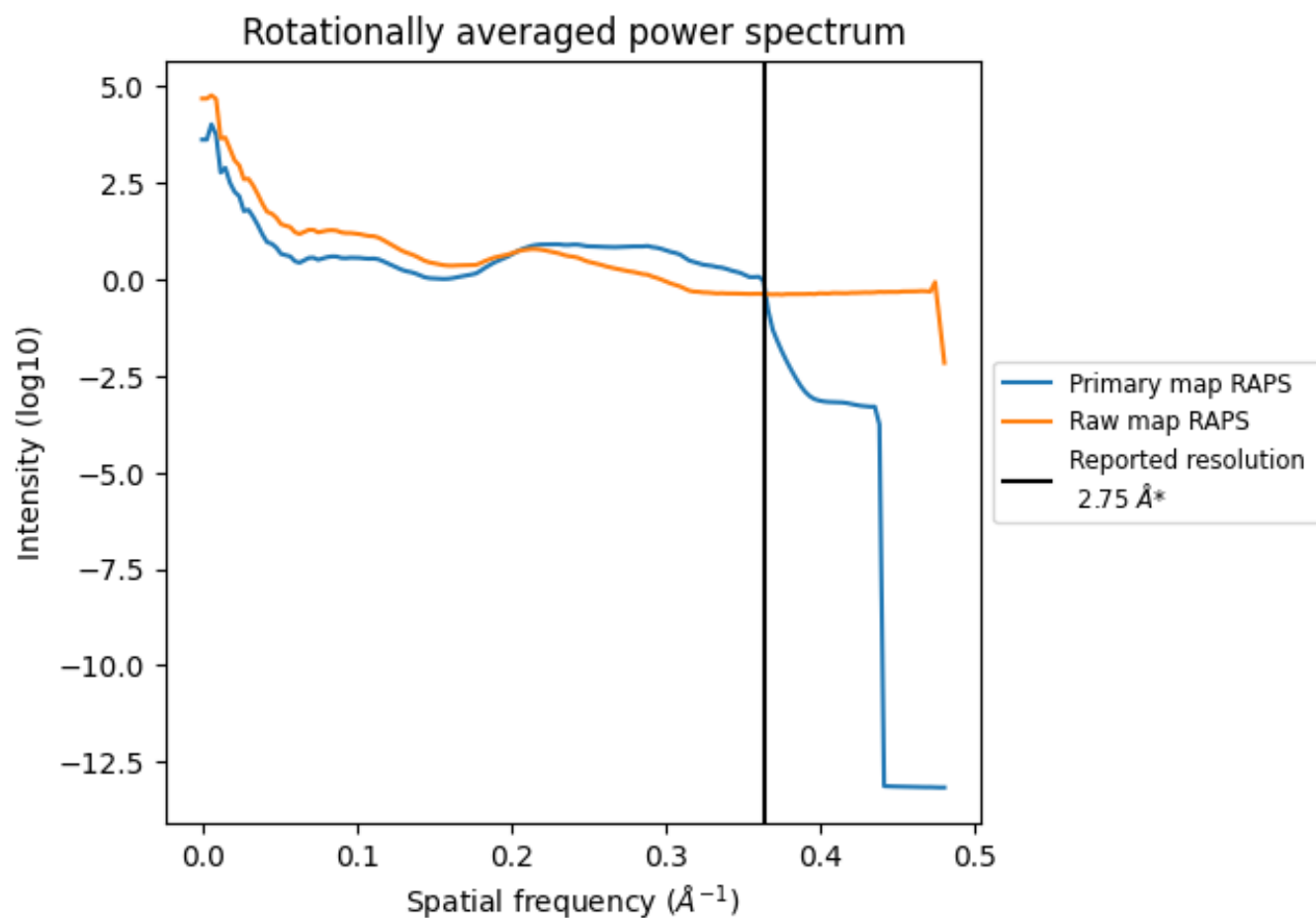
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 86 nm^3 ; this corresponds to an approximate mass of 78 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 ⓘ

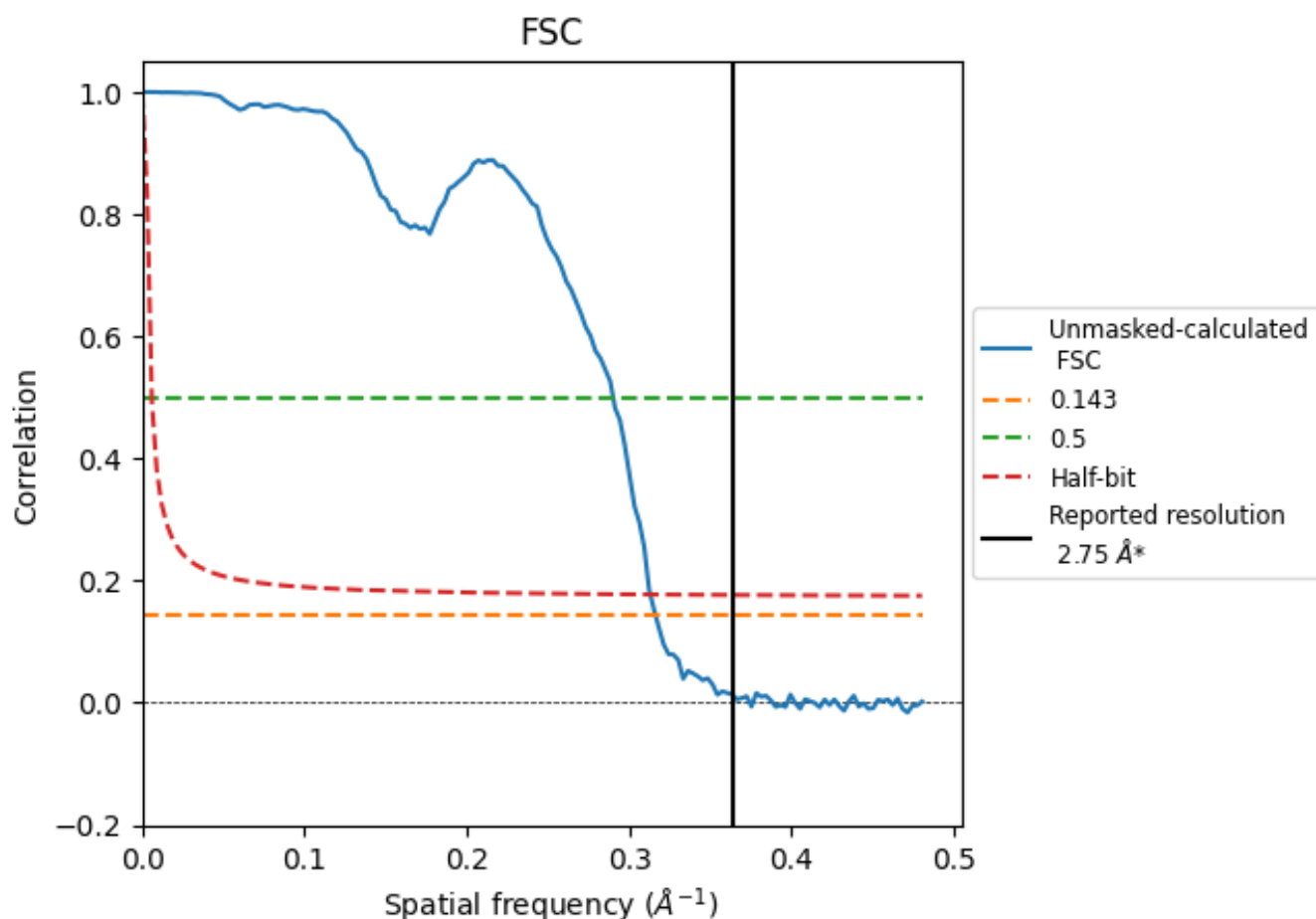


*Reported resolution corresponds to spatial frequency of 0.364 Å⁻¹

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 0.364 Å⁻¹

8.2 Resolution estimates [i](#)

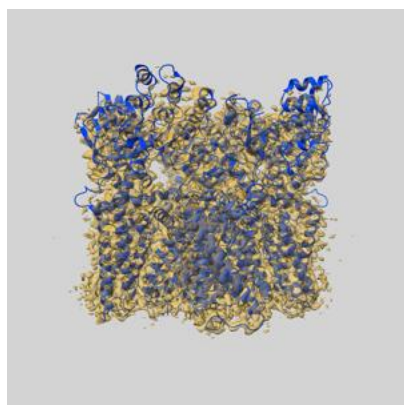
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.75	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.16	3.44	3.19

*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 3.16 differs from the reported value 2.75 by more than 10 %

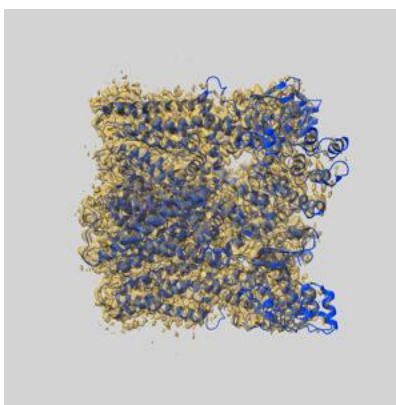
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36577 and PDB model 8JQR. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

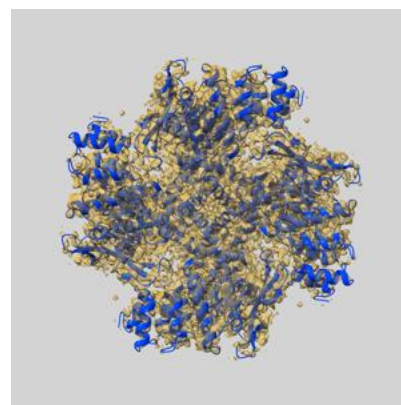
9.1 Map-model overlay [i](#)



X



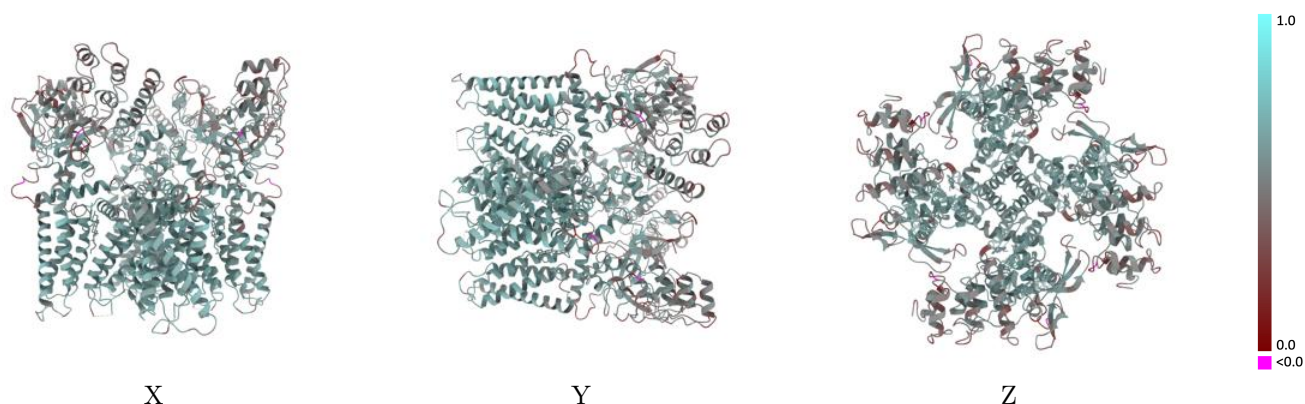
Y



Z

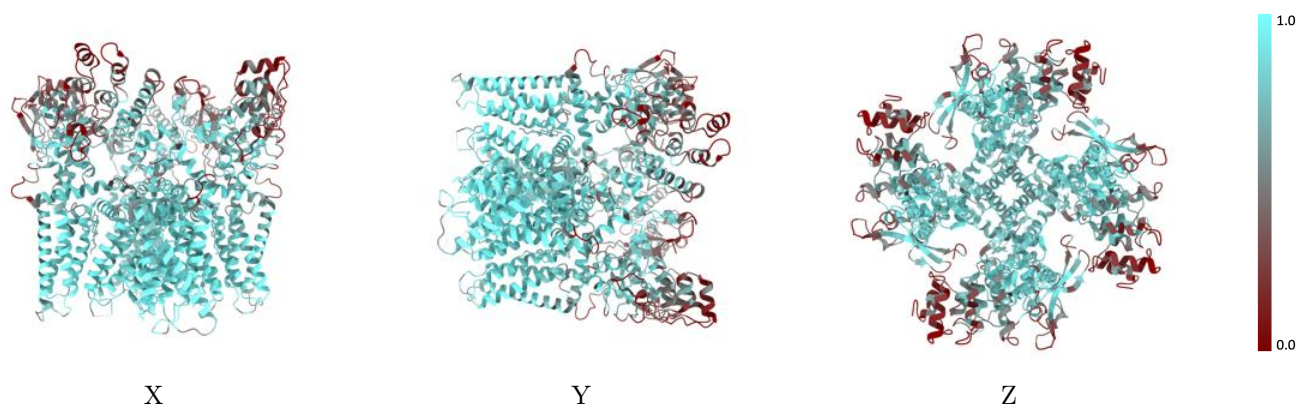
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



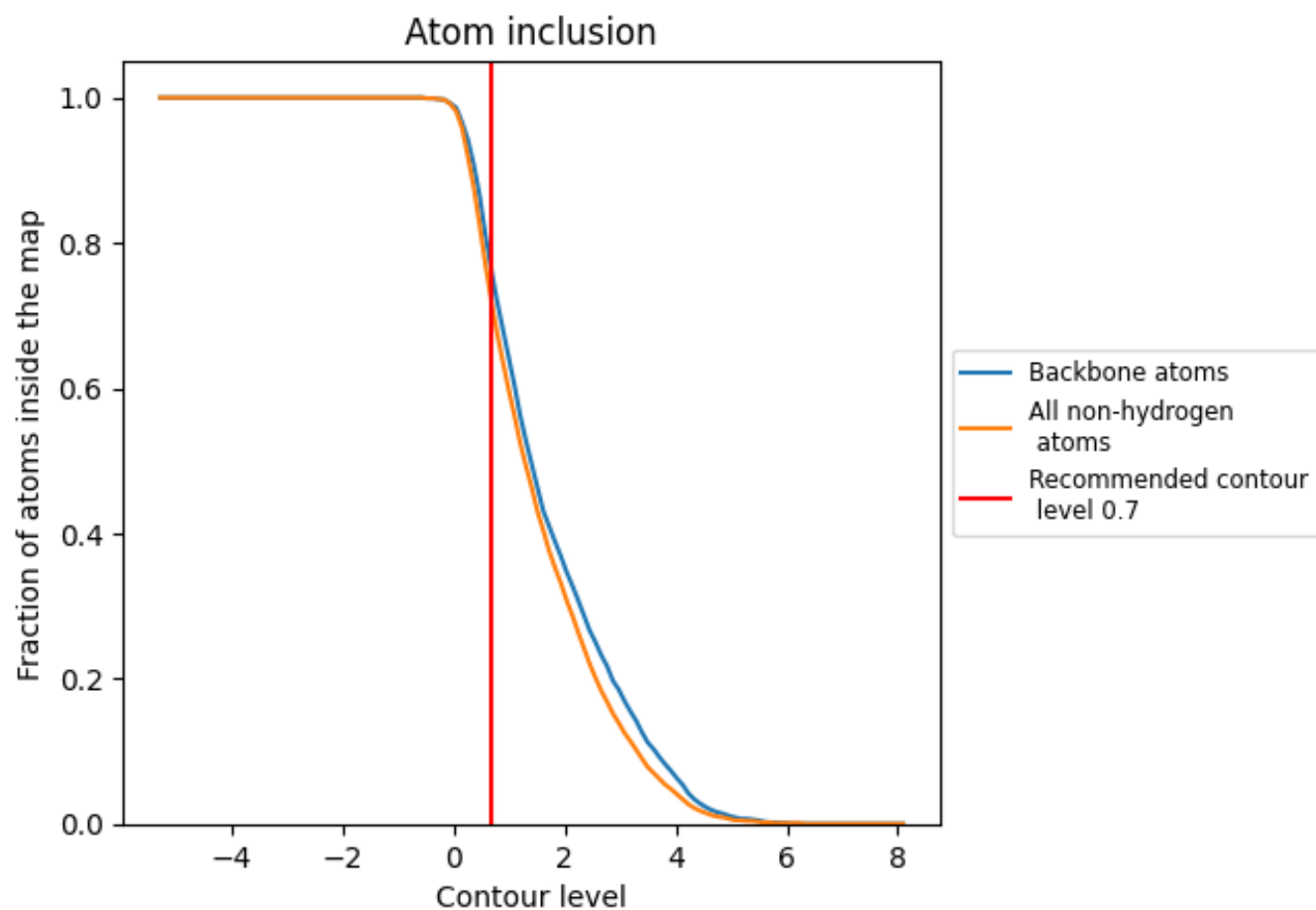
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 71% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7140	0.5490
A	0.7130	0.5500
B	0.7120	0.5480
C	0.7150	0.5480
D	0.7150	0.5510

