



## Full wwPDB EM Validation Report ⓘ

Oct 14, 2023 – 12:22 PM EDT

PDB ID : 8SDA  
EMDB ID : EMD-40350  
Title : CryoEM structure of rat Kv2.1(1-598) L403A mutant in nanodiscs  
Authors : Tan, X.; Swartz, K.J.  
Deposited on : 2023-04-06  
Resolution : 3.32 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev70  
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) : 2.36

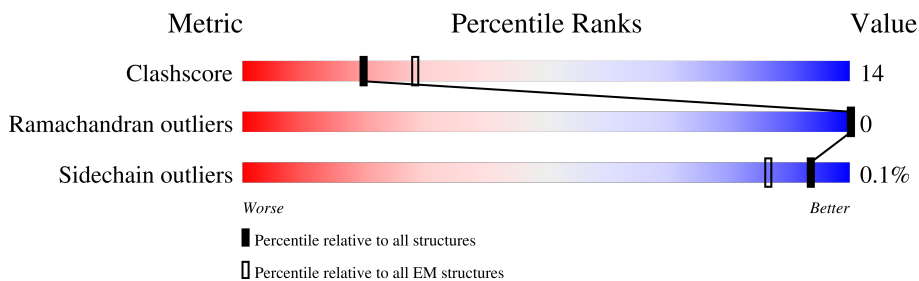
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.32 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  $\geq 3$ , 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	600	
1	B	600	
1	C	600	
1	D	600	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 7414 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.

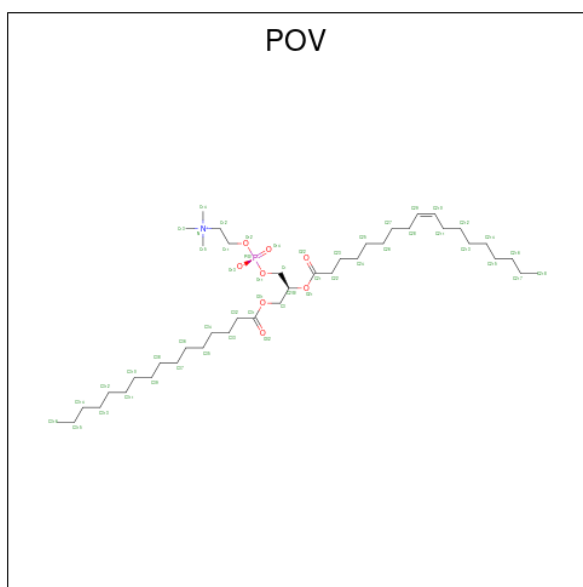
- Molecule 1 is a protein called Potassium voltage-gated channel subfamily B member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	236	1825	1221	286	309	9	0	0
1	B	236	1823	1217	286	311	9	0	0
1	D	233	1744	1165	271	299	9	0	0
1	C	234	1749	1167	271	302	9	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P15387
A	0	THR	-	expression tag	UNP P15387
A	403	ALA	LEU	engineered mutation	UNP P15387
B	-1	GLY	-	expression tag	UNP P15387
B	0	THR	-	expression tag	UNP P15387
B	403	ALA	LEU	engineered mutation	UNP P15387
D	-1	GLY	-	expression tag	UNP P15387
D	0	THR	-	expression tag	UNP P15387
D	403	ALA	LEU	engineered mutation	UNP P15387
C	-1	GLY	-	expression tag	UNP P15387
C	0	THR	-	expression tag	UNP P15387
C	403	ALA	LEU	engineered mutation	UNP P15387

- Molecule 2 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total C N O P 29 19 1 8 1	0
2	A	1	Total C O P 28 19 8 1	0
2	A	1	Total C O 15 13 2	0
2	A	1	Total C O 15 13 2	0
2	A	1	Total C O 7 6 1	0
2	A	1	Total C N O P 19 11 1 6 1	0
2	B	1	Total C O 7 6 1	0
2	B	1	Total C N O P 29 19 1 8 1	0
2	B	1	Total C O P 27 18 8 1	0
2	D	1	Total C O P 28 19 8 1	0
2	D	1	Total C O 15 13 2	0
2	D	1	Total C O 7 6 1	0
2	C	1	Total C O 7 6 1	0
2	C	1	Total C O P 21 12 8 1	0

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Mol	Chain	Residues	Atoms			AltConf
2	C	1	Total	C	O	0
			15	13	2	

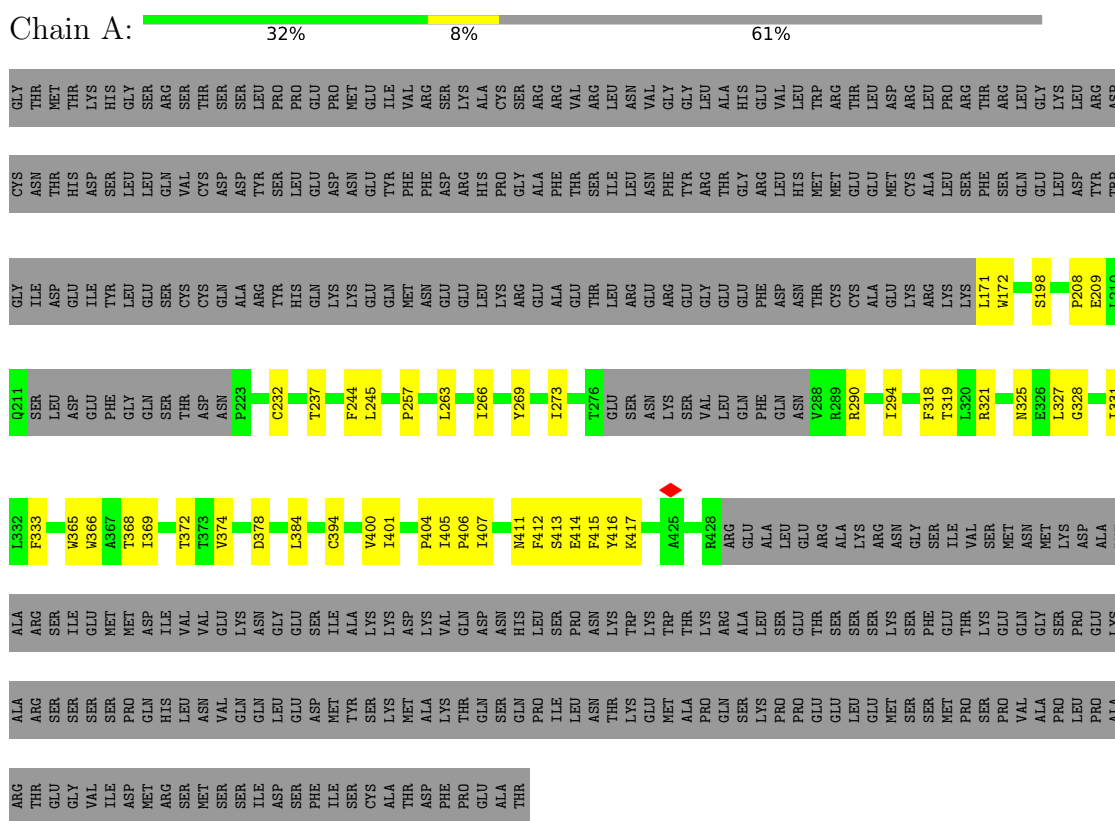
- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
3	A	3	Total	K	0
			3	3	
3	B	1	Total	K	0
			1	1	

### 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: Potassium voltage-gated channel subfamily B member 1



- Molecule 1: Potassium voltage-gated channel subfamily B member 1





CYS	ASN	THR	HIS	ASP	SER	LEU	LEU	GLN	SER	VAL	CYS	CYS	GLN	ASP	ASP	TYR	SER	LEU	GLU	ASP	ASN	GLN	TYR	GLN	TYR	PHE	PHE	ASN	ASP	GLU	ARG	HIS	PRO	LYS	GLY	ALA	ALA	PHE	THR	SER	ILE	ILE	LEU	ASN	GLU	TYR	ARG	THR	GLY	ARG	LEU	ASP	THR	HIS	MET	MET	CYS	CYS	GLU	GLU	MET	CYS	ALA	GLU	LEU	GLY	LYS	LYS	ARG	ALA	LEU	LYS	LYS	LEU	PHE	SER	GLN	GLU	LEU	ASP	TYR	TRP
GLY	ILE	ASP	GLU	ILE	TYR	LEU	LEU	GLU	SER	PHE	CYS	CYS	GLN	ALA	ARG	TYR	SER	LEU	GLU	LYS	LYS	GLU	GLN	TYR	GLN	TYR	PHE	ASN	GLU	GLY	ALA	ALA	PHE	THR	SER	ILE	ILE	LEU	ASN	GLU	TYR	ARG	THR	GLY	ARG	LEU	ASP	THR	HIS	MET	MET	CYS	CYS	GLU	GLU	MET	CYS	ALA	GLU	LEU	GLY	LYS	LYS	ARG	ALA	LEU	LYS	LYS	LEU	PHE	SER	GLN	GLU	LEU	ASP	TYR	TRP					
L197	S198	Q211	SER	LEU	ASP	GLU	PHE	GLY	GLN	SER	THR	ASP	ASN	F223	Q224	L225	V228	E229	A230	V231	C232	I233	A234	W235	F236	T237	W238	E239	P257	L258	I266	V271	T276	GLU	SER	ASN	LYS	SER	VAL	VAL	C394	I395	A396	G397	V398	L399	V400	I401	I405	P406	I407	I408	V409	W410	Q293	I294	F295	R296																								
R299	R302	I303	L304	R308	T311	G312	S323	L329	F333	K336	G337	V345	E349	S359	I360	P361	F364	K365	W366	A367	T368	T372	T373	V374	D378	G386	G391	C394	I395	A396	G397	V398	L399	V400	I401	I405	P406	I407	I408	V409	W410	Q293	I294	F295	R296																																					
W411	F415	Y416	I426	K427	ARG	ARG	GLU	ALA	GLU	LEU	GLU	ARG	ALA	SER	LYS	ARG	ASN	GLY	SER	ILE	VAL	VAL	SER	VAL	SER	ILE	VAL	VAL	GLU	LYS	ASN	VAL	VAL	GLN	LYS	GLY	GLU	SER	ILE	ILE	ALA	LYS	LYS	ASP	VAL	VAL	GLN	ASP	ASN	HIS	LEU	LEU	SER																													
PRO	ASN	THR	LYS	TRP	LYS	TRP	THR	LYS	ARG	ALA	LEU	ALA	SER	PRO	GLU	THR	THR	GLY	SER	PRO	PRO	GLU	ALA	ALA	ARG	ARG	SER	SER	ILE	VAL	VAL	GLN	LYS	GLY	GLU	ASP	THR	HIS	LEU	ASN	VAL	VAL	GLN	LEU	GLU	ASP	PHE	ILE	ILE	TYR	SER	LYS	ALA	THR	THR	ASP	ALA	PRO	PRO	GLU	ALA	THR																				
LEU	ASN	THR	LYS	GLU	MET	ALA	PRO	GLN	SER	LYS	PRO	PRO	GLU	THR	SER	SER	MET	PRO	SER	PRO	VAL	VAL	ALA	PRO	PRO	ALA	ARG	THR	GLU	VAL	VAL	ILE	ILE	ARG	SER	SER	ILE	VAL	VAL	PRO	PRO	GLN	HIS	LEU	ASN	VAL	VAL	GLN	LEU	GLU	ASP	PHE	ILE	ILE	TYR	SER	LYS	ALA	THR	THR	ASP	ALA	PRO	PRO	GLU	ALA	THR															



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	505078	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	48	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.048	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0055	Depositor
Map size ( $\text{\AA}$ )	249.0, 249.0, 249.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.83, 0.83, 0.83	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: POV, K

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	0/1867	0.46	0/2542
1	B	0.28	0/1864	0.45	0/2538
1	C	0.32	0/1785	0.50	0/2435
1	D	0.29	0/1780	0.44	0/2428
All	All	0.29	0/7296	0.47	0/9943

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	1825	0	1868	38	0
1	B	1823	0	1865	39	0
1	C	1749	0	1762	62	0
1	D	1744	0	1756	78	0
2	A	113	0	118	19	0
2	B	63	0	65	5	0
2	C	43	0	39	6	0
2	D	50	0	51	11	0
3	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
All	All	7414	0	7524	206	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 14.

All (206) 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:D:408:ILE:HG23	1:D:412:PHE:CD1	1.91	1.06
1:A:404:PRO:O	1:A:407:ILE:HG22	1.60	1.00
1:D:334:LEU:HD21	1:D:400:VAL:HG11	1.43	0.99
1:D:334:LEU:HD21	1:D:400:VAL:CG1	2.04	0.86
1:D:316:LEU:O	1:D:319:THR:HG22	1.79	0.83
1:D:319:THR:HG21	1:D:412:PHE:CZ	2.14	0.83
1:C:408:ILE:HG13	1:C:409:VAL:N	1.96	0.80
1:C:405:ILE:HA	1:C:408:ILE:HG12	1.63	0.79
1:D:307:ALA:HA	1:D:313:LEU:HD22	1.68	0.75
2:A:601:POV:H23	2:A:601:POV:H32	1.67	0.74
1:C:405:ILE:HA	1:C:408:ILE:CG1	2.18	0.74
1:D:407:ILE:HG23	1:D:411:ASN:ND2	2.03	0.73
1:B:384:LEU:CD1	2:C:603:POV:H22	2.19	0.72
1:B:317:GLY:HA3	2:B:603:POV:H24	1.70	0.72
1:A:318:PHE:HD1	1:A:415:PHE:HE2	1.36	0.71
1:D:409:VAL:HA	1:C:406:PRO:HB3	1.72	0.70
1:A:318:PHE:HD1	1:A:415:PHE:CE2	2.10	0.68
1:C:225:LEU:N	1:C:225:LEU:HD12	2.08	0.68
1:C:312:GLY:HA2	1:C:416:TYR:HE1	1.59	0.68
1:A:406:PRO:HG2	1:B:409:VAL:HG11	1.77	0.67
2:A:606:POV:H1A	1:D:329:LEU:CD2	2.25	0.66
1:C:174:LEU:HA	1:C:184:ALA:HB2	1.77	0.66
1:C:233:ILE:O	1:C:237:THR:HG23	1.96	0.65
1:C:408:ILE:HG13	1:C:409:VAL:H	1.59	0.65
1:D:319:THR:HA	1:D:415:PHE:CE1	2.32	0.65
1:A:321:ARG:CB	2:A:602:POV:H32	2.27	0.65
1:C:405:ILE:O	1:C:409:VAL:HG12	1.97	0.64
2:A:606:POV:H1A	1:D:329:LEU:HD23	1.80	0.64
1:C:237:THR:HG22	1:C:266:ILE:HG21	1.79	0.64
1:C:405:ILE:HA	1:C:408:ILE:CD1	2.28	0.64
1:A:319:THR:HG21	1:A:412:PHE:HB2	1.80	0.64
1:D:312:GLY:HA3	1:C:329:LEU:HD21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:SER:HB2	1:D:248:PRO:HD2	1.79	0.63
1:D:307:ALA:CB	1:D:313:LEU:HD22	2.29	0.63
1:D:407:ILE:O	1:D:411:ASN:ND2	2.28	0.62
1:D:318:PHE:HD1	1:D:415:PHE:HZ	1.47	0.62
1:D:320:LEU:HD13	1:D:327:LEU:HD13	1.81	0.62
1:D:407:ILE:O	1:D:411:ASN:HB2	2.00	0.62
1:A:372:THR:HG21	1:D:394:CYS:HB3	1.82	0.61
1:A:333:PHE:HB3	1:A:400:VAL:HG13	1.82	0.61
1:A:328:GLY:HA3	2:A:601:POV:H3	1.83	0.60
1:D:307:ALA:CA	1:D:313:LEU:HD22	2.31	0.60
1:B:313:LEU:O	2:B:603:POV:H25A	2.02	0.59
1:C:405:ILE:CA	1:C:408:ILE:HG12	2.32	0.59
1:B:396:ALA:O	1:B:400:VAL:HG12	2.03	0.58
1:D:320:LEU:CD1	1:D:327:LEU:HD13	2.33	0.58
2:D:601:POV:H21B	1:C:337:GLY:HA2	1.84	0.58
1:C:405:ILE:HA	1:C:408:ILE:HD11	1.86	0.58
1:D:317:GLY:HA3	2:D:601:POV:H23A	1.86	0.58
1:D:405:ILE:O	1:D:409:VAL:HG23	2.02	0.58
1:D:317:GLY:HA3	2:D:601:POV:O22	2.04	0.57
1:C:397:GLY:HA2	1:C:400:VAL:HG12	1.86	0.57
1:D:243:ARG:HH12	1:D:308:ARG:NH2	2.03	0.56
1:B:293:GLN:OE1	1:B:296:ARG:NH1	2.38	0.56
1:D:415:PHE:O	1:D:418:GLU:HG3	2.06	0.56
1:D:407:ILE:HG23	1:D:411:ASN:HD21	1.71	0.56
1:D:407:ILE:CG2	1:D:411:ASN:ND2	2.69	0.55
1:B:250:LYS:O	1:B:253:PHE:HB3	2.07	0.55
1:D:319:THR:HA	1:D:415:PHE:HE1	1.72	0.55
1:C:174:LEU:HA	1:C:184:ALA:CB	2.36	0.54
1:D:372:THR:HG21	1:C:394:CYS:HB3	1.89	0.54
1:A:208:PRO:HD2	1:A:209:GLU:OE1	2.07	0.54
1:D:257:PRO:HG3	2:D:601:POV:H3A	1.90	0.54
1:C:333:PHE:HE2	1:C:400:VAL:HB	1.73	0.53
1:B:406:PRO:HB2	1:C:409:VAL:HG23	1.90	0.53
1:C:236:PHE:O	1:C:239:GLU:HG3	2.08	0.53
1:C:230:ALA:O	1:C:233:ILE:HG22	2.08	0.53
1:D:258:LEU:HD23	2:D:601:POV:O14	2.09	0.53
1:D:313:LEU:HD23	2:D:601:POV:H23	1.90	0.53
1:B:233:ILE:HG21	1:B:269:TYR:CD2	2.44	0.53
1:A:384:LEU:CD1	2:A:604:POV:H22	2.39	0.52
1:C:368:THR:HG21	2:C:603:POV:H27	1.90	0.52
1:A:198:SER:HB2	1:A:232:CYS:SG	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:ASP:N	1:D:378:ASP:OD1	2.43	0.52
1:B:373:THR:HA	1:C:374:VAL:HG22	1.90	0.52
2:A:605:POV:H24	2:A:606:POV:H32A	1.91	0.51
1:C:258:LEU:HD23	2:C:602:POV:O14	2.10	0.51
1:C:378:ASP:OD1	1:C:378:ASP:N	2.43	0.51
1:C:225:LEU:N	1:C:225:LEU:CD1	2.73	0.51
1:B:263:LEU:HA	1:B:266:ILE:HG22	1.92	0.51
1:C:308:ARG:HG3	1:C:308:ARG:HH11	1.76	0.50
1:D:395:ILE:O	1:D:399:LEU:HG	2.11	0.50
1:B:394:CYS:HB3	1:C:372:THR:HG21	1.94	0.50
1:C:192:ILE:HG21	2:C:601:POV:H24A	1.94	0.50
1:D:234:ALA:O	1:D:237:THR:HB	2.12	0.50
1:D:318:PHE:HD1	1:D:415:PHE:CZ	2.29	0.50
1:C:235:TRP:CZ3	1:C:239:GLU:HG2	2.47	0.50
1:B:378:ASP:N	1:B:378:ASP:OD1	2.43	0.49
1:A:290:ARG:O	1:A:294:ILE:HG12	2.12	0.49
1:D:263:LEU:O	1:D:267:LEU:HD23	2.13	0.49
1:A:413:SER:O	1:A:417:LYS:HG2	2.12	0.49
2:A:606:POV:H1A	1:D:329:LEU:HD21	1.95	0.49
1:A:257:PRO:HD2	2:A:602:POV:O13	2.13	0.49
1:C:397:GLY:O	1:C:401:ILE:HG12	2.13	0.49
1:D:372:THR:HG23	1:C:398:VAL:HG23	1.95	0.49
1:A:378:ASP:OD1	1:A:378:ASP:N	2.44	0.48
1:A:384:LEU:HD11	2:A:604:POV:H22	1.95	0.48
1:B:241:LEU:O	1:B:245:LEU:HG	2.12	0.48
1:A:333:PHE:HB3	1:A:400:VAL:CG1	2.44	0.48
1:C:257:PRO:HD2	2:C:602:POV:O12	2.13	0.48
1:B:237:THR:OG1	1:B:266:ILE:HD11	2.13	0.48
1:C:304:LEU:HD11	2:C:602:POV:C26	2.43	0.48
1:B:412:PHE:HA	1:B:415:PHE:HD2	1.79	0.48
1:D:243:ARG:C	1:D:245:LEU:H	2.17	0.48
1:C:198:SER:HB3	1:C:302:ARG:HH11	1.78	0.48
2:D:601:POV:H29	1:C:336:MET:CE	2.44	0.47
1:D:345:VAL:HG21	1:D:366:TRP:CZ3	2.48	0.47
1:C:271:VAL:HG11	1:C:295:PHE:CE2	2.49	0.47
1:C:411:ASN:O	1:C:415:PHE:HD1	1.96	0.47
1:C:345:VAL:HG21	1:C:366:TRP:CZ3	2.49	0.47
1:B:365:TRP:CH2	1:B:369:ILE:HD11	2.49	0.47
1:A:263:LEU:HA	1:A:266:ILE:HG22	1.96	0.47
1:B:404:PRO:O	1:B:407:ILE:HG22	2.15	0.47
1:D:313:LEU:CD2	2:D:601:POV:H23	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:ALA:HB1	2:B:603:POV:H25	1.96	0.47
1:A:405:ILE:HG13	1:A:406:PRO:HD3	1.97	0.47
1:C:408:ILE:CG1	1:C:409:VAL:N	2.72	0.47
1:D:310:SER:HB2	2:D:603:POV:C21	2.45	0.46
1:C:197:LEU:HD11	1:C:228:VAL:HG11	1.97	0.46
1:A:257:PRO:HG2	2:A:602:POV:H1	1.98	0.46
1:A:365:TRP:O	1:A:369:ILE:HG12	2.15	0.46
1:D:359:SER:HB2	1:D:361:PRO:HD2	1.97	0.46
2:A:605:POV:C24	2:A:606:POV:H32A	2.46	0.46
1:B:192:ILE:HD11	1:B:309:HIS:CG	2.51	0.46
1:D:402:ALA:HA	1:D:405:ILE:HD12	1.98	0.46
1:D:396:ALA:O	1:D:400:VAL:HG23	2.16	0.45
1:C:391:GLY:O	1:C:395:ILE:HG12	2.16	0.45
1:A:325:ASN:ND2	2:A:601:POV:O14	2.38	0.45
1:C:372:THR:O	1:C:373:THR:OG1	2.33	0.45
1:A:328:GLY:HA3	2:A:601:POV:C3	2.46	0.45
1:A:394:CYS:SG	1:B:374:VAL:HG21	2.57	0.45
1:C:323:SER:OG	1:C:411:ASN:ND2	2.45	0.45
1:A:366:TRP:HE1	1:B:376:TYR:HH	1.61	0.44
1:D:243:ARG:HH22	1:D:308:ARG:NE	2.15	0.44
1:D:247:SER:HG	1:D:253:PHE:HD1	1.65	0.44
2:A:603:POV:H22	1:D:384:LEU:CD1	2.48	0.44
1:B:233:ILE:HG12	1:B:269:TYR:HD2	1.82	0.44
1:D:243:ARG:C	1:D:245:LEU:N	2.70	0.44
1:A:269:TYR:O	1:A:273:ILE:HG12	2.18	0.44
1:D:334:LEU:HD21	1:D:400:VAL:HG13	1.95	0.44
1:C:290:ARG:O	1:C:294:ILE:HG12	2.16	0.44
1:A:237:THR:OG1	1:A:266:ILE:HD11	2.17	0.44
1:D:312:GLY:C	1:C:329:LEU:HD11	2.38	0.44
1:D:385:LEU:HD12	1:D:385:LEU:H	1.83	0.44
1:D:385:LEU:O	1:D:389:VAL:HG12	2.18	0.44
1:C:224:GLN:O	1:C:228:VAL:HG23	2.18	0.44
1:C:296:ARG:O	1:C:299:ARG:HG2	2.17	0.44
1:B:307:ALA:HB2	2:B:603:POV:H26A	2.00	0.44
1:A:171:LEU:HG	1:A:172:TRP:H	1.82	0.43
2:A:602:POV:H26	2:A:602:POV:H29	1.60	0.43
1:B:383:THR:O	1:B:387:LYS:N	2.39	0.43
1:B:369:ILE:HG23	1:B:374:VAL:HB	2.00	0.43
1:C:233:ILE:CD1	1:C:266:ILE:HG23	2.49	0.43
1:B:291:VAL:HA	1:B:294:ILE:HG22	2.00	0.43
1:B:319:THR:O	1:B:323:SER:OG	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405:ILE:N	1:C:406:PRO:HD2	2.34	0.43
1:A:411:ASN:O	1:A:414:GLU:HB3	2.18	0.43
1:B:323:SER:HB2	1:B:326:GLU:OE2	2.18	0.43
1:B:385:LEU:HD12	1:B:385:LEU:H	1.84	0.43
1:D:251:TRP:O	1:D:255:LYS:N	2.52	0.43
1:C:197:LEU:HD21	1:C:228:VAL:HG13	2.00	0.43
1:A:368:THR:HG23	1:A:369:ILE:N	2.34	0.42
1:B:391:GLY:O	1:B:395:ILE:HG12	2.19	0.42
1:D:241:LEU:O	1:D:245:LEU:HG	2.18	0.42
1:D:403:ALA:O	1:D:406:PRO:HD2	2.19	0.42
1:D:372:THR:O	1:D:373:THR:OG1	2.36	0.42
1:B:327:LEU:HD23	1:B:408:ILE:HD13	2.01	0.42
1:D:391:GLY:O	1:D:395:ILE:HG12	2.20	0.42
1:B:366:TRP:NE1	1:B:381:PRO:HD3	2.34	0.42
1:B:369:ILE:HG21	1:B:376:TYR:H	1.85	0.42
2:B:602:POV:H12	1:C:311:THR:H	1.85	0.42
1:D:405:ILE:HD13	1:C:405:ILE:HD12	2.02	0.42
1:C:308:ARG:HG3	1:C:308:ARG:NH1	2.34	0.42
1:A:327:LEU:O	1:A:331:ILE:HG12	2.20	0.42
1:D:198:SER:HB2	1:D:302:ARG:HH11	1.85	0.42
1:D:319:THR:HG21	1:D:412:PHE:CE1	2.55	0.42
1:A:328:GLY:CA	2:A:601:POV:H32A	2.50	0.42
1:B:330:LEU:HD13	1:B:404:PRO:HG2	2.00	0.42
1:D:224:GLN:O	1:D:227:HIS:HB2	2.20	0.42
1:A:416:TYR:CE1	1:D:329:LEU:HD11	2.55	0.41
1:B:296:ARG:O	1:B:299:ARG:HG2	2.20	0.41
1:A:401:ILE:HG21	1:D:398:VAL:HG11	2.01	0.41
1:A:411:ASN:O	1:A:415:PHE:CD1	2.74	0.41
2:A:606:POV:H13B	2:A:606:POV:H11A	1.70	0.41
1:A:244:PHE:HD2	1:A:245:LEU:HD12	1.85	0.41
1:D:173:ASP:OD1	1:D:173:ASP:N	2.54	0.41
1:D:257:PRO:CG	2:D:601:POV:H3A	2.50	0.41
1:D:400:VAL:O	1:D:404:PRO:HD3	2.21	0.41
1:D:271:VAL:HG11	1:D:295:PHE:CE2	2.55	0.41
1:D:294:ILE:HA	1:D:297:ILE:HG12	2.02	0.41
1:D:306:LEU:HD22	2:D:603:POV:H22	2.02	0.41
2:A:601:POV:H15B	2:A:601:POV:H11A	1.50	0.41
1:B:397:GLY:O	1:B:401:ILE:HB	2.20	0.41
1:C:361:PRO:HA	1:C:364:PHE:CD2	2.56	0.41
1:A:374:VAL:HG21	1:D:394:CYS:SG	2.61	0.41
1:D:200:ILE:HD13	1:D:200:ILE:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:VAL:O	1:D:234:ALA:HB3	2.20	0.40
1:D:327:LEU:O	1:D:327:LEU:HD23	2.21	0.40
1:C:198:SER:OG	1:C:232:CYS:HB3	2.21	0.40
1:C:349:GLU:OE2	1:C:386:GLY:HA3	2.21	0.40
1:C:233:ILE:HD11	1:C:266:ILE:HG23	2.03	0.40
1:B:319:THR:HG21	1:B:412:PHE:HB2	2.02	0.40
1:D:208:PRO:HD3	1:C:359:SER:HB3	2.01	0.40
1:B:369:ILE:HG22	1:B:375:GLY:H	1.86	0.40
1:D:402:ALA:O	1:D:406:PRO:CD	2.69	0.40
1:C:290:ARG:O	1:C:293:GLN:HG2	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	230/600 (38%)	227 (99%)	3 (1%)	0	100	100
1	B	230/600 (38%)	225 (98%)	5 (2%)	0	100	100
1	C	228/600 (38%)	219 (96%)	9 (4%)	0	100	100
1	D	227/600 (38%)	219 (96%)	8 (4%)	0	100	100
All	All	915/2400 (38%)	890 (97%)	25 (3%)	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	191/537 (36%)	191 (100%)	0	100	100
1	B	191/537 (36%)	191 (100%)	0	100	100
1	C	178/537 (33%)	178 (100%)	0	100	100
1	D	177/537 (33%)	176 (99%)	1 (1%)	86	92
All	All	737/2148 (34%)	736 (100%)	1 (0%)	93	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	415	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	411	ASN
1	C	411	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	POV	A	604	-	14,14,51	1.24	1 (7%)	14,14,59	1.22	1 (7%)
2	POV	D	601	-	27,27,51	1.53	4 (14%)	31,32,59	1.42	2 (6%)
2	POV	C	603	-	14,14,51	1.15	1 (7%)	14,14,59	1.53	2 (14%)
2	POV	C	601	-	6,6,51	0.34	0	5,5,59	0.78	0
2	POV	B	602	-	28,28,51	1.41	3 (10%)	34,36,59	1.08	4 (11%)
2	POV	D	603	-	6,6,51	0.33	0	5,5,59	0.80	0
2	POV	A	606	-	18,18,51	1.32	2 (11%)	23,24,59	1.04	1 (4%)
2	POV	A	605	-	6,6,51	0.28	0	5,5,59	0.85	0
2	POV	A	601	-	28,28,51	1.39	4 (14%)	34,36,59	1.41	4 (11%)
2	POV	A	603	-	14,14,51	1.24	1 (7%)	14,14,59	1.22	1 (7%)
2	POV	D	602	-	14,14,51	1.25	1 (7%)	14,14,59	1.21	1 (7%)
2	POV	B	603	-	26,26,51	1.54	4 (15%)	29,31,59	1.32	2 (6%)
2	POV	C	602	-	20,20,51	1.68	4 (20%)	24,25,59	1.37	2 (8%)
2	POV	A	602	-	27,27,51	1.52	4 (14%)	31,32,59	1.27	2 (6%)
2	POV	B	601	-	6,6,51	0.34	0	5,5,59	0.74	0

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
2	POV	A	604	-	-	1/13/13/55	-
2	POV	D	601	-	-	18/29/29/55	-
2	POV	C	603	-	-	0/13/13/55	-
2	POV	C	601	-	-	0/3/4/55	-
2	POV	B	602	-	-	18/32/32/55	-
2	POV	D	603	-	-	0/3/4/55	-
2	POV	A	606	-	-	8/19/19/55	-
2	POV	A	605	-	-	0/3/4/55	-
2	POV	A	601	-	-	14/32/32/55	-
2	POV	A	603	-	-	1/13/13/55	-
2	POV	D	602	-	-	1/13/13/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	B	603	-	-	16/28/28/55	-
2	POV	C	602	-	-	13/22/22/55	-
2	POV	A	602	-	-	17/29/29/55	-
2	POV	B	601	-	-	3/3/4/55	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	602	POV	O21-C21	4.42	1.46	1.33
2	A	603	POV	O21-C21	4.42	1.46	1.33
2	A	604	POV	O21-C21	4.39	1.46	1.33
2	A	606	POV	O31-C31	4.26	1.45	1.33
2	C	603	POV	O21-C21	3.95	1.44	1.33
2	C	602	POV	P-O12	3.89	1.69	1.54
2	D	601	POV	P-O12	3.89	1.69	1.54
2	B	603	POV	P-O12	3.88	1.69	1.54
2	A	602	POV	P-O12	3.87	1.69	1.54
2	D	601	POV	O31-C31	3.84	1.44	1.33
2	B	603	POV	O31-C31	3.82	1.44	1.33
2	A	602	POV	O31-C31	3.82	1.44	1.33
2	C	602	POV	O31-C31	3.81	1.44	1.33
2	B	602	POV	O31-C31	3.58	1.43	1.33
2	A	601	POV	O31-C31	3.58	1.43	1.33
2	B	602	POV	O21-C21	2.83	1.42	1.34
2	D	601	POV	O21-C21	2.67	1.41	1.34
2	A	601	POV	O21-C21	2.64	1.41	1.34
2	B	603	POV	O21-C21	2.60	1.41	1.34
2	C	602	POV	O21-C21	2.56	1.41	1.34
2	A	602	POV	O21-C21	2.56	1.41	1.34
2	A	606	POV	P-O12	2.44	1.69	1.59
2	B	602	POV	P-O12	2.32	1.68	1.59
2	A	601	POV	P-O12	2.25	1.68	1.59
2	D	601	POV	P-O11	2.20	1.67	1.60
2	C	602	POV	P-O11	2.18	1.67	1.60
2	A	602	POV	P-O11	2.18	1.67	1.60
2	B	603	POV	P-O11	2.13	1.67	1.60
2	A	601	POV	C12-C11	2.02	1.57	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	POV	O21-C21-C22	4.89	122.05	111.50
2	D	601	POV	O21-C21-C22	4.70	121.62	111.50
2	A	602	POV	O21-C21-C22	4.03	120.19	111.50
2	C	602	POV	O21-C21-C22	3.84	119.78	111.50
2	B	603	POV	O21-C21-C22	3.73	119.55	111.50
2	B	603	POV	O31-C31-C32	3.43	120.39	111.38
2	D	601	POV	O31-C31-C32	3.41	120.33	111.38
2	C	602	POV	O31-C31-C32	3.34	120.14	111.38
2	A	606	POV	O31-C31-C32	3.33	120.12	111.38
2	C	603	POV	O21-C21-C22	3.10	121.64	111.91
2	A	602	POV	O31-C31-C32	3.01	119.27	111.38
2	B	602	POV	O31-C31-C32	2.75	120.55	111.91
2	B	602	POV	O21-C21-C22	2.75	117.42	111.50
2	A	604	POV	O21-C21-C22	2.73	120.48	111.91
2	A	603	POV	O21-C21-C22	2.71	120.42	111.91
2	D	602	POV	O21-C21-C22	2.71	120.41	111.91
2	A	601	POV	C11-C12-N	-2.58	107.15	115.78
2	A	601	POV	O31-C31-C32	2.56	119.94	111.91
2	C	603	POV	C23-C22-C21	-2.11	105.95	113.62
2	B	602	POV	C11-C12-N	-2.11	108.75	115.78
2	B	602	POV	C2-O21-C21	2.05	122.84	117.79
2	A	601	POV	C2-O21-C21	-2.01	112.84	117.79

There are no chirality outliers.

All (110) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	POV	C1-O11-P-O12
2	A	601	POV	C1-O11-P-O13
2	A	601	POV	C1-O11-P-O14
2	A	601	POV	O12-C11-C12-N
2	A	602	POV	C210-C211-C212-C213
2	A	602	POV	C26-C27-C28-C29
2	A	606	POV	C1-O11-P-O12
2	A	606	POV	C1-O11-P-O13
2	A	606	POV	C1-O11-P-O14
2	A	606	POV	C11-O12-P-O11
2	A	606	POV	C11-O12-P-O13
2	A	606	POV	C11-O12-P-O14
2	B	601	POV	C21-C22-C23-C24
2	B	603	POV	C1-O11-P-O14
2	B	603	POV	O11-C1-C2-O21
2	D	601	POV	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
2	D	601	POV	C210-C211-C212-C213
2	A	601	POV	O32-C31-O31-C3
2	A	601	POV	C32-C31-O31-C3
2	A	602	POV	C24-C25-C26-C27
2	B	603	POV	O21-C2-C3-O31
2	C	602	POV	O21-C2-C3-O31
2	D	601	POV	C21-C22-C23-C24
2	A	606	POV	C1-C2-C3-O31
2	B	602	POV	C21-C22-C23-C24
2	B	602	POV	C1-O11-P-O12
2	C	602	POV	O22-C21-O21-C2
2	C	602	POV	C22-C21-O21-C2
2	B	602	POV	C23-C24-C25-C26
2	D	601	POV	C26-C27-C28-C29
2	A	601	POV	C23-C24-C25-C26
2	B	603	POV	C23-C24-C25-C26
2	D	601	POV	C23-C24-C25-C26
2	B	603	POV	C32-C31-O31-C3
2	D	601	POV	C32-C31-O31-C3
2	A	602	POV	C23-C24-C25-C26
2	B	603	POV	O32-C31-O31-C3
2	A	602	POV	C32-C31-O31-C3
2	C	602	POV	C32-C31-O31-C3
2	D	601	POV	O32-C31-O31-C3
2	A	602	POV	O32-C31-O31-C3
2	C	602	POV	O32-C31-O31-C3
2	C	602	POV	C21-C22-C23-C24
2	A	602	POV	C22-C21-O21-C2
2	B	603	POV	C24-C25-C26-C27
2	A	602	POV	O22-C21-O21-C2
2	B	603	POV	C26-C27-C28-C29
2	A	601	POV	C21-C22-C23-C24
2	B	603	POV	C21-C22-C23-C24
2	B	603	POV	C1-C2-C3-O31
2	C	602	POV	C1-C2-C3-O31
2	C	602	POV	C23-C24-C25-C26
2	B	602	POV	C31-C32-C33-C34
2	B	602	POV	C24-C25-C26-C27
2	A	601	POV	C24-C25-C26-C27
2	A	602	POV	C1-O11-P-O14
2	C	602	POV	C1-O11-P-O14
2	B	601	POV	C23-C24-C25-C26

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	A	602	POV	O11-C1-C2-C3
2	B	602	POV	O11-C1-C2-C3
2	B	602	POV	C32-C31-O31-C3
2	A	602	POV	C21-C22-C23-C24
2	B	603	POV	C29-C210-C211-C212
2	B	603	POV	O11-C1-C2-C3
2	D	601	POV	O11-C1-C2-C3
2	B	603	POV	C1-O11-P-O12
2	B	601	POV	C22-C23-C24-C25
2	D	601	POV	C24-C25-C26-C27
2	B	602	POV	C1-C2-O21-C21
2	D	601	POV	O11-C1-C2-O21
2	B	602	POV	O21-C2-C3-O31
2	B	602	POV	O32-C31-O31-C3
2	A	601	POV	C31-C32-C33-C34
2	A	601	POV	C11-O12-P-O11
2	B	602	POV	C1-O11-P-O13
2	B	602	POV	C1-O11-P-O14
2	A	602	POV	O11-C1-C2-O21
2	B	602	POV	O11-C1-C2-O21
2	A	606	POV	O12-C11-C12-N
2	B	602	POV	O12-C11-C12-N
2	B	602	POV	C11-O12-P-O11
2	D	601	POV	O31-C31-C32-C33
2	D	601	POV	O32-C31-C32-C33
2	A	602	POV	C29-C210-C211-C212
2	D	601	POV	C27-C28-C29-C210
2	D	601	POV	O22-C21-O21-C2
2	D	601	POV	C25-C26-C27-C28
2	D	601	POV	C1-O11-P-O12
2	C	602	POV	C1-O11-P-O12
2	A	601	POV	O22-C21-O21-C2
2	A	602	POV	C27-C28-C29-C210
2	B	603	POV	C27-C28-C29-C210
2	B	602	POV	O31-C31-C32-C33
2	A	602	POV	O21-C21-C22-C23
2	D	601	POV	C22-C21-O21-C2
2	D	601	POV	C29-C210-C211-C212
2	C	602	POV	O21-C21-C22-C23
2	B	602	POV	O32-C31-C32-C33
2	A	601	POV	C22-C21-O21-C2
2	B	602	POV	O21-C21-C22-C23

*Continued on next page...*

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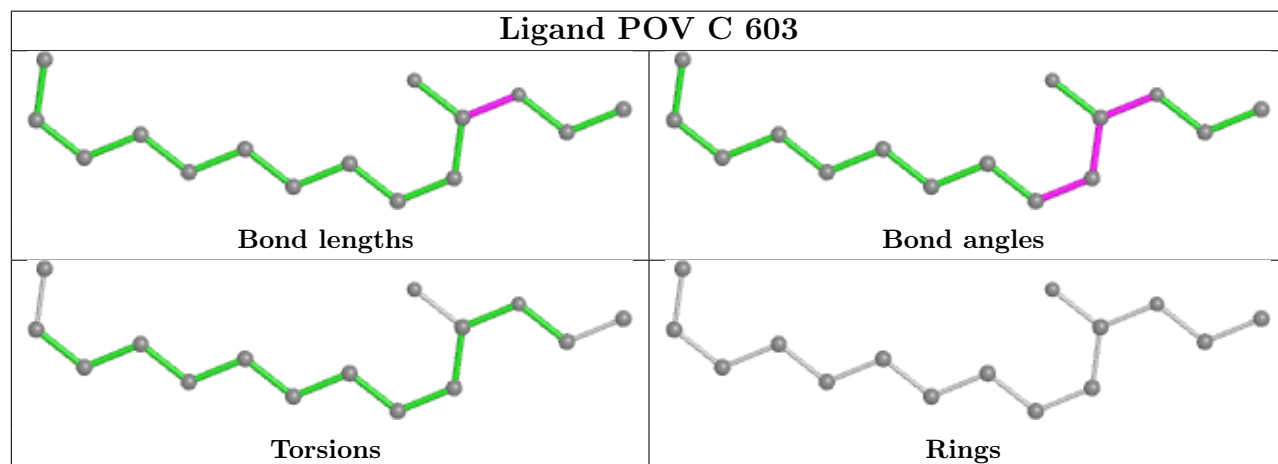
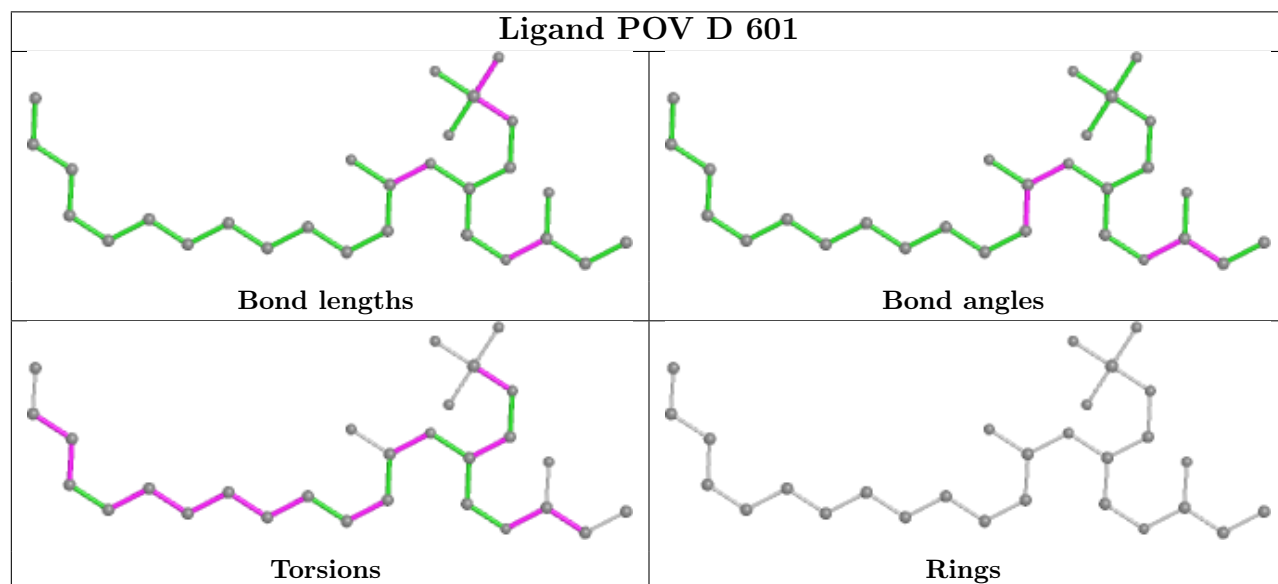
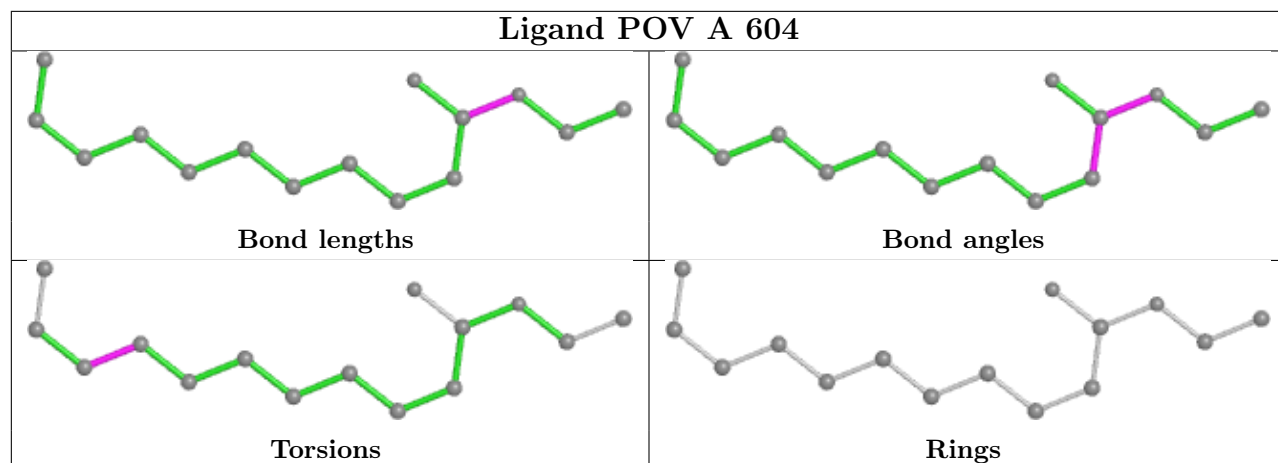
Mol	Chain	Res	Type	Atoms
2	A	601	POV	O21-C21-C22-C23
2	A	603	POV	C27-C28-C29-C210
2	A	604	POV	C27-C28-C29-C210
2	D	602	POV	C27-C28-C29-C210
2	A	602	POV	O31-C31-C32-C33
2	B	603	POV	O31-C31-C32-C33
2	C	602	POV	O31-C31-C32-C33
2	A	602	POV	O22-C21-C22-C23
2	C	602	POV	O22-C21-C22-C23
2	B	603	POV	O21-C21-C22-C23

There are no ring outliers.

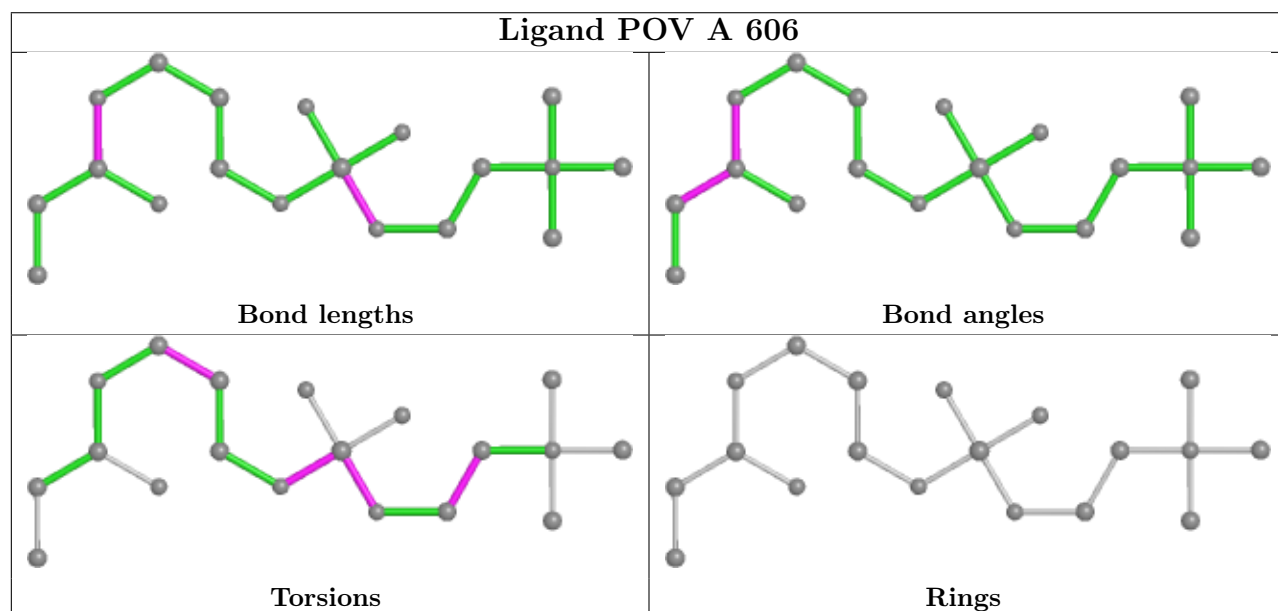
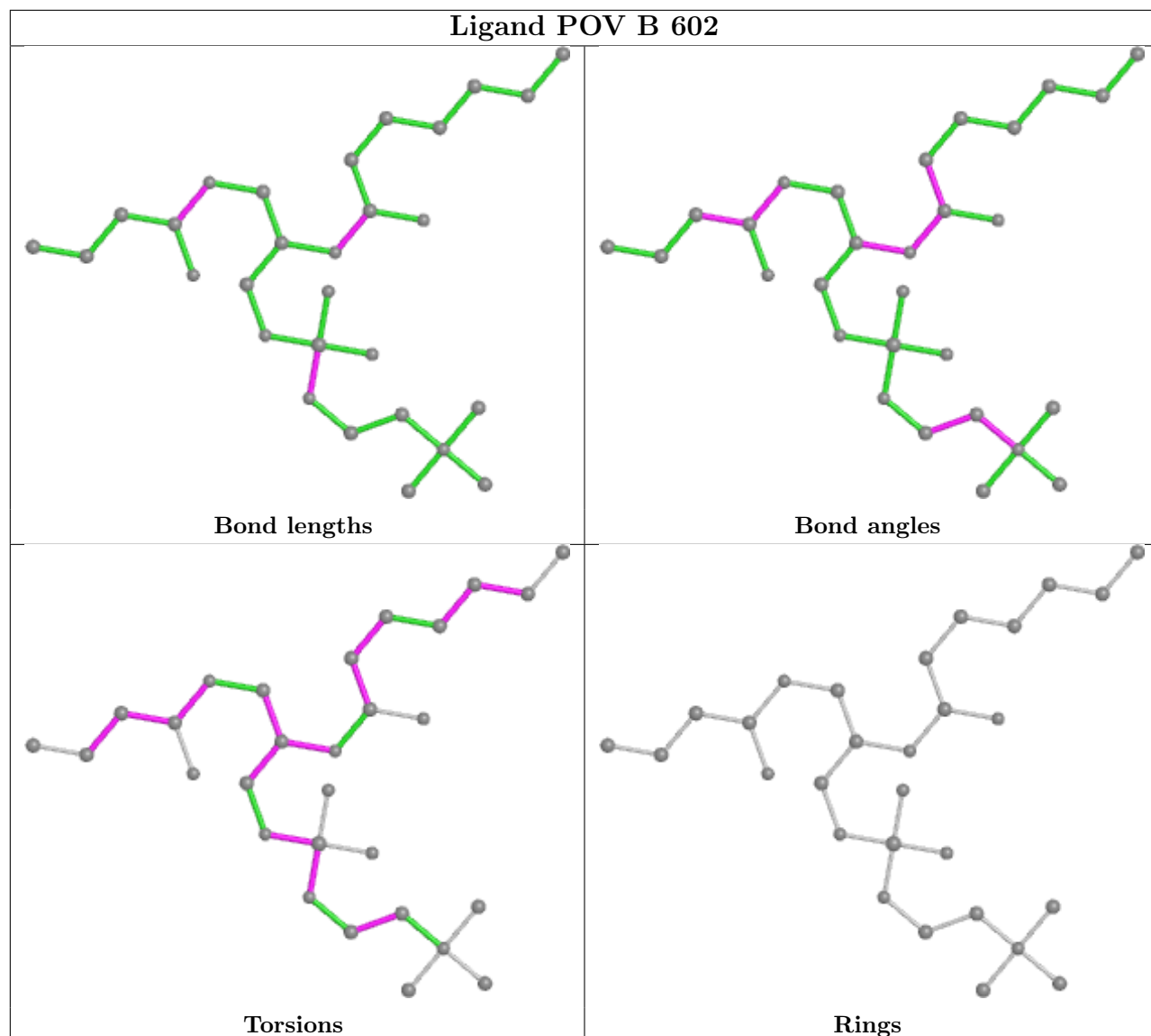
13 monomers are involved in 41 short contacts:

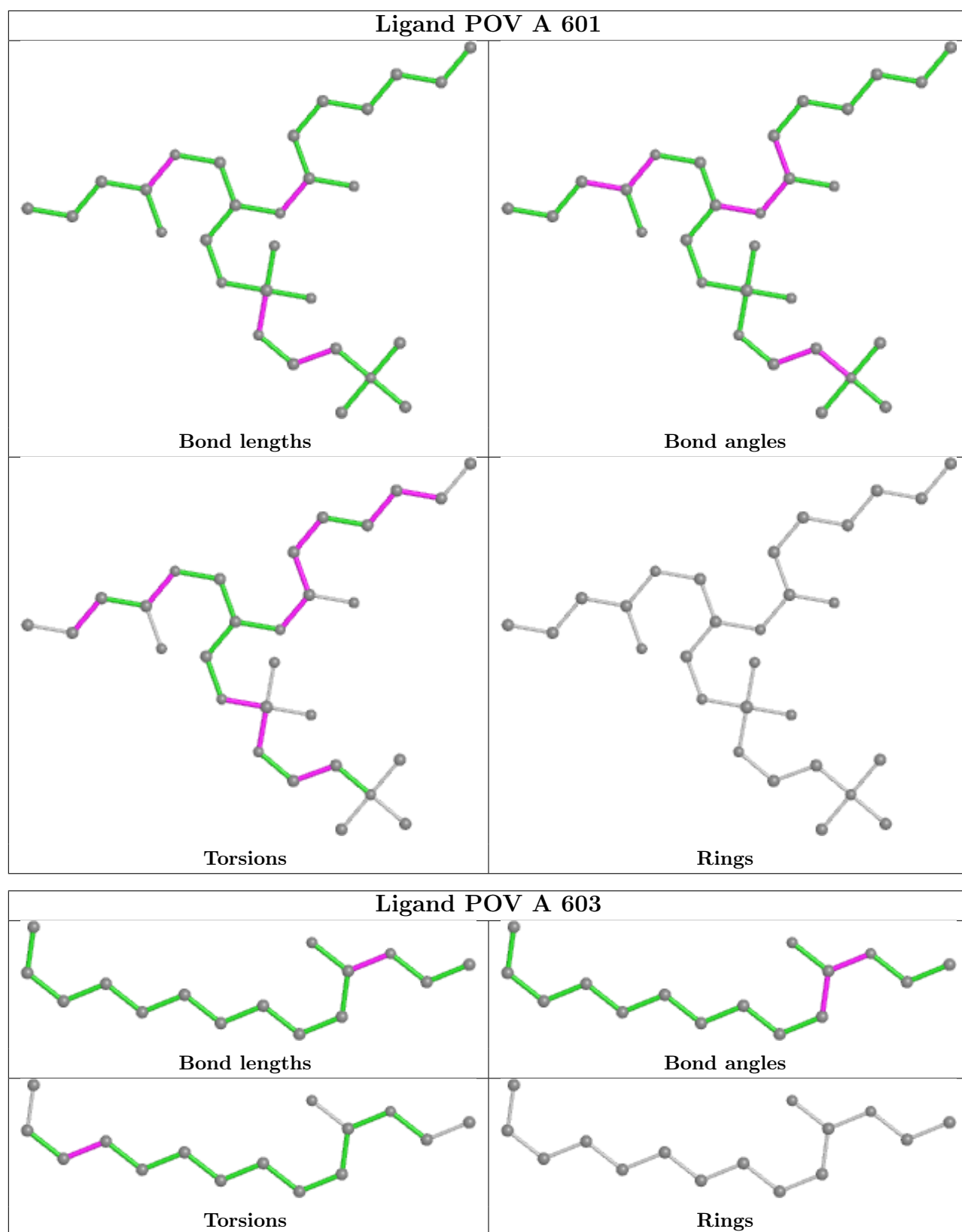
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	604	POV	2	0
2	D	601	POV	9	0
2	C	603	POV	2	0
2	C	601	POV	1	0
2	B	602	POV	1	0
2	D	603	POV	2	0
2	A	606	POV	6	0
2	A	605	POV	2	0
2	A	601	POV	6	0
2	A	603	POV	1	0
2	B	603	POV	4	0
2	C	602	POV	3	0
2	A	602	POV	4	0

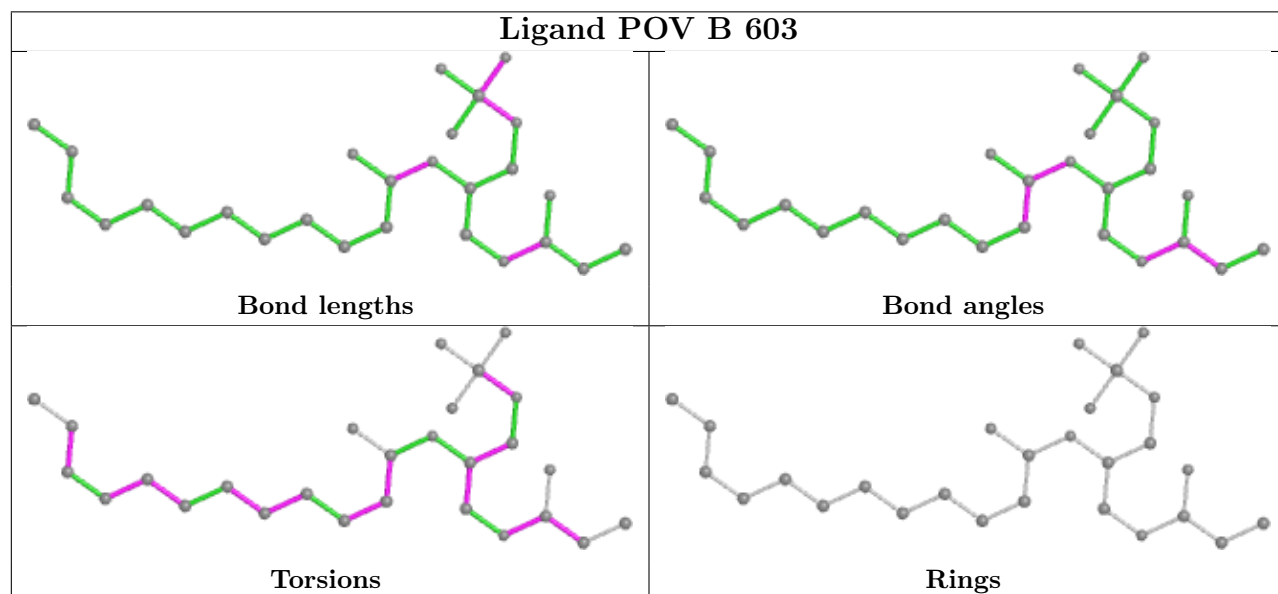
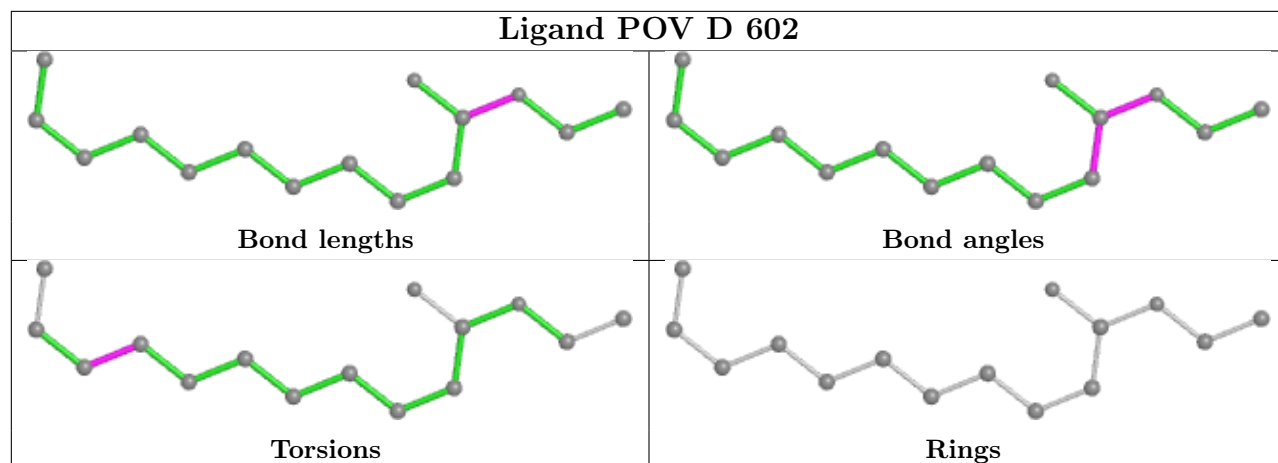
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

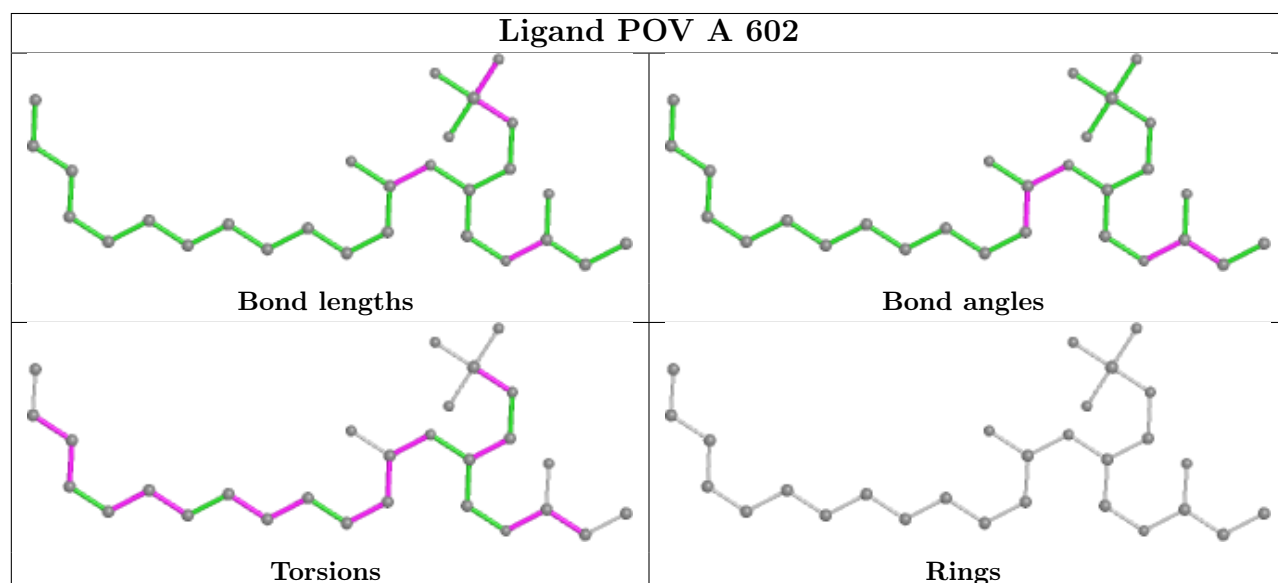
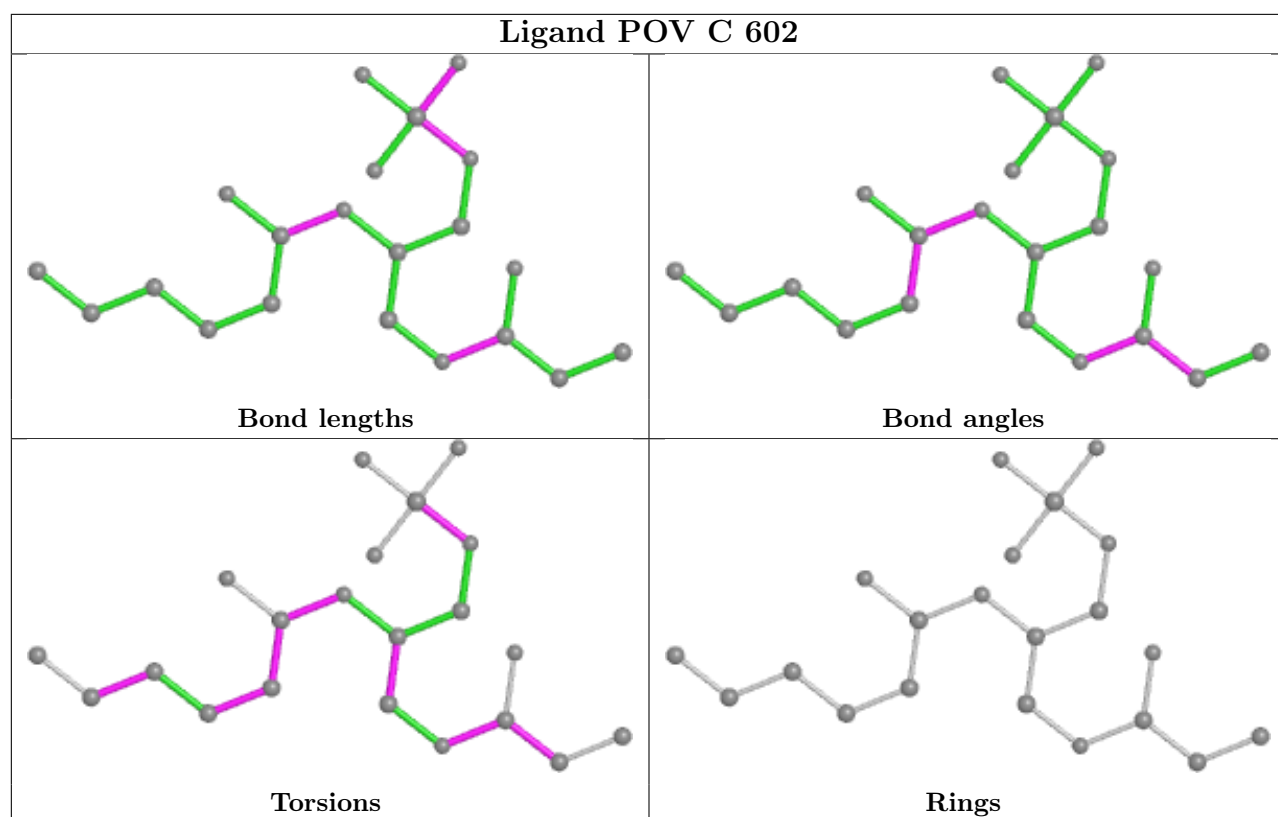


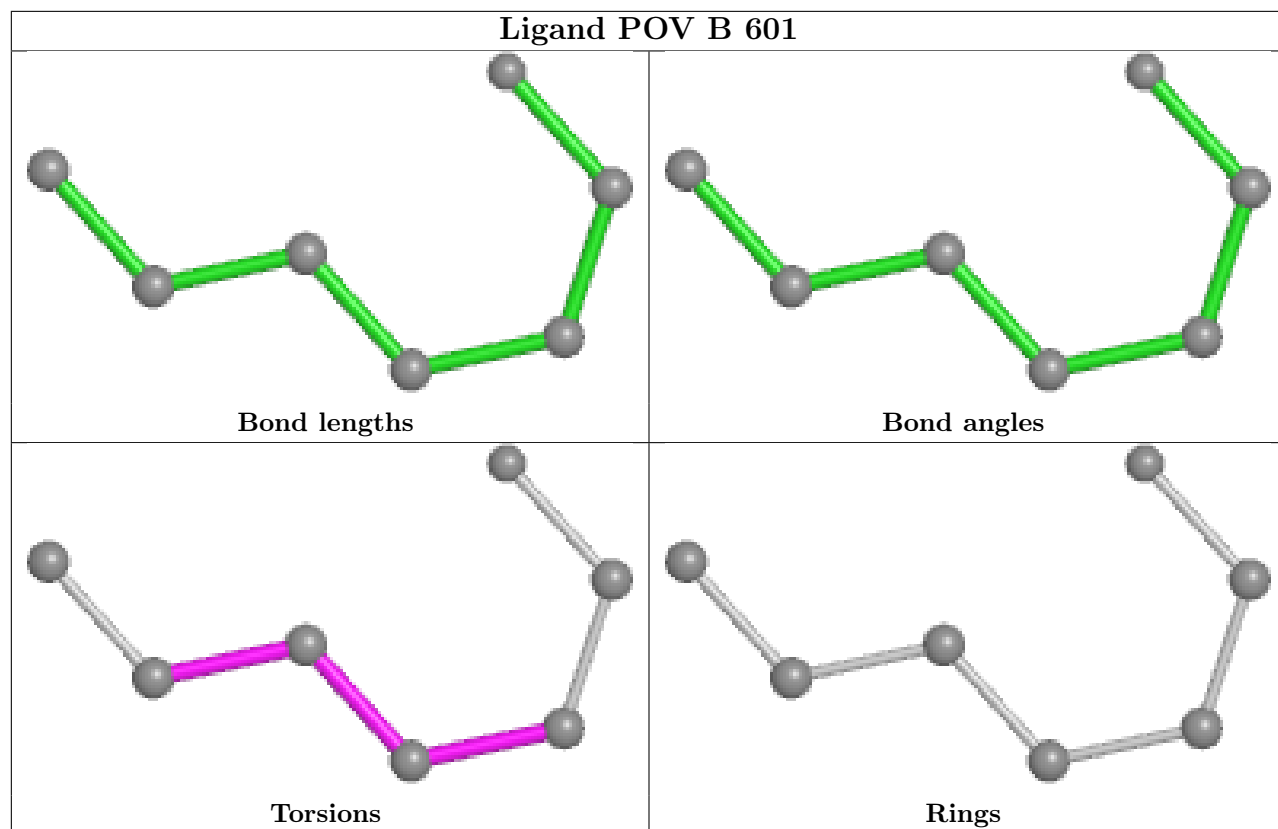












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

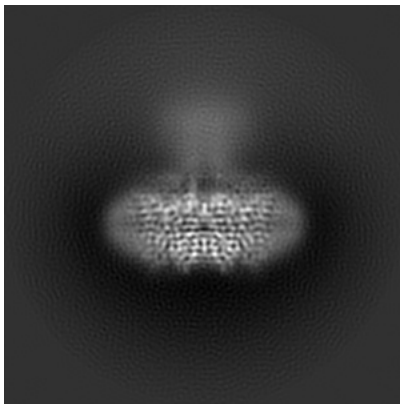
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40350. These allow visual inspection of the internal detail of the map and identification of artifacts.

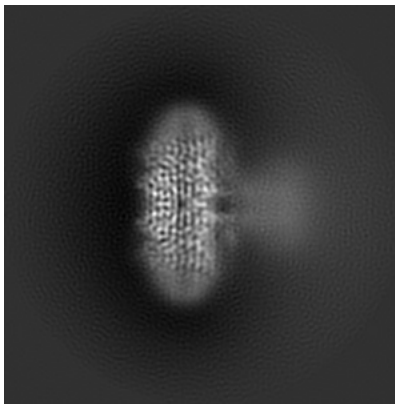
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

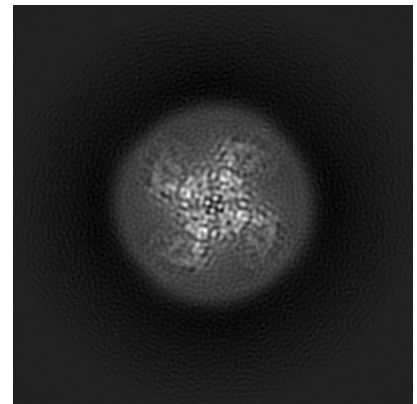
#### 6.1.1 Primary map



X

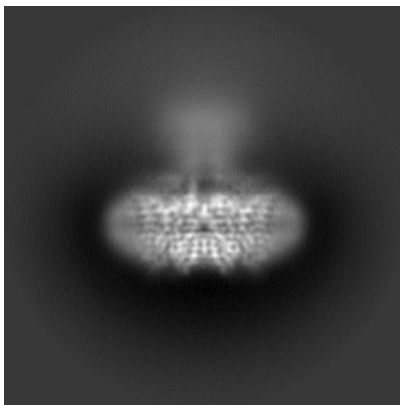


Y

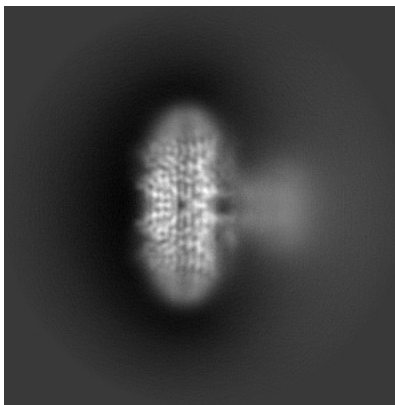


Z

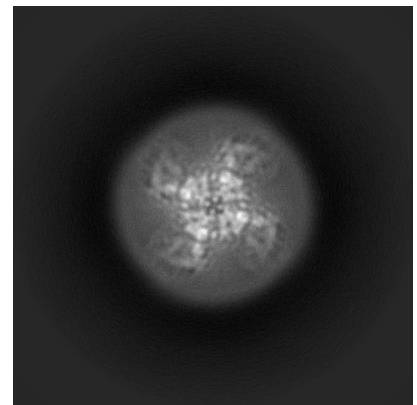
#### 6.1.2 Raw map



X



Y

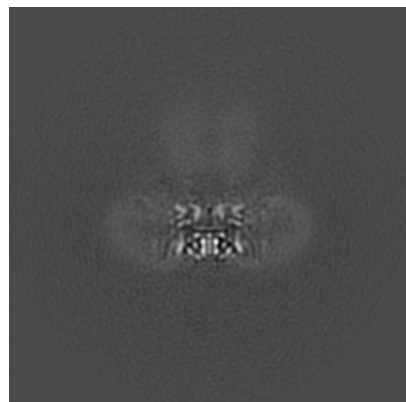


Z

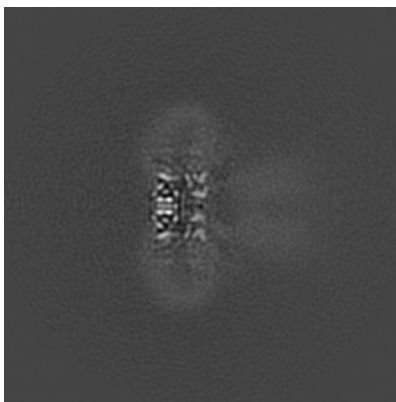
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

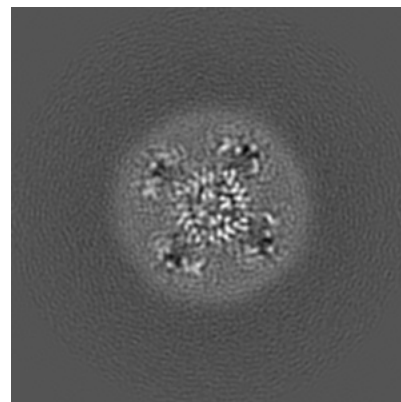
### 6.2.1 Primary map



X Index: 150

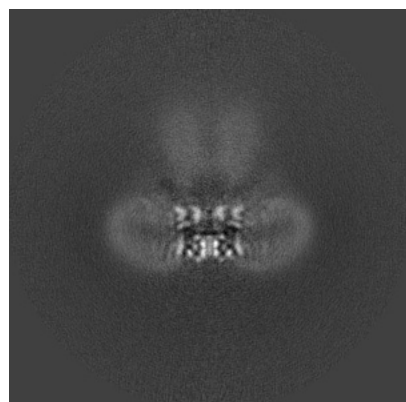


Y Index: 150

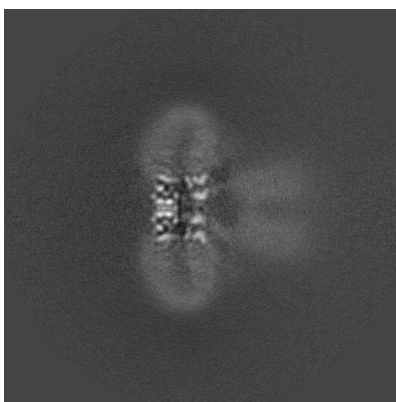


Z Index: 150

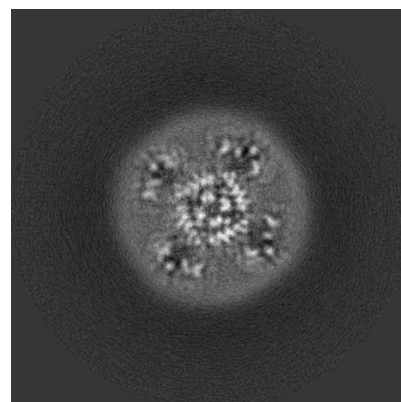
### 6.2.2 Raw map



X Index: 150



Y Index: 150

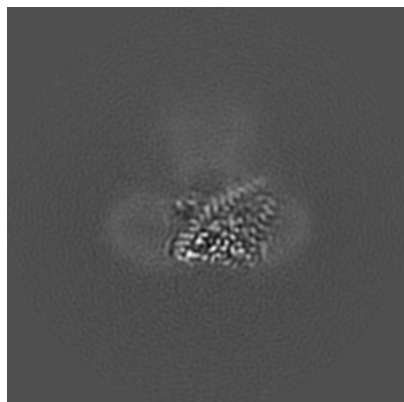


Z Index: 150

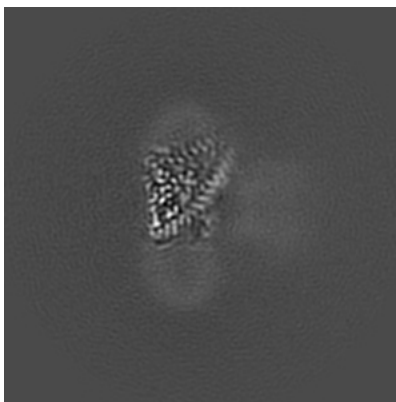
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

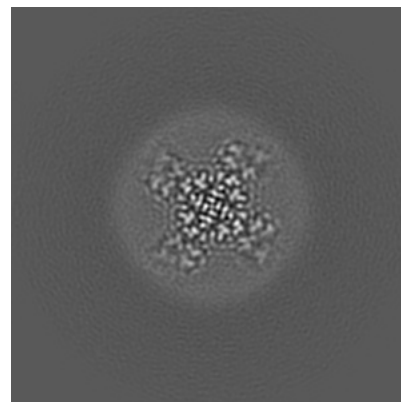
### 6.3.1 Primary map



X Index: 158

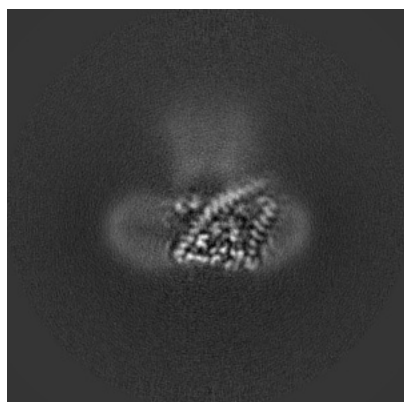


Y Index: 142

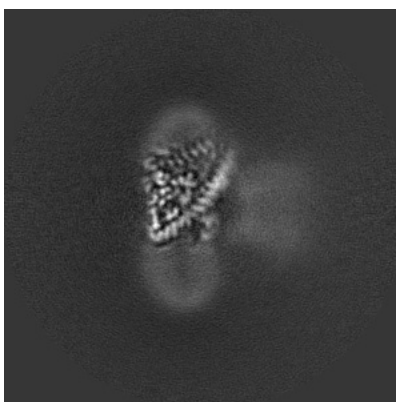


Z Index: 122

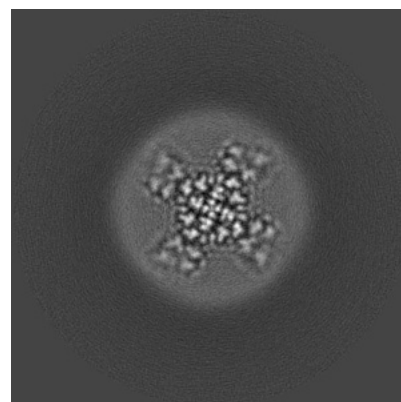
### 6.3.2 Raw map



X Index: 159



Y Index: 142



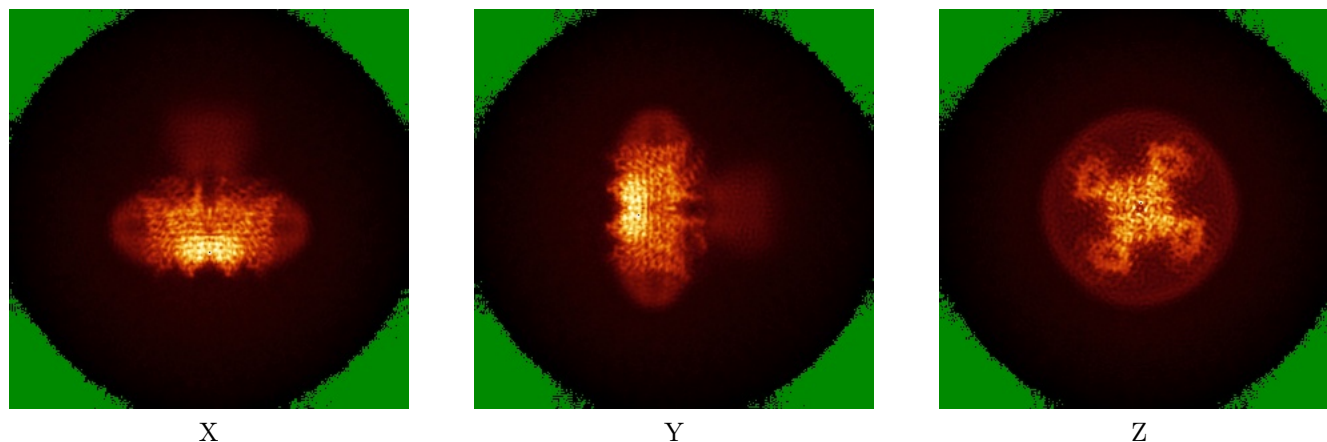
Z Index: 122

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

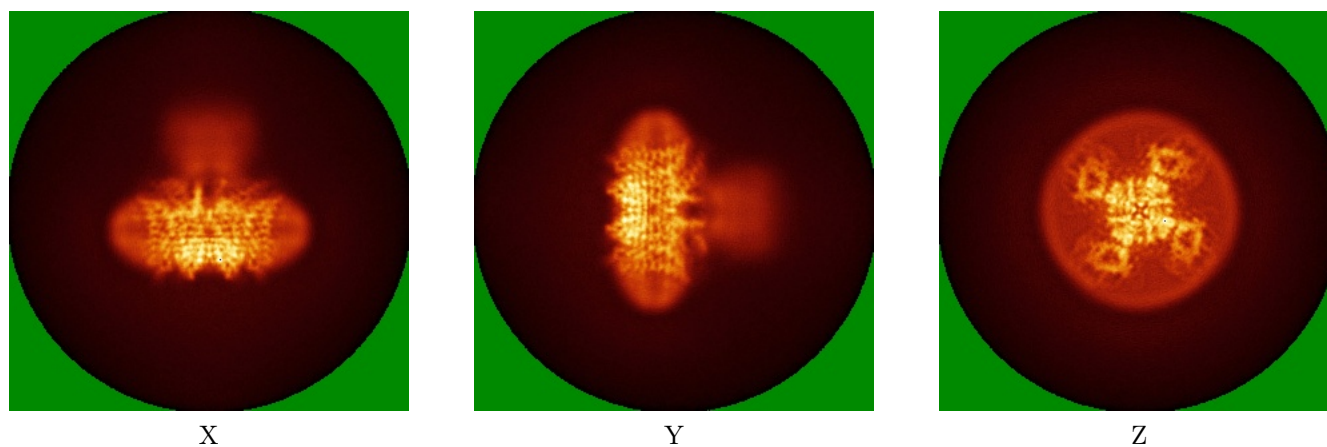


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



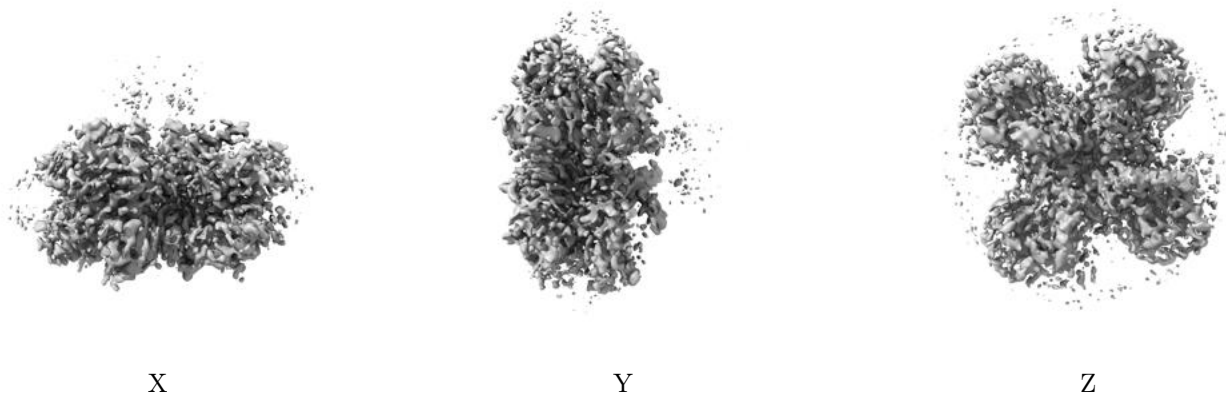
### 6.4.2 Raw map



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.

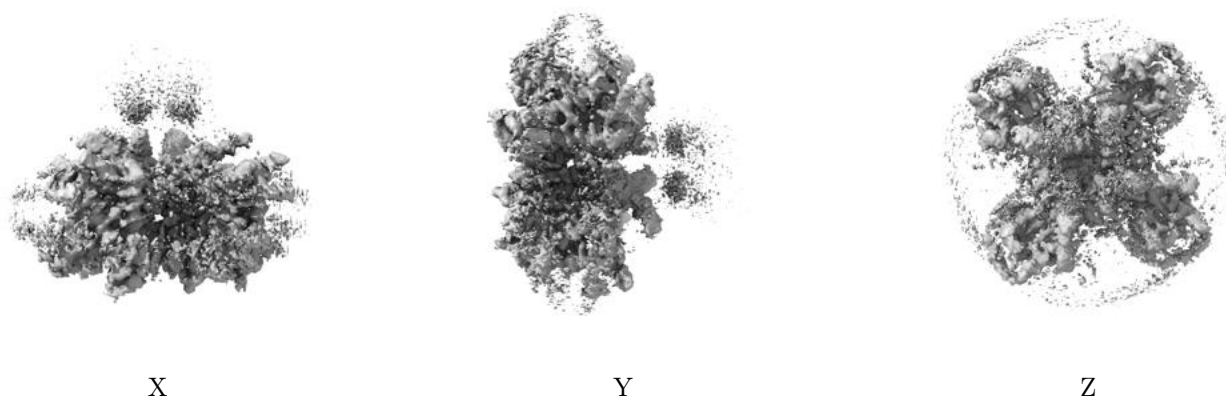
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0055. 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.

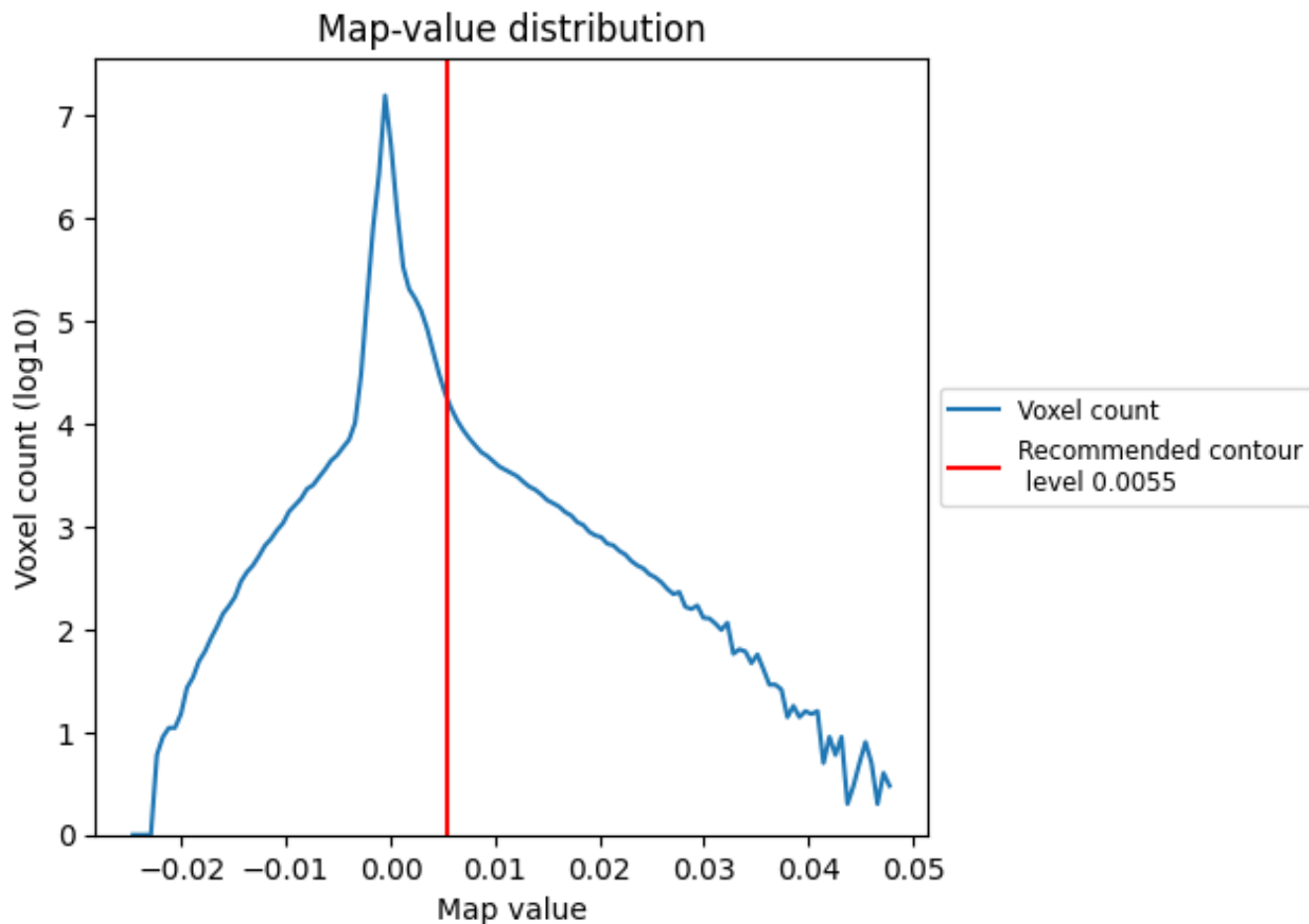
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

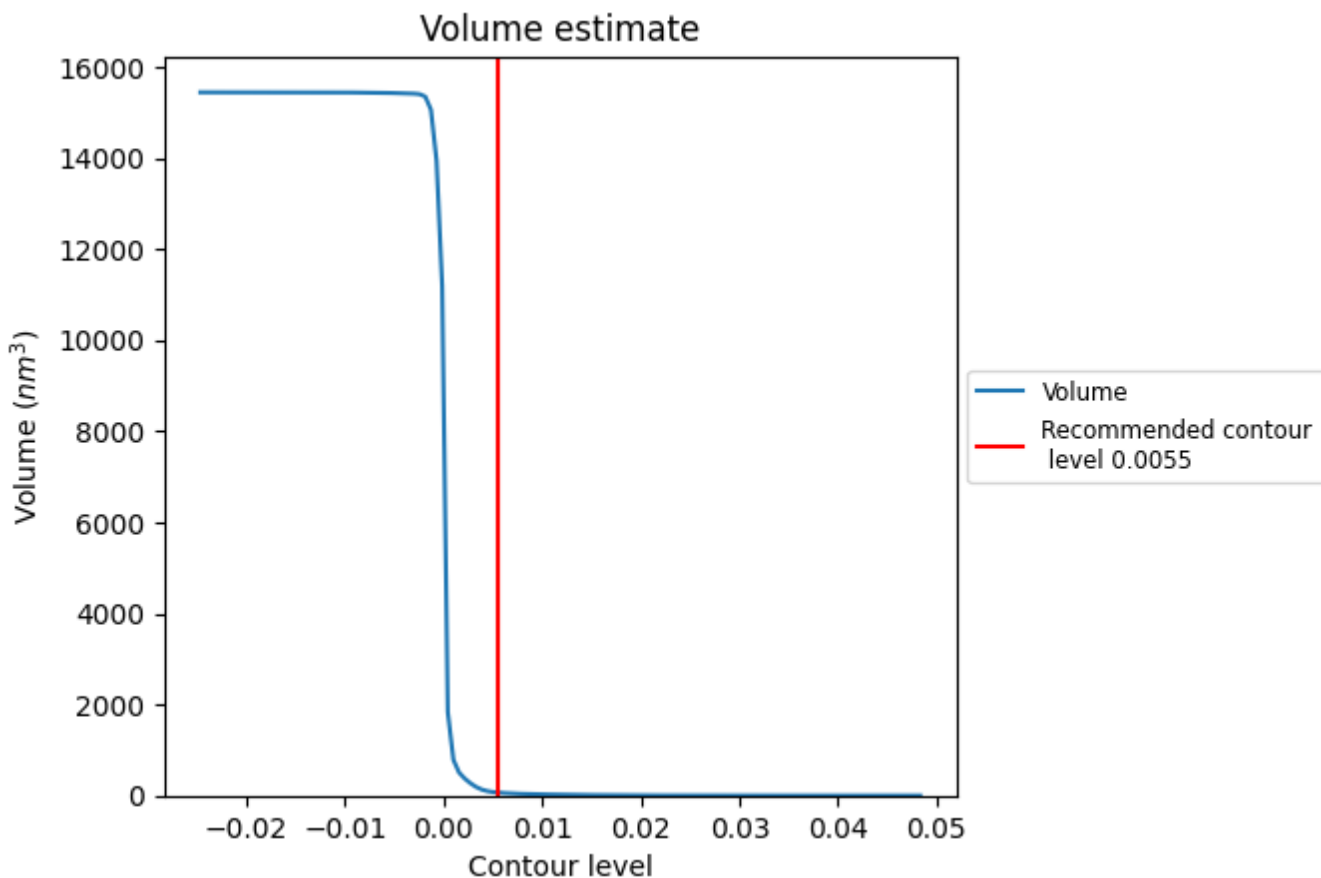
This section contains the results of statistical analysis of the map.

### 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.

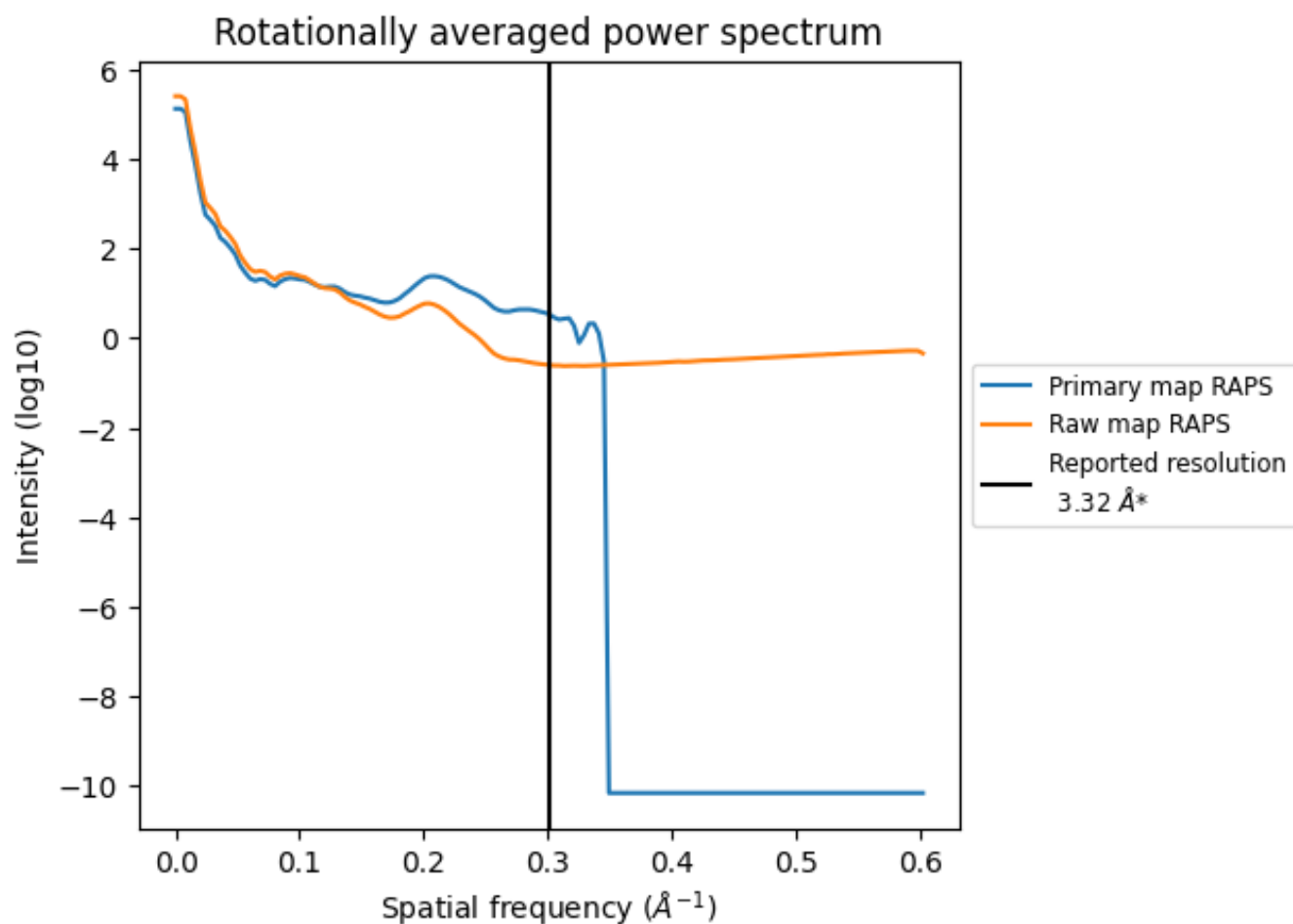
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 66 nm<sup>3</sup>; this corresponds to an approximate mass of 59 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 [\(i\)](#)

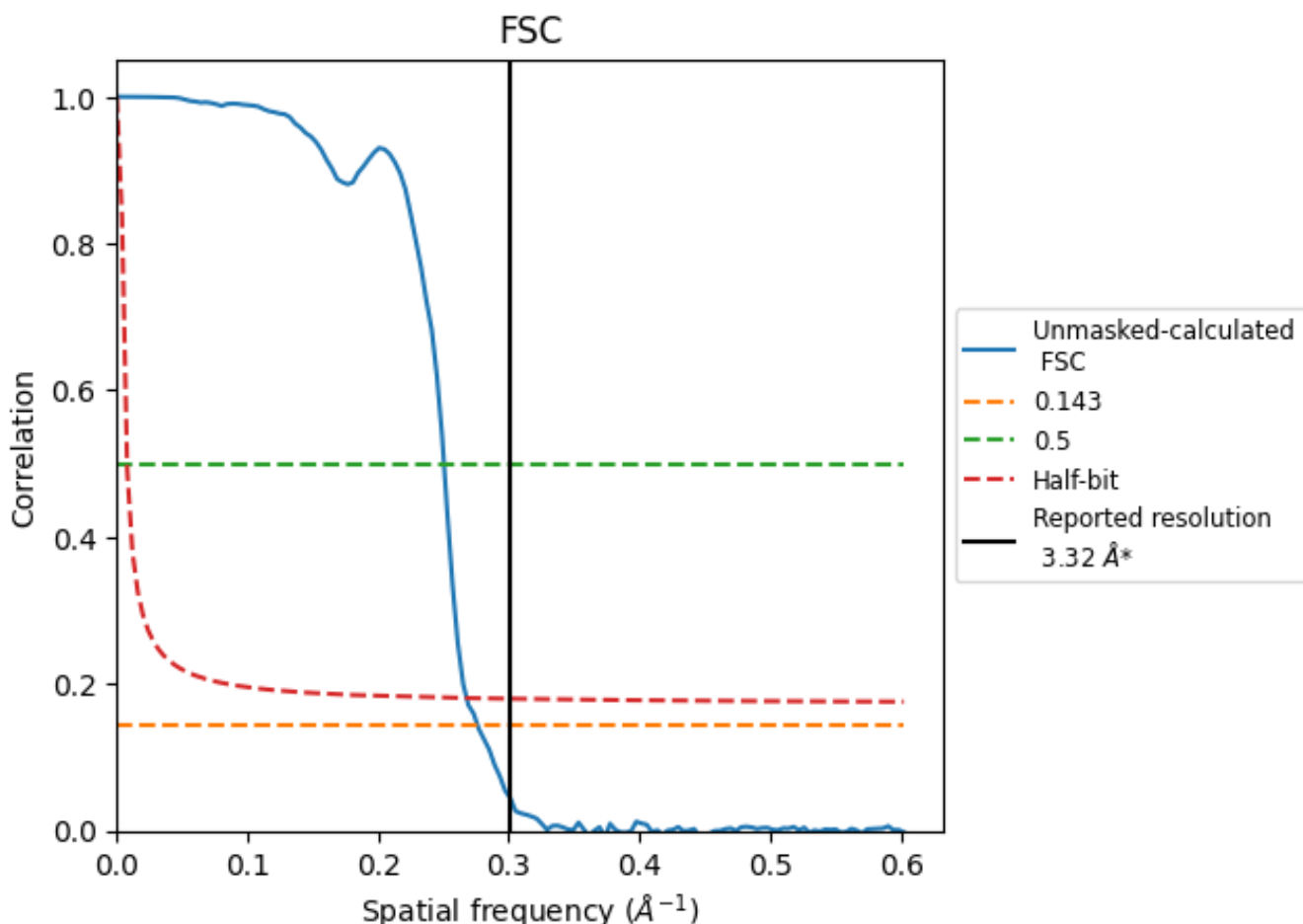


\*Reported resolution corresponds to spatial frequency of 0.301 Å<sup>-1</sup>

## 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 0.301  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

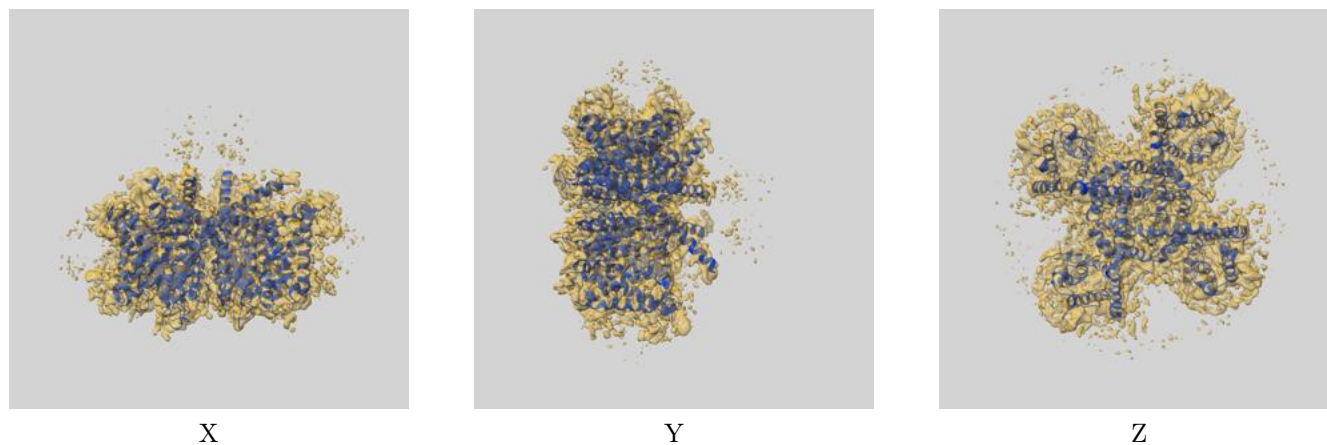
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.32	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.62	3.99	3.74

\*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-40350 and PDB model 8SDA. Per-residue inclusion information can be found in section 3 on page 6.

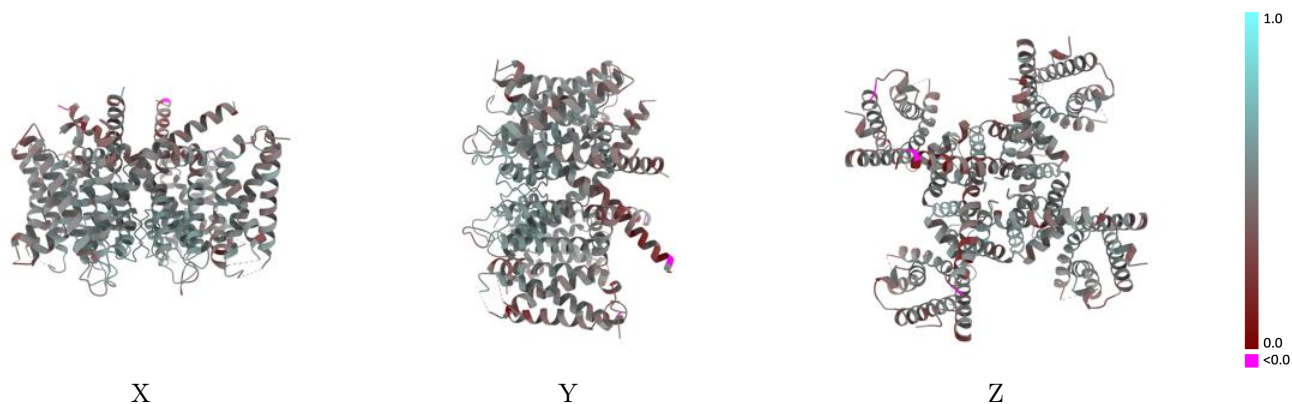
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0055 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.

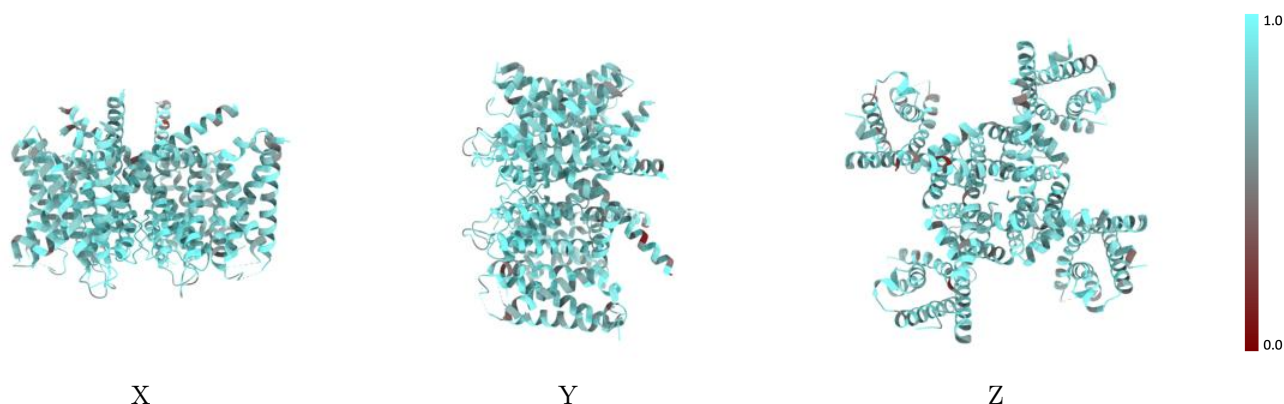


## 9.2 Q-score mapped to coordinate model [\(i\)](#)



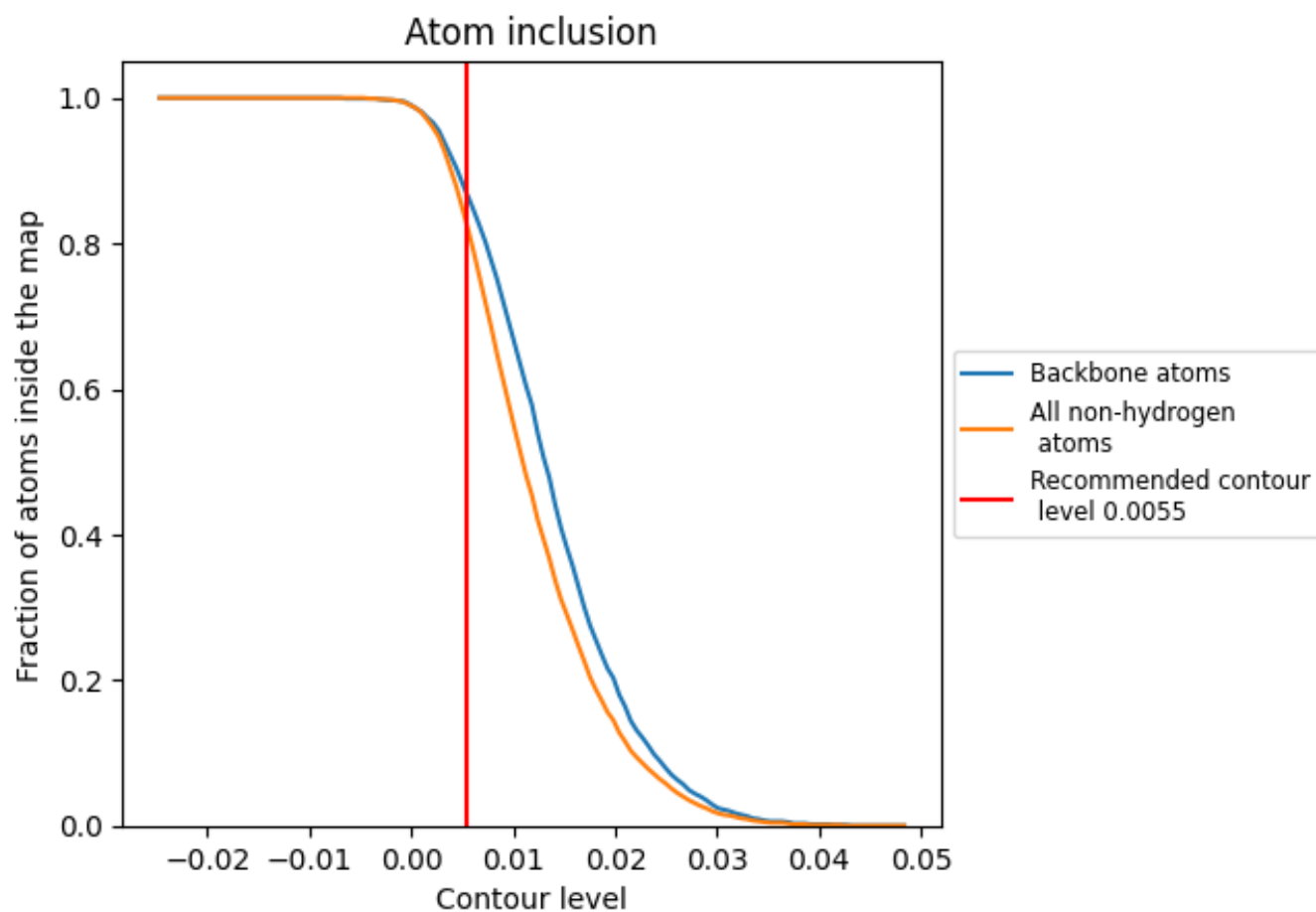
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0055).











## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 82% 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 (0.0055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8230	 0.4780
A	 0.8300	 0.4920
B	 0.8310	 0.4890
C	 0.8300	 0.4740
D	 0.7990	 0.4540

