



## Full wwPDB EM Validation Report ⓘ

May 25, 2024 – 09:08 AM EDT

PDB ID : 7RAS  
EMDB ID : EMD-24385  
Title : Structure of TRPV3 in complex with osthole  
Authors : Neuberger, A.; Nadezhdin, K.D.; Sobolevsky, A.I.  
Deposited on : 2021-07-02  
Resolution : 3.64 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.dev92  
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 : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

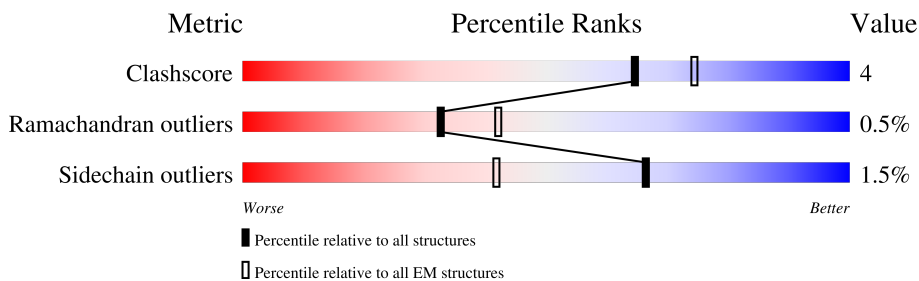
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.64 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	808	
1	B	808	
1	C	808	
1	D	808	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	A00	A	901	-	X	-	-

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
2	A0O	A	902	-	X	-	-
2	A0O	B	901	-	X	-	-
2	A0O	B	902	-	X	-	-
2	A0O	C	901	-	X	-	-
2	A0O	C	902	-	X	-	-
2	A0O	D	901	-	X	-	-
2	A0O	D	902	-	X	-	-

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 20000 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 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	610	4964	3238	818	879	29	0	0
1	B	610	4964	3238	818	879	29	0	0
1	C	610	4964	3238	818	879	29	0	0
1	D	610	4964	3238	818	879	29	0	0

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	ASN	conflict	UNP Q8K424
A	564	ALA	TYR	engineered mutation	UNP Q8K424
A	792	LEU	-	expression tag	UNP Q8K424
A	793	VAL	-	expression tag	UNP Q8K424
A	794	PRO	-	expression tag	UNP Q8K424
A	795	ARG	-	expression tag	UNP Q8K424
A	796	GLY	-	expression tag	UNP Q8K424
A	797	SER	-	expression tag	UNP Q8K424
A	798	ALA	-	expression tag	UNP Q8K424
A	799	ALA	-	expression tag	UNP Q8K424
A	800	ALA	-	expression tag	UNP Q8K424
A	801	TRP	-	expression tag	UNP Q8K424
A	802	SER	-	expression tag	UNP Q8K424
A	803	HIS	-	expression tag	UNP Q8K424
A	804	PRO	-	expression tag	UNP Q8K424
A	805	GLN	-	expression tag	UNP Q8K424
A	806	PHE	-	expression tag	UNP Q8K424
A	807	GLU	-	expression tag	UNP Q8K424
A	808	LYS	-	expression tag	UNP Q8K424
B	2	GLY	ASN	conflict	UNP Q8K424
B	564	ALA	TYR	engineered mutation	UNP Q8K424

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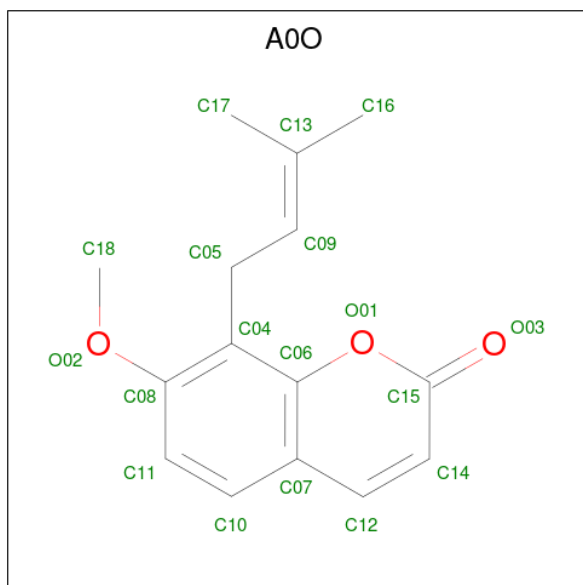
Chain	Residue	Modelled	Actual	Comment	Reference
B	792	LEU	-	expression tag	UNP Q8K424
B	793	VAL	-	expression tag	UNP Q8K424
B	794	PRO	-	expression tag	UNP Q8K424
B	795	ARG	-	expression tag	UNP Q8K424
B	796	GLY	-	expression tag	UNP Q8K424
B	797	SER	-	expression tag	UNP Q8K424
B	798	ALA	-	expression tag	UNP Q8K424
B	799	ALA	-	expression tag	UNP Q8K424
B	800	ALA	-	expression tag	UNP Q8K424
B	801	TRP	-	expression tag	UNP Q8K424
B	802	SER	-	expression tag	UNP Q8K424
B	803	HIS	-	expression tag	UNP Q8K424
B	804	PRO	-	expression tag	UNP Q8K424
B	805	GLN	-	expression tag	UNP Q8K424
B	806	PHE	-	expression tag	UNP Q8K424
B	807	GLU	-	expression tag	UNP Q8K424
B	808	LYS	-	expression tag	UNP Q8K424
C	2	GLY	ASN	conflict	UNP Q8K424
C	564	ALA	TYR	engineered mutation	UNP Q8K424
C	792	LEU	-	expression tag	UNP Q8K424
C	793	VAL	-	expression tag	UNP Q8K424
C	794	PRO	-	expression tag	UNP Q8K424
C	795	ARG	-	expression tag	UNP Q8K424
C	796	GLY	-	expression tag	UNP Q8K424
C	797	SER	-	expression tag	UNP Q8K424
C	798	ALA	-	expression tag	UNP Q8K424
C	799	ALA	-	expression tag	UNP Q8K424
C	800	ALA	-	expression tag	UNP Q8K424
C	801	TRP	-	expression tag	UNP Q8K424
C	802	SER	-	expression tag	UNP Q8K424
C	803	HIS	-	expression tag	UNP Q8K424
C	804	PRO	-	expression tag	UNP Q8K424
C	805	GLN	-	expression tag	UNP Q8K424
C	806	PHE	-	expression tag	UNP Q8K424
C	807	GLU	-	expression tag	UNP Q8K424
C	808	LYS	-	expression tag	UNP Q8K424
D	2	GLY	ASN	conflict	UNP Q8K424
D	564	ALA	TYR	engineered mutation	UNP Q8K424
D	792	LEU	-	expression tag	UNP Q8K424
D	793	VAL	-	expression tag	UNP Q8K424
D	794	PRO	-	expression tag	UNP Q8K424
D	795	ARG	-	expression tag	UNP Q8K424

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Chain	Residue	Modelled	Actual	Comment	Reference
D	796	GLY	-	expression tag	UNP Q8K424
D	797	SER	-	expression tag	UNP Q8K424
D	798	ALA	-	expression tag	UNP Q8K424
D	799	ALA	-	expression tag	UNP Q8K424
D	800	ALA	-	expression tag	UNP Q8K424
D	801	TRP	-	expression tag	UNP Q8K424
D	802	SER	-	expression tag	UNP Q8K424
D	803	HIS	-	expression tag	UNP Q8K424
D	804	PRO	-	expression tag	UNP Q8K424
D	805	GLN	-	expression tag	UNP Q8K424
D	806	PHE	-	expression tag	UNP Q8K424
D	807	GLU	-	expression tag	UNP Q8K424
D	808	LYS	-	expression tag	UNP Q8K424

- Molecule 2 is 7-methoxy-8-(3-methylbut-2-enyl)chromen-2-one (three-letter code: A00) (formula: C<sub>15</sub>H<sub>16</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			18	15	3	
2	A	1	Total	C	O	0
			18	15	3	
2	B	1	Total	C	O	0
			18	15	3	
2	B	1	Total	C	O	0
			18	15	3	

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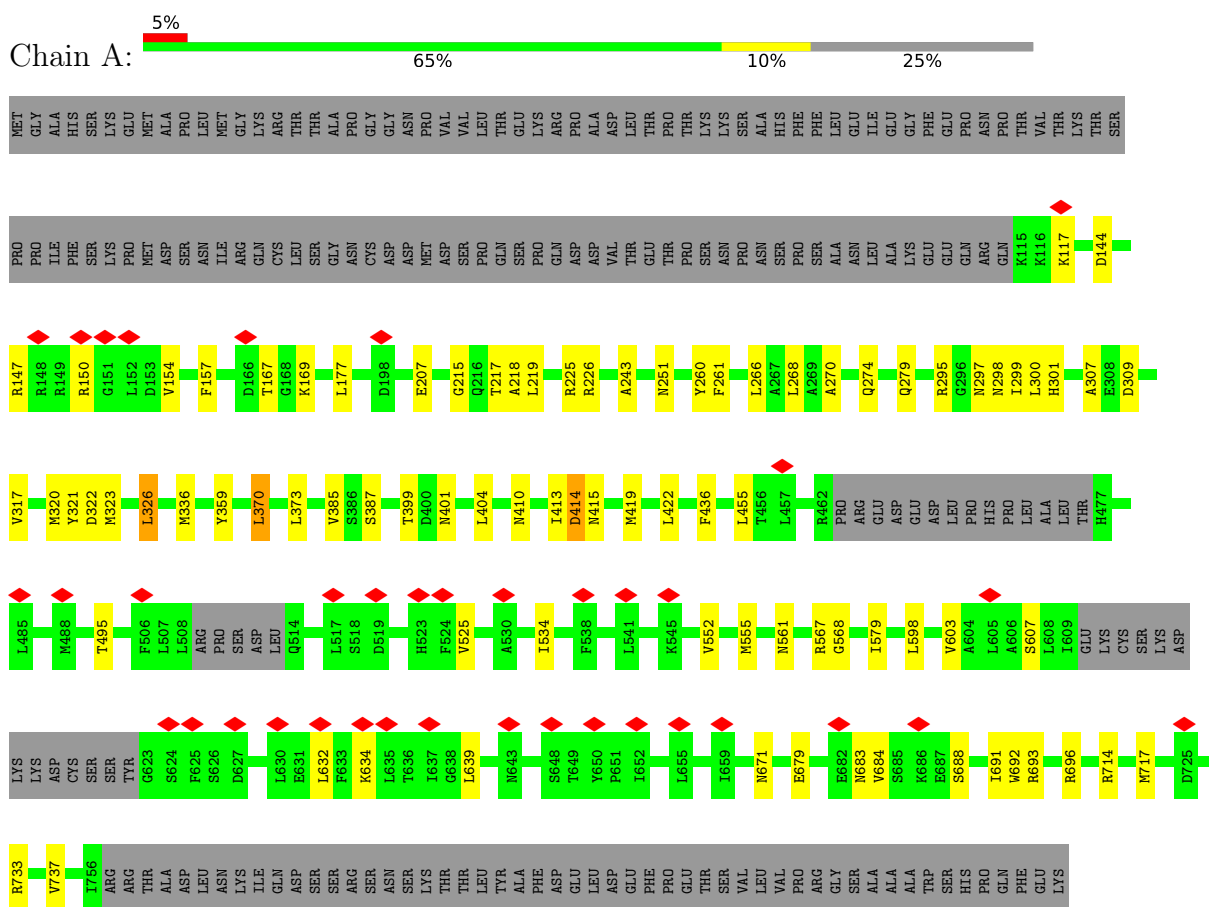
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>			<b>AltConf</b>
2	C	1	Total	C	O	0
			18	15	3	
2	C	1	Total	C	O	0
			18	15	3	
2	D	1	Total	C	O	0
			18	15	3	
2	D	1	Total	C	O	0
			18	15	3	

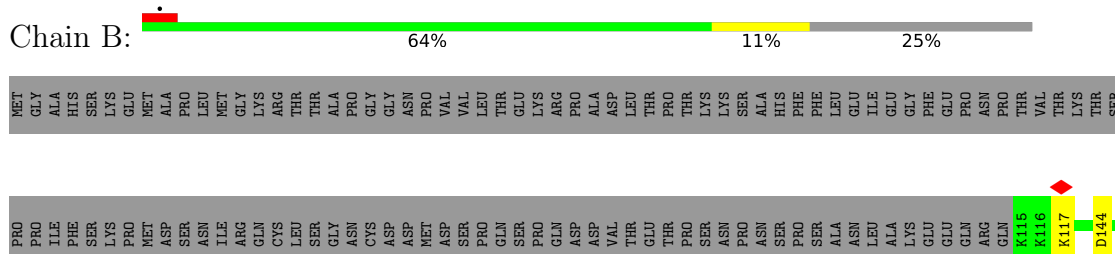
### 3 Residue-property plots

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.

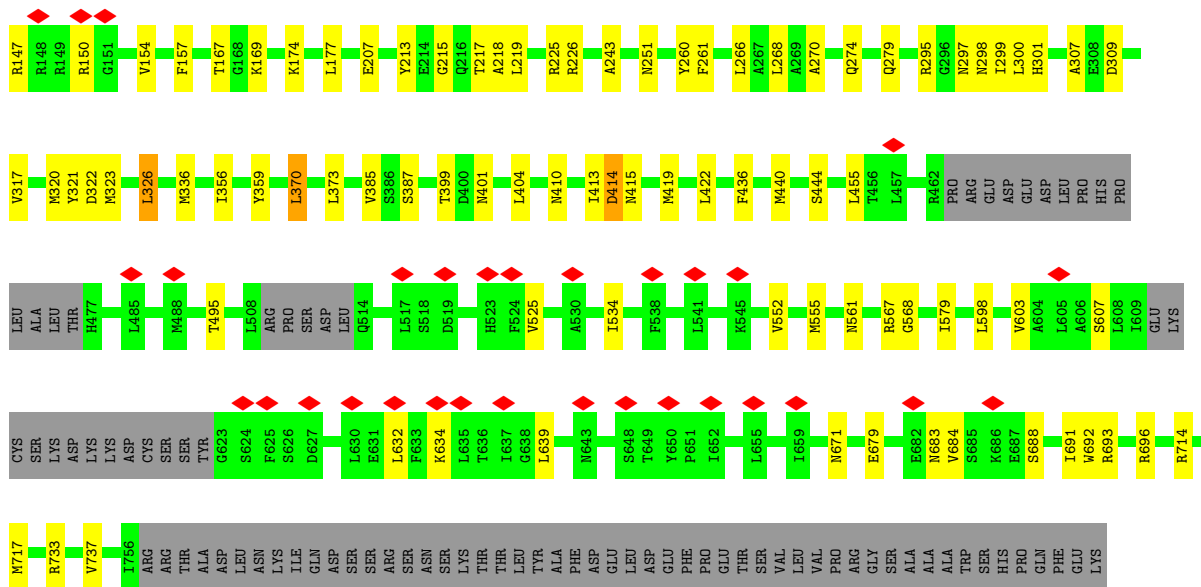
- Molecule 1: Transient receptor potential cation channel subfamily V member 3



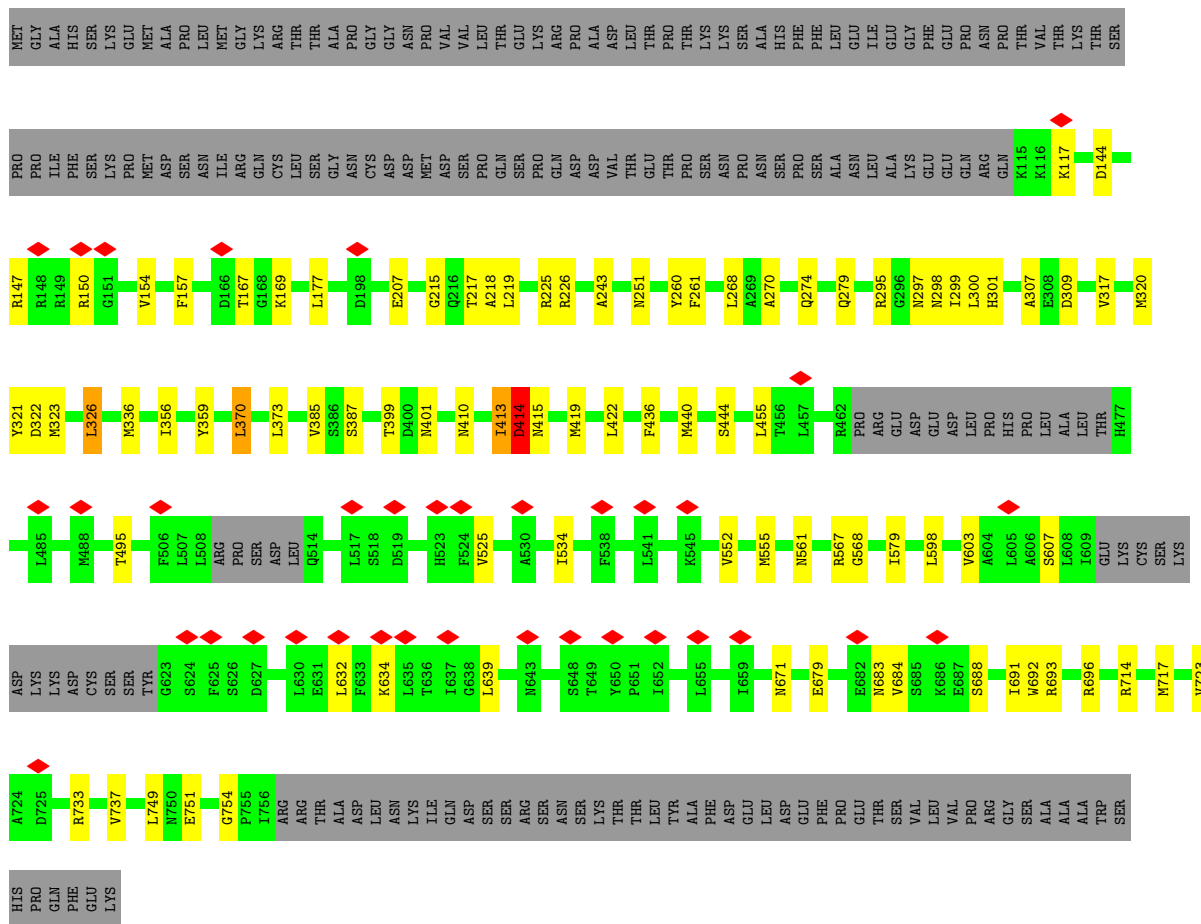
- Molecule 1: Transient receptor potential cation channel subfamily V member 3







• Molecule 1: Transient receptor potential cation channel subfamily V member 3



• Molecule 1: Transient receptor potential cation channel subfamily V member 3



MET	PRO	R147	M320	L485	CYS	M717	PRO
GLY	ILE	R148	Y321	L488	SER	W723	GLN
ALA	PHE	R149	D322	M488	LYS	A724	PHE
HIS	SER	R150	M323	T495	ASP	D725	GLU
SER	LYS	G151	L326	F506	LYS	R733	LYS
LYS	PRO	V154	M336	L507	ASP	V737	
GLU	MET	F157	Y359	L508	CYS	L749	
MET	ASP	D166	L370	ARG	TYR	I756	
ALA	ASN	T167	L373	PRO	G623	ARG	
LEU	SER	G168	V385	ASP	S624	THR	
MET	ILE	K169	S387	LEU	S626	ALA	
GLY	ARG	L177	T399	Q514	D627	ASP	
LYS	CYS	D198	M401	L517	L630	LEU	
ARG	LEU	E207	M410	S518	E631	LEU	
THR	GLY	G215	M413	D519	L632	ASN	
THR	ASN	Q216	M414	HE23	F633	LYS	
LEU	PRO	A218	M415	F524	K634	ILE	
THR	GLN	R225	M419	V525	L635	GLN	
GLU	SER	A226	M422	A530	T636	ASP	
LYS	ASN	N251	F436	V534	I637	ARG	
SER	ALA	Y260	M440	F538	L638	ARG	
SER	VAL	F261	S444	L541	L639	ASN	
LEU	THR	L266	L455	K545	M643	LYS	
ILE	THR	A267	T456	V552	S648	THR	
GLY	PRO	L268	L457	M555	T649	LEU	
PHE	LYS	A270	R462	N561	V650	ALA	
GLU	ASN	Q274	PRO	R567	P651	PHE	
PHE	ALA	Q279	ARG	G568	I652	ASP	
GLY	LEU	G296	GLU	I579	L655	LEU	
PHE	LYS	N297	ASP	L596	L659	GLU	
GLU	GLU	M298	ASP	F597	M671	PHE	
PRO	GLN	L299	LEU	L598	E679	PRO	
ASN	GLN	L300	PRO	L599	E682	THR	
PRO	ARG	H301	HIS	G600	N683	SER	
THR	ASN	A307	PRO	V603	V684	LEU	
VAL	GLN	E308	LEU	A604	S685	VAL	
THR	ALA	D309	ALA	L605	K686	LEU	
LYS	THR	V317	THR	A606	E687	LEU	
SER	THR		LYS	S607	S688	VAL	
				L608	I691	VAL	
				L609	H692	PRO	
				GLU	R693	ARG	
				LYS	R696	GLY	
					R714	SER	
						HIS	

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68101	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.054	Depositor
Minimum map value	-1.070	Depositor
Average map value	0.026	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.325	Depositor
Map size ( $\text{\AA}$ )	239.04, 239.04, 239.04	wwPDB
Map dimensions	288, 288, 288	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: A00

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	0.36	0/5068	0.58	2/6853 (0.0%)
1	B	0.36	0/5068	0.58	2/6853 (0.0%)
1	C	0.36	0/5068	0.59	2/6853 (0.0%)
1	D	0.36	0/5068	0.59	2/6853 (0.0%)
All	All	0.36	0/20272	0.59	8/27412 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	LEU	CA-CB-CG	5.61	128.21	115.30
1	B	373	LEU	CA-CB-CG	5.61	128.20	115.30
1	C	373	LEU	CA-CB-CG	5.59	128.16	115.30
1	D	373	LEU	CA-CB-CG	5.59	128.16	115.30
1	A	370	LEU	CA-CB-CG	5.27	127.42	115.30
1	D	370	LEU	CA-CB-CG	5.27	127.42	115.30
1	B	370	LEU	CA-CB-CG	5.27	127.42	115.30
1	C	370	LEU	CA-CB-CG	5.26	127.40	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	414	ASP	Peptide
1	A	436	PHE	Peptide
1	B	414	ASP	Peptide
1	B	436	PHE	Peptide
1	C	414	ASP	Peptide
1	C	436	PHE	Peptide
1	D	414	ASP	Peptide
1	D	436	PHE	Peptide

## 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	4964	0	5053	42	0
1	B	4964	0	5053	47	0
1	C	4964	0	5053	46	0
1	D	4964	0	5053	43	0
2	A	36	0	0	0	0
2	B	36	0	0	0	0
2	C	36	0	0	0	0
2	D	36	0	0	0	0
All	All	20000	0	20212	168	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 (168) 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:A:251:ASN:OD1	1:A:295:ARG:NH2	2.32	0.63
1:C:251:ASN:OD1	1:C:295:ARG:NH2	2.32	0.63
1:B:251:ASN:OD1	1:B:295:ARG:NH2	2.32	0.63
1:D:251:ASN:OD1	1:D:295:ARG:NH2	2.32	0.62
1:B:607:SER:HB3	1:C:552:VAL:HG11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:GLU:HB2	1:B:215:GLY:HA2	1.84	0.60
1:C:607:SER:HB3	1:D:552:VAL:HG11	1.84	0.60
1:B:568:GLY:O	1:B:696:ARG:NH2	2.35	0.60
1:A:607:SER:HB3	1:B:552:VAL:HG11	1.83	0.59
1:A:207:GLU:HB2	1:A:215:GLY:HA2	1.84	0.59
1:A:568:GLY:O	1:A:696:ARG:NH2	2.35	0.59
1:D:568:GLY:O	1:D:696:ARG:NH2	2.35	0.59
1:C:568:GLY:O	1:C:696:ARG:NH2	2.35	0.58
1:A:552:VAL:HG11	1:D:607:SER:HB3	1.83	0.58
1:D:207:GLU:HB2	1:D:215:GLY:HA2	1.84	0.58
1:A:226:ARG:HG2	1:A:274:GLN:HE21	1.69	0.58
1:D:226:ARG:HG2	1:D:274:GLN:HE21	1.69	0.58
1:C:207:GLU:HB2	1:C:215:GLY:HA2	1.84	0.58
1:C:226:ARG:HG2	1:C:274:GLN:HE21	1.69	0.57
1:B:226:ARG:HG2	1:B:274:GLN:HE21	1.69	0.57
1:D:279:GLN:NE2	1:D:323:MET:SD	2.78	0.57
1:B:279:GLN:NE2	1:B:323:MET:SD	2.78	0.56
1:A:279:GLN:NE2	1:A:323:MET:SD	2.78	0.56
1:C:279:GLN:NE2	1:C:323:MET:SD	2.78	0.56
1:C:579:ILE:HD13	1:C:684:VAL:HG11	1.88	0.56
1:B:579:ILE:HD13	1:B:684:VAL:HG11	1.88	0.55
1:D:579:ILE:HD13	1:D:684:VAL:HG11	1.88	0.55
1:A:167:THR:HG23	1:A:169:LYS:H	1.72	0.55
1:D:167:THR:HG23	1:D:169:LYS:H	1.72	0.55
1:A:579:ILE:HD13	1:A:684:VAL:HG11	1.88	0.54
1:B:167:THR:HG23	1:B:169:LYS:H	1.72	0.54
1:D:679:GLU:OE2	1:D:683:ASN:ND2	2.39	0.54
1:C:679:GLU:OE2	1:C:683:ASN:ND2	2.39	0.54
1:C:167:THR:HG23	1:C:169:LYS:H	1.72	0.53
1:A:634:LYS:HD2	1:A:639:LEU:HD13	1.91	0.53
1:C:525:VAL:HG12	1:C:561:ASN:HD21	1.74	0.52
1:A:525:VAL:HG12	1:A:561:ASN:HD21	1.74	0.52
1:D:525:VAL:HG12	1:D:561:ASN:HD21	1.74	0.52
1:A:144:ASP:OD1	1:A:147:ARG:NH2	2.42	0.52
1:B:525:VAL:HG12	1:B:561:ASN:HD21	1.74	0.52
1:D:634:LYS:HD2	1:D:639:LEU:HD13	1.91	0.52
1:B:144:ASP:OD1	1:B:147:ARG:NH2	2.42	0.52
1:B:634:LYS:HD2	1:B:639:LEU:HD13	1.91	0.52
1:C:144:ASP:OD1	1:C:147:ARG:NH2	2.42	0.52
1:C:598:LEU:HD12	1:C:632:LEU:HD23	1.92	0.52
1:D:598:LEU:HD12	1:D:632:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:THR:OG1	1:A:401:ASN:O	2.28	0.51
1:D:322:ASP:OD1	1:D:359:TYR:OH	2.29	0.51
1:D:144:ASP:OD1	1:D:147:ARG:NH2	2.42	0.51
1:B:598:LEU:HD12	1:B:632:LEU:HD23	1.92	0.51
1:D:399:THR:OG1	1:D:401:ASN:O	2.28	0.51
1:A:322:ASP:OD1	1:A:359:TYR:OH	2.29	0.51
1:B:679:GLU:OE2	1:B:683:ASN:ND2	2.39	0.51
1:C:322:ASP:OD1	1:C:359:TYR:OH	2.29	0.51
1:B:399:THR:OG1	1:B:401:ASN:O	2.28	0.51
1:C:634:LYS:HD2	1:C:639:LEU:HD13	1.91	0.51
1:A:679:GLU:OE2	1:A:683:ASN:ND2	2.39	0.50
1:B:322:ASP:OD1	1:B:359:TYR:OH	2.29	0.50
1:A:598:LEU:HD12	1:A:632:LEU:HD23	1.92	0.50
1:A:270:ALA:HB1	1:A:320:MET:HB3	1.95	0.49
1:D:270:ALA:HB1	1:D:320:MET:HB3	1.95	0.49
1:A:260:TYR:OH	1:A:297:ASN:OD1	2.30	0.48
1:B:270:ALA:HB1	1:B:320:MET:HB3	1.95	0.48
1:C:270:ALA:HB1	1:C:320:MET:HB3	1.95	0.48
1:C:399:THR:OG1	1:C:401:ASN:O	2.28	0.48
1:B:260:TYR:OH	1:B:297:ASN:OD1	2.30	0.48
1:B:385:VAL:HG22	1:B:737:VAL:HG22	1.96	0.47
1:C:260:TYR:OH	1:C:297:ASN:OD1	2.30	0.47
1:B:387:SER:OG	1:B:733:ARG:NH1	2.48	0.47
1:B:174:LYS:NZ	1:C:751:GLU:OE1	2.38	0.47
1:A:385:VAL:HG22	1:A:737:VAL:HG22	1.96	0.46
1:A:387:SER:OG	1:A:733:ARG:NH1	2.48	0.46
1:C:385:VAL:HG22	1:C:737:VAL:HG22	1.96	0.46
1:C:309:ASP:OD1	1:C:309:ASP:N	2.48	0.46
1:D:260:TYR:OH	1:D:297:ASN:OD1	2.30	0.46
1:B:309:ASP:OD1	1:B:309:ASP:N	2.48	0.46
1:D:298:ASN:ND2	1:D:336:MET:SD	2.77	0.46
1:B:217:THR:HG21	1:B:243:ALA:HB1	1.98	0.46
1:C:387:SER:OG	1:C:733:ARG:NH1	2.48	0.46
1:D:385:VAL:HG22	1:D:737:VAL:HG22	1.96	0.46
1:D:217:THR:HG21	1:D:243:ALA:HB1	1.98	0.46
1:B:326:LEU:HD12	1:B:370:LEU:HD11	1.98	0.46
1:C:217:THR:HG21	1:C:243:ALA:HB1	1.98	0.46
1:A:217:THR:HG21	1:A:243:ALA:HB1	1.98	0.45
1:D:387:SER:OG	1:D:733:ARG:NH1	2.48	0.45
1:A:309:ASP:OD1	1:A:309:ASP:N	2.48	0.45
1:A:326:LEU:HD12	1:A:370:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:LEU:HD12	1:D:370:LEU:HD11	1.99	0.45
1:B:154:VAL:HG12	1:B:157:PHE:HB3	1.99	0.45
1:A:154:VAL:HG12	1:A:157:PHE:HB3	1.99	0.44
1:C:326:LEU:HD12	1:C:370:LEU:HD11	1.99	0.44
1:D:419:MET:HA	1:D:422:LEU:HD23	2.00	0.44
1:C:455:LEU:HD13	1:C:555:MET:HG2	1.99	0.44
1:C:154:VAL:HG12	1:C:157:PHE:HB3	1.99	0.44
1:B:603:VAL:HG12	1:C:552:VAL:HG13	1.98	0.44
1:C:413:ILE:HB	1:C:414:ASP:H	1.63	0.44
1:C:717:MET:SD	1:C:717:MET:N	2.91	0.44
1:A:552:VAL:HG13	1:D:603:VAL:HG12	2.00	0.43
1:D:717:MET:SD	1:D:717:MET:N	2.91	0.43
1:A:717:MET:SD	1:A:717:MET:N	2.91	0.43
1:C:419:MET:HA	1:C:422:LEU:HD23	2.00	0.43
1:C:440:MET:O	1:C:444:SER:N	2.49	0.43
1:D:154:VAL:HG12	1:D:157:PHE:HB3	1.99	0.43
1:A:419:MET:HA	1:A:422:LEU:HD23	2.00	0.43
1:B:298:ASN:ND2	1:B:336:MET:SD	2.77	0.43
1:B:717:MET:SD	1:B:717:MET:N	2.91	0.43
1:B:299:ILE:HG23	1:B:300:LEU:HD22	2.01	0.43
1:D:455:LEU:HD13	1:D:555:MET:HG2	1.99	0.43
1:B:419:MET:HA	1:B:422:LEU:HD23	2.00	0.43
1:B:455:LEU:HD13	1:B:555:MET:HG2	1.99	0.43
1:C:299:ILE:HG23	1:C:300:LEU:HD22	2.01	0.43
1:A:299:ILE:HG23	1:A:300:LEU:HD22	2.01	0.43
1:B:300:LEU:HD12	1:B:321:TYR:CE1	2.54	0.43
1:B:404:LEU:HD13	1:B:404:LEU:HA	1.81	0.43
1:A:455:LEU:HD13	1:A:555:MET:HG2	1.99	0.43
1:C:688:SER:HA	1:C:691:ILE:HG22	2.01	0.42
1:A:688:SER:HA	1:A:691:ILE:HG22	2.01	0.42
1:C:261:PHE:CG	1:C:268:LEU:HD12	2.55	0.42
1:D:300:LEU:HD12	1:D:321:TYR:CE1	2.54	0.42
1:A:177:LEU:HD13	1:A:225:ARG:HH11	1.85	0.42
1:B:688:SER:HA	1:B:691:ILE:HG22	2.01	0.42
1:D:688:SER:HA	1:D:691:ILE:HG22	2.01	0.42
1:B:261:PHE:CG	1:B:268:LEU:HD12	2.55	0.42
1:C:603:VAL:HG12	1:D:552:VAL:HG13	2.01	0.42
1:D:177:LEU:HD13	1:D:225:ARG:HH11	1.85	0.42
1:D:261:PHE:CG	1:D:268:LEU:HD12	2.55	0.42
1:D:297:ASN:HB3	1:D:301:HIS:HB2	2.02	0.42
1:D:440:MET:O	1:D:444:SER:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ASN:HB3	1:A:301:HIS:HB2	2.02	0.42
1:C:300:LEU:HD12	1:C:321:TYR:CE1	2.54	0.42
1:D:299:ILE:HG23	1:D:300:LEU:HD22	2.01	0.42
1:A:261:PHE:CG	1:A:268:LEU:HD12	2.55	0.42
1:A:298:ASN:ND2	1:A:336:MET:SD	2.77	0.42
1:A:300:LEU:HD12	1:A:321:TYR:CE1	2.54	0.42
1:D:309:ASP:OD1	1:D:309:ASP:N	2.48	0.42
1:C:297:ASN:HB3	1:C:301:HIS:HB2	2.02	0.41
1:D:266:LEU:HG	1:D:299:ILE:HD12	2.02	0.41
1:A:404:LEU:HA	1:A:404:LEU:HD13	1.81	0.41
1:D:495:THR:HA	1:D:534:ILE:HD11	2.02	0.41
1:B:217:THR:O	1:B:219:LEU:N	2.54	0.41
1:B:307:ALA:HB2	1:B:317:VAL:HG11	2.03	0.41
1:B:356:ILE:HD12	1:B:356:ILE:HA	1.96	0.41
1:A:692:TRP:CE3	1:A:693:ARG:HD2	2.56	0.41
1:B:213:TYR:OH	1:C:754:GLY:N	2.54	0.41
1:C:307:ALA:HB2	1:C:317:VAL:HG11	2.03	0.41
1:C:356:ILE:HD12	1:C:356:ILE:HA	1.96	0.41
1:C:692:TRP:CE3	1:C:693:ARG:HD2	2.56	0.41
1:D:307:ALA:HB2	1:D:317:VAL:HG11	2.03	0.41
1:D:692:TRP:CE3	1:D:693:ARG:HD2	2.56	0.41
1:C:217:THR:O	1:C:219:LEU:N	2.54	0.41
1:B:266:LEU:HG	1:B:299:ILE:HD12	2.02	0.41
1:B:495:THR:HA	1:B:534:ILE:HD11	2.02	0.41
1:C:177:LEU:HD13	1:C:225:ARG:HH11	1.85	0.41
1:B:177:LEU:HD13	1:B:225:ARG:HH11	1.85	0.41
1:B:297:ASN:HB3	1:B:301:HIS:HB2	2.02	0.41
1:B:422:LEU:HD13	1:B:422:LEU:HA	1.87	0.41
1:A:266:LEU:HG	1:A:299:ILE:HD12	2.02	0.40
1:A:217:THR:O	1:A:219:LEU:N	2.54	0.40
1:A:307:ALA:HB2	1:A:317:VAL:HG11	2.03	0.40
1:A:603:VAL:HG12	1:B:552:VAL:HG13	2.03	0.40
1:B:440:MET:O	1:B:444:SER:N	2.49	0.40
1:D:723:VAL:HA	1:D:749:LEU:HD21	2.03	0.40
1:B:692:TRP:CE3	1:B:693:ARG:HD2	2.56	0.40
1:C:495:THR:HA	1:C:534:ILE:HD11	2.02	0.40
1:D:596:LEU:O	1:D:600:GLY:N	2.54	0.40
1:A:495:THR:HA	1:A:534:ILE:HD11	2.02	0.40
1:C:298:ASN:ND2	1:C:336:MET:SD	2.77	0.40
1:C:723:VAL:HA	1:C:749:LEU:HD21	2.03	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	602/808 (74%)	561 (93%)	38 (6%)	3 (0%)	29	67
1	B	602/808 (74%)	561 (93%)	38 (6%)	3 (0%)	29	67
1	C	602/808 (74%)	561 (93%)	38 (6%)	3 (0%)	29	67
1	D	602/808 (74%)	561 (93%)	38 (6%)	3 (0%)	29	67
All	All	2408/3232 (74%)	2244 (93%)	152 (6%)	12 (0%)	32	67

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	ALA
1	A	414	ASP
1	B	218	ALA
1	B	414	ASP
1	C	218	ALA
1	C	414	ASP
1	D	218	ALA
1	D	414	ASP
1	A	413	ILE
1	B	413	ILE
1	C	413	ILE
1	D	413	ILE

### 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	540/719 (75%)	532 (98%)	8 (2%)	65	83
1	B	540/719 (75%)	532 (98%)	8 (2%)	65	83
1	C	540/719 (75%)	532 (98%)	8 (2%)	65	83
1	D	540/719 (75%)	532 (98%)	8 (2%)	65	83
All	All	2160/2876 (75%)	2128 (98%)	32 (2%)	66	83

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	LYS
1	A	150	ARG
1	A	326	LEU
1	A	410	ASN
1	A	415	ASN
1	A	567	ARG
1	A	671	ASN
1	A	714	ARG
1	B	117	LYS
1	B	150	ARG
1	B	326	LEU
1	B	410	ASN
1	B	415	ASN
1	B	567	ARG
1	B	671	ASN
1	B	714	ARG
1	C	117	LYS
1	C	150	ARG
1	C	326	LEU
1	C	410	ASN
1	C	415	ASN
1	C	567	ARG
1	C	671	ASN
1	C	714	ARG
1	D	117	LYS
1	D	150	ARG
1	D	326	LEU
1	D	410	ASN
1	D	415	ASN
1	D	567	ARG
1	D	671	ASN
1	D	714	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	410	ASN
1	A	415	ASN
1	A	561	ASN
1	A	671	ASN
1	B	410	ASN
1	B	415	ASN
1	B	561	ASN
1	B	671	ASN
1	C	410	ASN
1	C	415	ASN
1	C	671	ASN
1	D	410	ASN
1	D	415	ASN
1	D	671	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](#)

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
2	A0O	A	902	-	19,19,19	4.84	12 (63%)	26,26,26	7.11	17 (65%)
2	A0O	C	901	-	19,19,19	4.88	12 (63%)	26,26,26	7.04	19 (73%)
2	A0O	D	901	-	19,19,19	4.87	12 (63%)	26,26,26	7.02	19 (73%)
2	A0O	D	902	-	19,19,19	4.85	12 (63%)	26,26,26	7.13	17 (65%)
2	A0O	B	902	-	19,19,19	4.84	12 (63%)	26,26,26	7.11	17 (65%)
2	A0O	A	901	-	19,19,19	4.86	12 (63%)	26,26,26	7.01	19 (73%)
2	A0O	B	901	-	19,19,19	4.88	12 (63%)	26,26,26	7.04	19 (73%)
2	A0O	C	902	-	19,19,19	4.84	12 (63%)	26,26,26	7.11	17 (65%)

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	A0O	A	902	-	-	2/7/7/7	0/2/2/2
2	A0O	C	901	-	-	2/7/7/7	0/2/2/2
2	A0O	D	901	-	-	2/7/7/7	0/2/2/2
2	A0O	D	902	-	-	2/7/7/7	0/2/2/2
2	A0O	B	902	-	-	2/7/7/7	0/2/2/2
2	A0O	A	901	-	-	2/7/7/7	0/2/2/2
2	A0O	B	901	-	-	2/7/7/7	0/2/2/2
2	A0O	C	902	-	-	2/7/7/7	0/2/2/2

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	902	A0O	C06-C04	10.19	1.56	1.39
2	B	902	A0O	C06-C04	10.18	1.56	1.39
2	C	902	A0O	C06-C04	10.16	1.56	1.39
2	A	902	A0O	C06-C04	10.15	1.56	1.39
2	B	901	A0O	C06-C04	10.06	1.56	1.39
2	D	901	A0O	C06-C04	10.05	1.56	1.39
2	C	901	A0O	C06-C04	10.00	1.55	1.39
2	A	901	A0O	C06-C04	9.96	1.55	1.39
2	C	902	A0O	C07-C12	9.62	1.65	1.44
2	A	902	A0O	C07-C12	9.59	1.65	1.44
2	D	902	A0O	C07-C12	9.57	1.65	1.44
2	B	902	A0O	C07-C12	9.56	1.65	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	A00	C07-C12	9.54	1.65	1.44
2	D	901	A00	C07-C12	9.53	1.65	1.44
2	A	901	A00	C07-C12	9.52	1.64	1.44
2	C	901	A00	C07-C12	9.50	1.64	1.44
2	C	901	A00	C08-C04	8.02	1.51	1.40
2	B	901	A00	C08-C04	7.98	1.51	1.40
2	D	901	A00	C08-C04	7.93	1.51	1.40
2	A	901	A00	C08-C04	7.93	1.51	1.40
2	D	902	A00	C08-C04	7.51	1.50	1.40
2	B	902	A00	C08-C04	7.49	1.50	1.40
2	A	902	A00	C08-C04	7.47	1.50	1.40
2	C	902	A00	C08-C04	7.43	1.50	1.40
2	D	901	A00	O01-C15	-7.06	1.26	1.38
2	A	901	A00	O01-C15	-7.06	1.26	1.38
2	C	901	A00	O01-C15	-7.03	1.26	1.38
2	D	902	A00	O01-C15	-7.02	1.26	1.38
2	B	901	A00	O01-C15	-7.01	1.26	1.38
2	A	902	A00	O01-C15	-7.00	1.26	1.38
2	C	902	A00	O01-C15	-6.98	1.26	1.38
2	B	902	A00	O01-C15	-6.95	1.26	1.38
2	C	901	A00	C11-C10	-6.54	1.26	1.38
2	B	901	A00	C11-C10	-6.49	1.26	1.38
2	A	901	A00	C11-C10	-6.49	1.26	1.38
2	A	902	A00	C11-C10	-6.48	1.27	1.38
2	D	902	A00	C11-C10	-6.47	1.27	1.38
2	D	901	A00	C11-C10	-6.47	1.27	1.38
2	B	902	A00	C11-C10	-6.44	1.27	1.38
2	C	902	A00	C11-C10	-6.43	1.27	1.38
2	C	901	A00	C10-C07	-6.41	1.29	1.41
2	B	901	A00	C10-C07	-6.40	1.29	1.41
2	D	901	A00	C10-C07	-6.37	1.29	1.41
2	A	901	A00	C10-C07	-6.29	1.29	1.41
2	C	902	A00	C10-C07	-5.96	1.30	1.41
2	A	902	A00	C10-C07	-5.96	1.30	1.41
2	D	902	A00	C10-C07	-5.94	1.30	1.41
2	B	902	A00	C10-C07	-5.93	1.30	1.41
2	A	902	A00	C07-C06	4.83	1.50	1.41
2	D	902	A00	C07-C06	4.82	1.50	1.41
2	C	902	A00	C07-C06	4.81	1.50	1.41
2	B	902	A00	C07-C06	4.80	1.50	1.41
2	B	901	A00	C07-C06	4.61	1.50	1.41
2	C	901	A00	C07-C06	4.61	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	A0O	C07-C06	4.61	1.50	1.41
2	A	901	A0O	C07-C06	4.60	1.50	1.41
2	D	902	A0O	C05-C04	4.21	1.56	1.51
2	B	902	A0O	C05-C04	4.18	1.56	1.51
2	A	902	A0O	C05-C04	4.17	1.56	1.51
2	C	902	A0O	C05-C04	4.14	1.56	1.51
2	A	901	A0O	C05-C04	3.88	1.55	1.51
2	C	901	A0O	C05-C04	3.84	1.55	1.51
2	B	901	A0O	C05-C04	3.84	1.55	1.51
2	D	901	A0O	C05-C04	3.82	1.55	1.51
2	A	901	A0O	O01-C06	-2.64	1.34	1.38
2	D	901	A0O	O01-C06	-2.59	1.34	1.38
2	A	901	A0O	O02-C08	2.58	1.41	1.37
2	C	901	A0O	O01-C06	-2.56	1.34	1.38
2	D	901	A0O	O02-C08	2.56	1.41	1.37
2	B	901	A0O	O02-C08	2.55	1.41	1.37
2	C	901	A0O	O02-C08	2.55	1.41	1.37
2	B	901	A0O	O01-C06	-2.54	1.34	1.38
2	D	902	A0O	O01-C06	-2.43	1.34	1.38
2	B	902	A0O	O01-C06	-2.43	1.34	1.38
2	C	902	A0O	O01-C06	-2.42	1.34	1.38
2	A	902	A0O	O01-C06	-2.39	1.34	1.38
2	C	902	A0O	C14-C15	-2.27	1.39	1.44
2	B	902	A0O	C14-C15	-2.27	1.39	1.44
2	A	902	A0O	C14-C15	-2.25	1.39	1.44
2	D	902	A0O	O02-C08	2.24	1.40	1.37
2	B	902	A0O	O02-C08	2.23	1.40	1.37
2	C	902	A0O	O02-C08	2.23	1.40	1.37
2	D	902	A0O	C14-C15	-2.22	1.39	1.44
2	B	902	A0O	C05-C09	2.21	1.55	1.50
2	A	902	A0O	O02-C08	2.20	1.40	1.37
2	D	902	A0O	C05-C09	2.19	1.55	1.50
2	A	902	A0O	C05-C09	2.17	1.55	1.50
2	C	902	A0O	C05-C09	2.13	1.55	1.50
2	B	901	A0O	C05-C09	2.11	1.55	1.50
2	C	901	A0O	C05-C09	2.11	1.55	1.50
2	D	901	A0O	C05-C09	2.08	1.55	1.50
2	A	901	A0O	C14-C15	-2.07	1.39	1.44
2	C	901	A0O	C14-C15	-2.07	1.39	1.44
2	A	901	A0O	C05-C09	2.07	1.55	1.50
2	B	901	A0O	C14-C15	-2.03	1.40	1.44
2	D	901	A0O	C14-C15	-2.01	1.40	1.44

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	902	A00	O01-C06-C04	25.41	144.79	115.96
2	C	902	A00	O01-C06-C04	25.38	144.76	115.96
2	B	902	A00	O01-C06-C04	25.35	144.72	115.96
2	B	901	A00	O01-C06-C04	25.35	144.72	115.96
2	A	902	A00	O01-C06-C04	25.32	144.69	115.96
2	D	901	A00	O01-C06-C04	25.29	144.66	115.96
2	C	901	A00	O01-C06-C04	25.22	144.58	115.96
2	A	901	A00	O01-C06-C04	25.22	144.57	115.96
2	B	902	A00	C06-O01-C15	14.27	134.18	121.99
2	D	902	A00	C06-O01-C15	14.23	134.15	121.99
2	A	902	A00	C06-O01-C15	14.21	134.13	121.99
2	C	902	A00	C06-O01-C15	14.11	134.05	121.99
2	C	901	A00	C06-O01-C15	13.44	133.47	121.99
2	B	901	A00	C06-O01-C15	13.15	133.22	121.99
2	D	901	A00	C06-O01-C15	13.10	133.18	121.99
2	A	901	A00	C06-O01-C15	13.08	133.16	121.99
2	C	902	A00	C07-C06-C04	-8.86	103.31	121.91
2	D	902	A00	C07-C06-C04	-8.85	103.33	121.91
2	A	902	A00	C07-C06-C04	-8.83	103.37	121.91
2	B	902	A00	C07-C06-C04	-8.83	103.38	121.91
2	C	901	A00	C07-C06-C04	-8.71	103.61	121.91
2	B	901	A00	C07-C06-C04	-8.71	103.62	121.91
2	D	901	A00	C07-C06-C04	-8.67	103.70	121.91
2	A	901	A00	C07-C06-C04	-8.67	103.71	121.91
2	C	901	A00	O02-C08-C04	8.46	124.30	115.35
2	D	901	A00	O02-C08-C04	8.45	124.29	115.35
2	B	901	A00	O02-C08-C04	8.40	124.24	115.35
2	A	901	A00	O02-C08-C04	8.39	124.23	115.35
2	D	901	A00	O01-C06-C07	-8.34	111.64	120.56
2	B	901	A00	O01-C06-C07	-8.33	111.66	120.56
2	A	901	A00	O01-C06-C07	-8.27	111.72	120.56
2	C	901	A00	O01-C06-C07	-8.19	111.81	120.56
2	D	902	A00	O01-C06-C07	-8.13	111.87	120.56
2	B	902	A00	O01-C06-C07	-8.11	111.89	120.56
2	C	902	A00	O01-C06-C07	-8.08	111.92	120.56
2	A	902	A00	O01-C06-C07	-8.08	111.93	120.56
2	C	901	A00	C08-C04-C06	8.05	126.27	116.63
2	A	901	A00	C08-C04-C06	8.04	126.25	116.63
2	D	901	A00	C08-C04-C06	8.01	126.22	116.63
2	B	901	A00	C08-C04-C06	8.01	126.22	116.63
2	C	902	A00	C08-C04-C06	8.01	126.22	116.63
2	D	902	A00	C08-C04-C06	7.94	126.14	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	902	A00	C08-C04-C06	7.90	126.10	116.63
2	B	902	A00	C08-C04-C06	7.89	126.08	116.63
2	A	902	A00	O02-C08-C04	7.58	123.37	115.35
2	D	902	A00	O02-C08-C04	7.50	123.29	115.35
2	B	902	A00	O02-C08-C04	7.45	123.24	115.35
2	C	902	A00	O02-C08-C04	7.42	123.21	115.35
2	B	902	A00	C10-C07-C06	6.31	127.22	119.76
2	D	902	A00	C10-C07-C06	6.30	127.20	119.76
2	C	902	A00	C10-C07-C06	6.29	127.19	119.76
2	A	902	A00	C10-C07-C06	6.29	127.19	119.76
2	C	901	A00	C11-C08-C04	-6.25	111.98	120.54
2	A	901	A00	C11-C08-C04	-6.22	112.02	120.54
2	D	901	A00	C11-C08-C04	-6.21	112.04	120.54
2	B	901	A00	C11-C08-C04	-6.20	112.05	120.54
2	B	901	A00	C10-C07-C06	5.96	126.80	119.76
2	A	901	A00	C10-C07-C06	5.90	126.74	119.76
2	C	901	A00	C10-C07-C06	5.90	126.73	119.76
2	D	901	A00	C10-C07-C06	5.88	126.71	119.76
2	C	901	A00	C05-C09-C13	-5.85	120.47	127.59
2	A	901	A00	C05-C09-C13	-5.84	120.49	127.59
2	D	901	A00	C05-C09-C13	-5.81	120.52	127.59
2	B	901	A00	C05-C09-C13	-5.76	120.58	127.59
2	C	902	A00	C11-C08-C04	-5.74	112.69	120.54
2	D	902	A00	C11-C08-C04	-5.71	112.72	120.54
2	A	902	A00	C11-C08-C04	-5.67	112.77	120.54
2	B	902	A00	C11-C08-C04	-5.67	112.77	120.54
2	D	902	A00	C05-C09-C13	-5.66	120.70	127.59
2	C	902	A00	C05-C09-C13	-5.65	120.71	127.59
2	A	902	A00	C05-C09-C13	-5.61	120.77	127.59
2	B	902	A00	C05-C09-C13	-5.59	120.79	127.59
2	A	902	A00	C06-C07-C12	-4.28	113.29	117.52
2	C	902	A00	C06-C07-C12	-4.25	113.32	117.52
2	D	902	A00	C06-C07-C12	-4.23	113.34	117.52
2	B	902	A00	C06-C07-C12	-4.20	113.37	117.52
2	C	902	A00	C05-C04-C08	-3.84	115.68	121.67
2	A	902	A00	C18-O02-C08	-3.80	111.79	117.53
2	B	902	A00	C05-C04-C08	-3.76	115.80	121.67
2	D	902	A00	C05-C04-C08	-3.76	115.81	121.67
2	B	902	A00	C18-O02-C08	-3.75	111.86	117.53
2	D	902	A00	C18-O02-C08	-3.70	111.94	117.53
2	A	902	A00	C05-C04-C08	-3.69	115.91	121.67
2	A	901	A00	C06-C07-C12	-3.67	113.90	117.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	A00	C06-C07-C12	-3.65	113.91	117.52
2	D	901	A00	C06-C07-C12	-3.60	113.96	117.52
2	C	902	A00	C18-O02-C08	-3.57	112.14	117.53
2	C	901	A00	C06-C07-C12	-3.55	114.02	117.52
2	D	902	A00	O01-C15-O03	3.35	120.71	116.44
2	C	901	A00	C11-C10-C07	3.33	126.24	121.74
2	B	902	A00	O01-C15-O03	3.33	120.68	116.44
2	C	902	A00	O01-C15-O03	3.29	120.64	116.44
2	A	902	A00	O01-C15-O03	3.29	120.64	116.44
2	D	901	A00	C11-C10-C07	3.26	126.16	121.74
2	B	901	A00	C11-C10-C07	3.26	126.15	121.74
2	A	901	A00	C11-C10-C07	3.18	126.05	121.74
2	C	901	A00	O03-C15-C14	-3.02	120.39	126.00
2	B	901	A00	C05-C04-C08	-3.02	116.97	121.67
2	B	901	A00	O03-C15-C14	-3.01	120.41	126.00
2	D	901	A00	C05-C04-C08	-2.97	117.04	121.67
2	D	901	A00	O03-C15-C14	-2.93	120.55	126.00
2	A	901	A00	C05-C04-C08	-2.93	117.10	121.67
2	D	902	A00	C12-C14-C15	-2.92	117.66	121.43
2	C	901	A00	C05-C04-C08	-2.91	117.13	121.67
2	B	902	A00	O03-C15-C14	-2.88	120.65	126.00
2	D	902	A00	O03-C15-C14	-2.88	120.65	126.00
2	A	901	A00	O03-C15-C14	-2.87	120.66	126.00
2	A	902	A00	C12-C14-C15	-2.84	117.76	121.43
2	A	902	A00	O03-C15-C14	-2.84	120.73	126.00
2	C	902	A00	O03-C15-C14	-2.83	120.75	126.00
2	B	902	A00	C12-C14-C15	-2.80	117.81	121.43
2	A	902	A00	C11-C10-C07	2.80	125.53	121.74
2	C	902	A00	C12-C14-C15	-2.79	117.82	121.43
2	C	902	A00	C11-C10-C07	2.79	125.51	121.74
2	D	902	A00	C11-C10-C07	2.79	125.51	121.74
2	B	902	A00	C11-C10-C07	2.75	125.46	121.74
2	A	901	A00	C10-C11-C08	2.72	125.23	120.06
2	C	901	A00	C05-C04-C06	-2.71	116.59	121.37
2	D	901	A00	C10-C11-C08	2.69	125.18	120.06
2	A	901	A00	C05-C04-C06	-2.68	116.64	121.37
2	B	901	A00	C10-C11-C08	2.68	125.16	120.06
2	C	901	A00	C10-C11-C08	2.68	125.16	120.06
2	D	902	A00	C10-C11-C08	2.64	125.09	120.06
2	B	902	A00	C10-C11-C08	2.64	125.09	120.06
2	C	902	A00	C10-C11-C08	2.64	125.08	120.06
2	D	901	A00	C05-C04-C06	-2.63	116.73	121.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	902	A00	C10-C11-C08	2.61	125.03	120.06
2	B	901	A00	C05-C04-C06	-2.59	116.81	121.37
2	B	901	A00	O01-C15-O03	2.34	119.42	116.44
2	D	901	A00	C18-O02-C08	-2.26	114.12	117.53
2	C	901	A00	O01-C15-C14	2.26	120.56	117.12
2	A	901	A00	C18-O02-C08	-2.23	114.16	117.53
2	B	901	A00	C18-O02-C08	-2.23	114.17	117.53
2	C	901	A00	C18-O02-C08	-2.19	114.22	117.53
2	D	901	A00	O01-C15-O03	2.17	119.21	116.44
2	A	901	A00	O01-C15-C14	2.11	120.33	117.12
2	C	901	A00	O01-C15-O03	2.05	119.06	116.44
2	D	901	A00	O01-C15-C14	2.05	120.24	117.12
2	B	901	A00	C16-C13-C17	2.05	119.13	114.60
2	A	901	A00	C16-C13-C17	2.04	119.11	114.60
2	D	901	A00	C16-C13-C17	2.03	119.10	114.60
2	A	901	A00	O01-C15-O03	2.01	119.01	116.44
2	C	901	A00	C16-C13-C17	2.01	119.05	114.60
2	B	901	A00	O01-C15-C14	2.00	120.17	117.12

There are no chirality outliers.

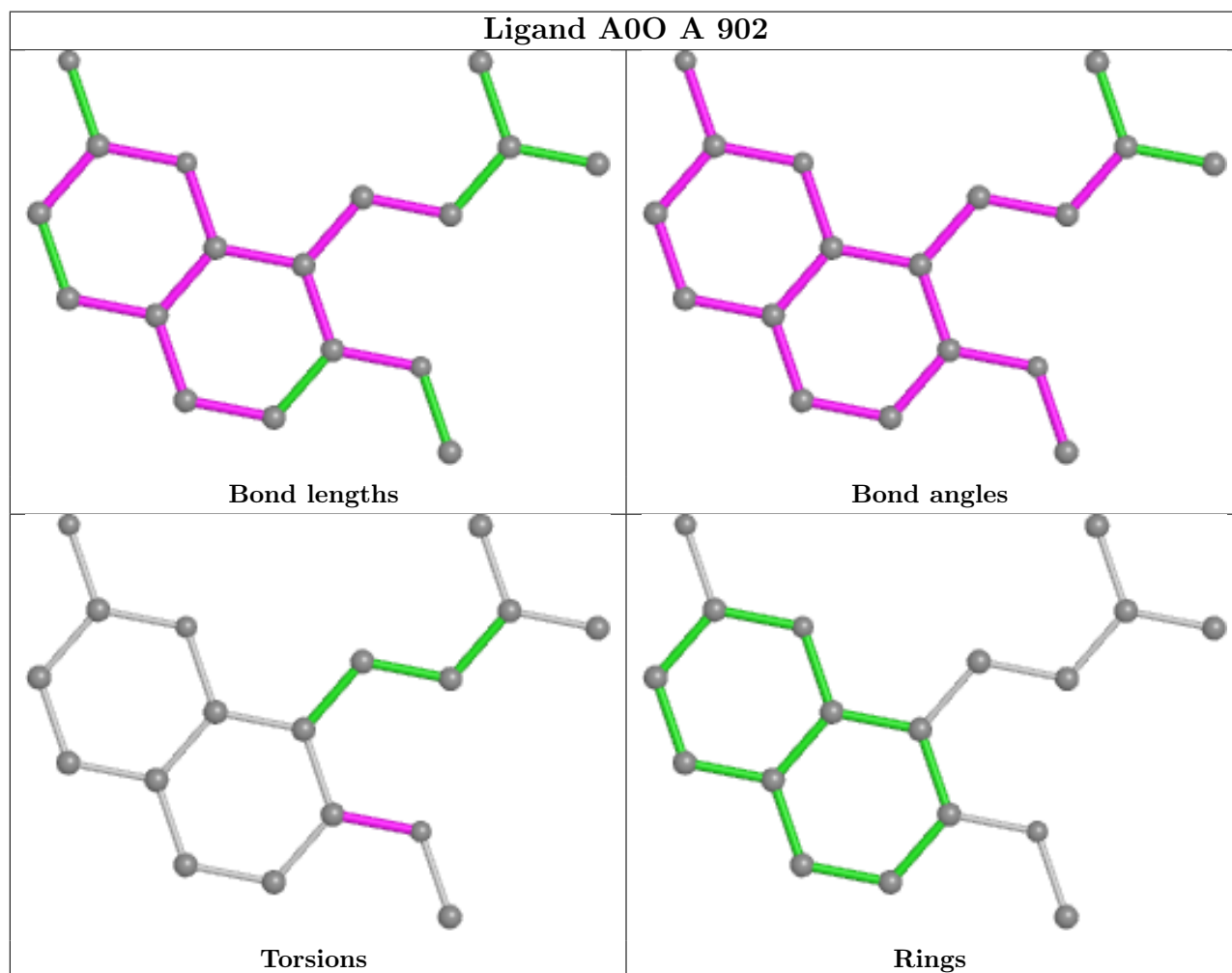
All (16) torsion outliers are listed below:

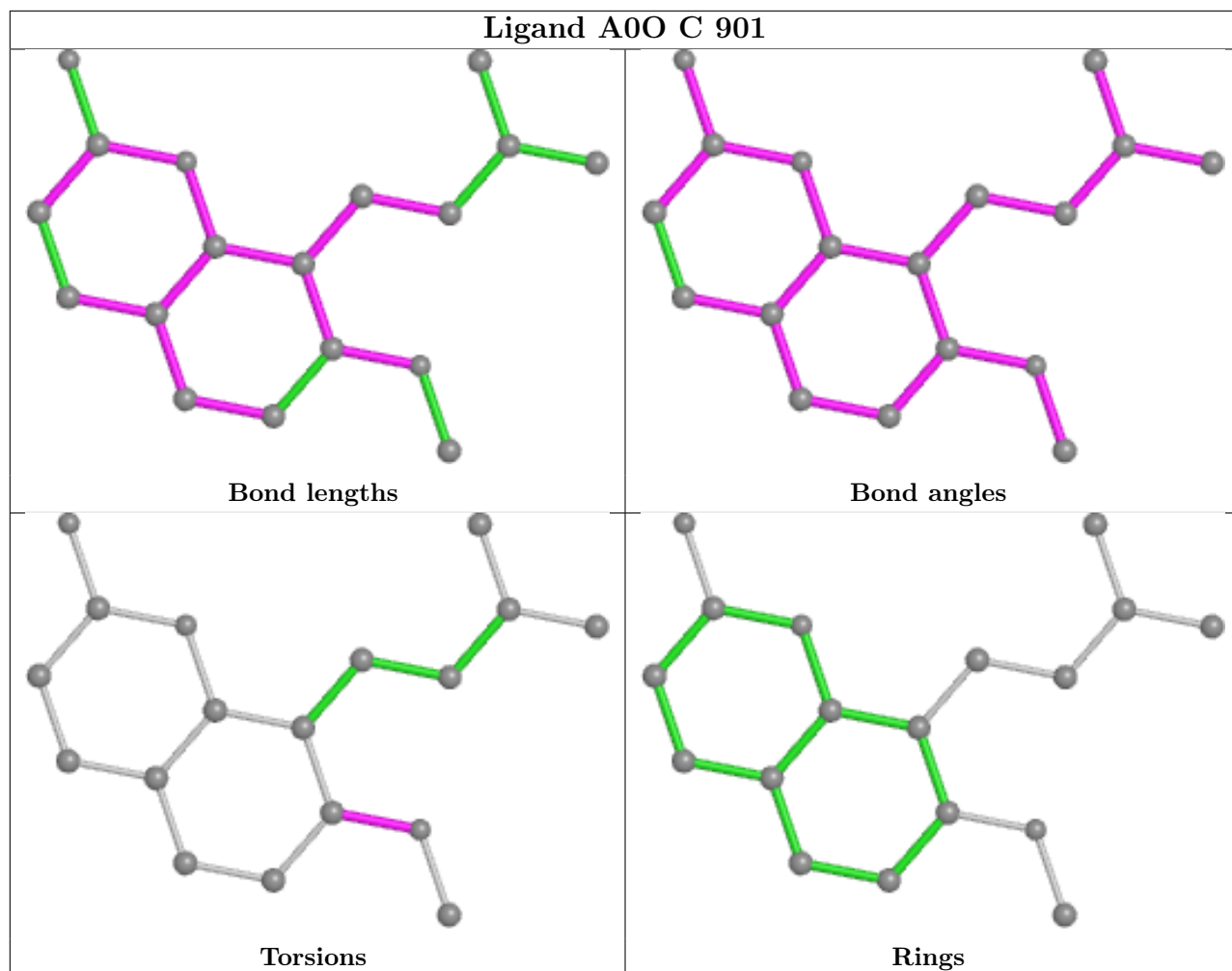
Mol	Chain	Res	Type	Atoms
2	C	902	A00	C11-C08-O02-C18
2	A	902	A00	C11-C08-O02-C18
2	B	902	A00	C11-C08-O02-C18
2	D	902	A00	C11-C08-O02-C18
2	A	902	A00	C04-C08-O02-C18
2	B	902	A00	C04-C08-O02-C18
2	C	902	A00	C04-C08-O02-C18
2	D	902	A00	C04-C08-O02-C18
2	D	901	A00	C11-C08-O02-C18
2	A	901	A00	C11-C08-O02-C18
2	B	901	A00	C11-C08-O02-C18
2	C	901	A00	C11-C08-O02-C18
2	D	901	A00	C04-C08-O02-C18
2	A	901	A00	C04-C08-O02-C18
2	B	901	A00	C04-C08-O02-C18
2	C	901	A00	C04-C08-O02-C18

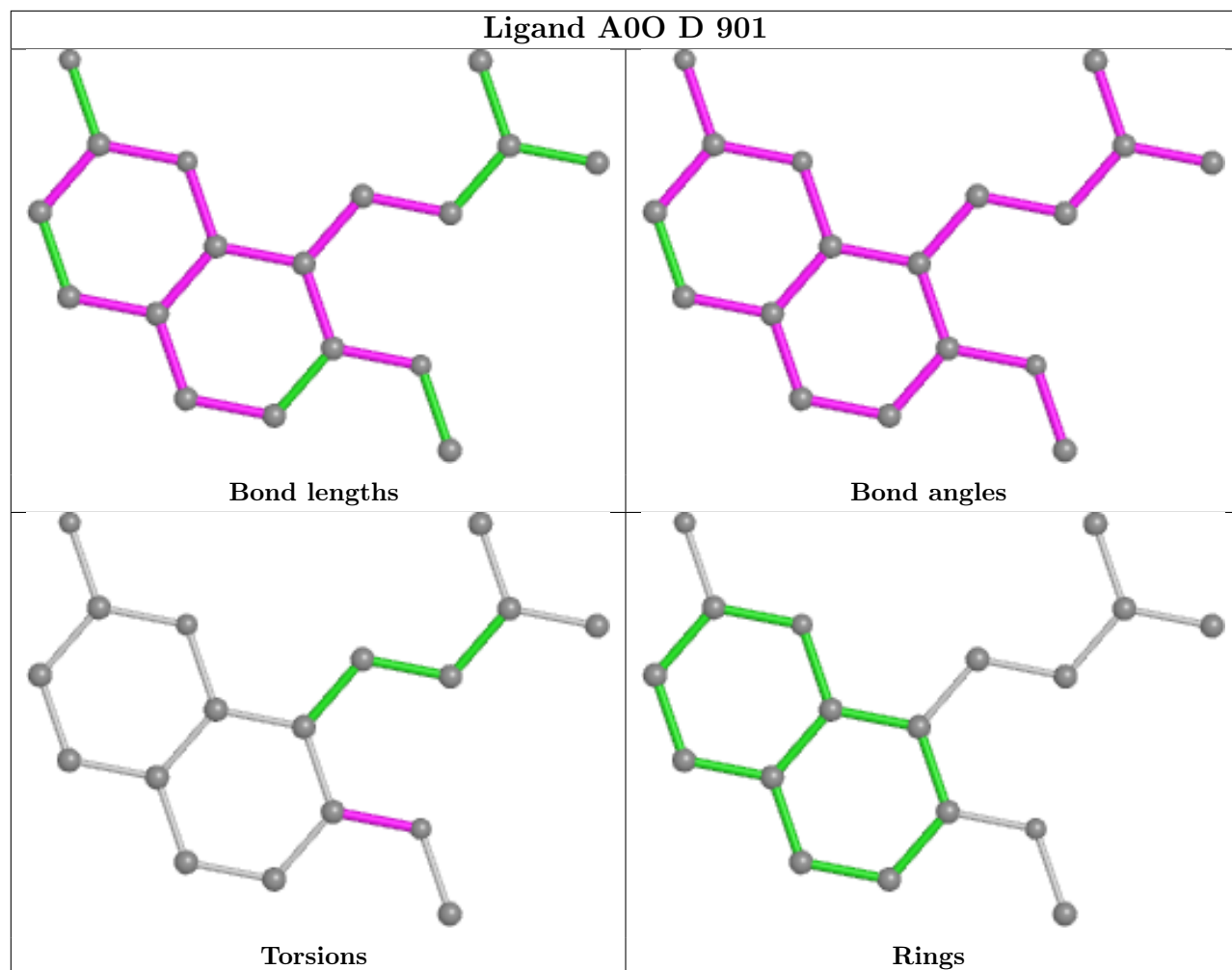
There are no ring outliers.

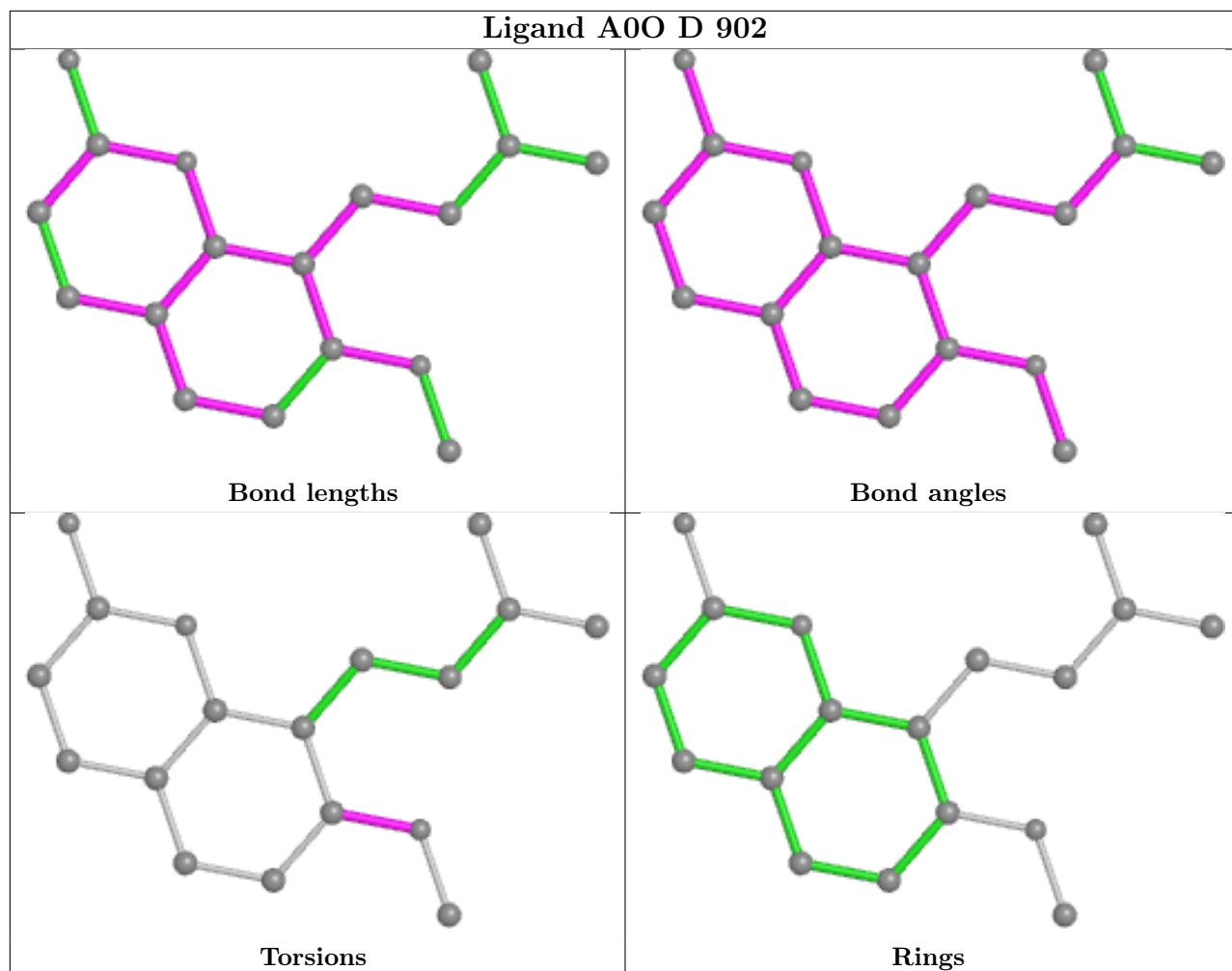
No monomer is involved in short contacts.

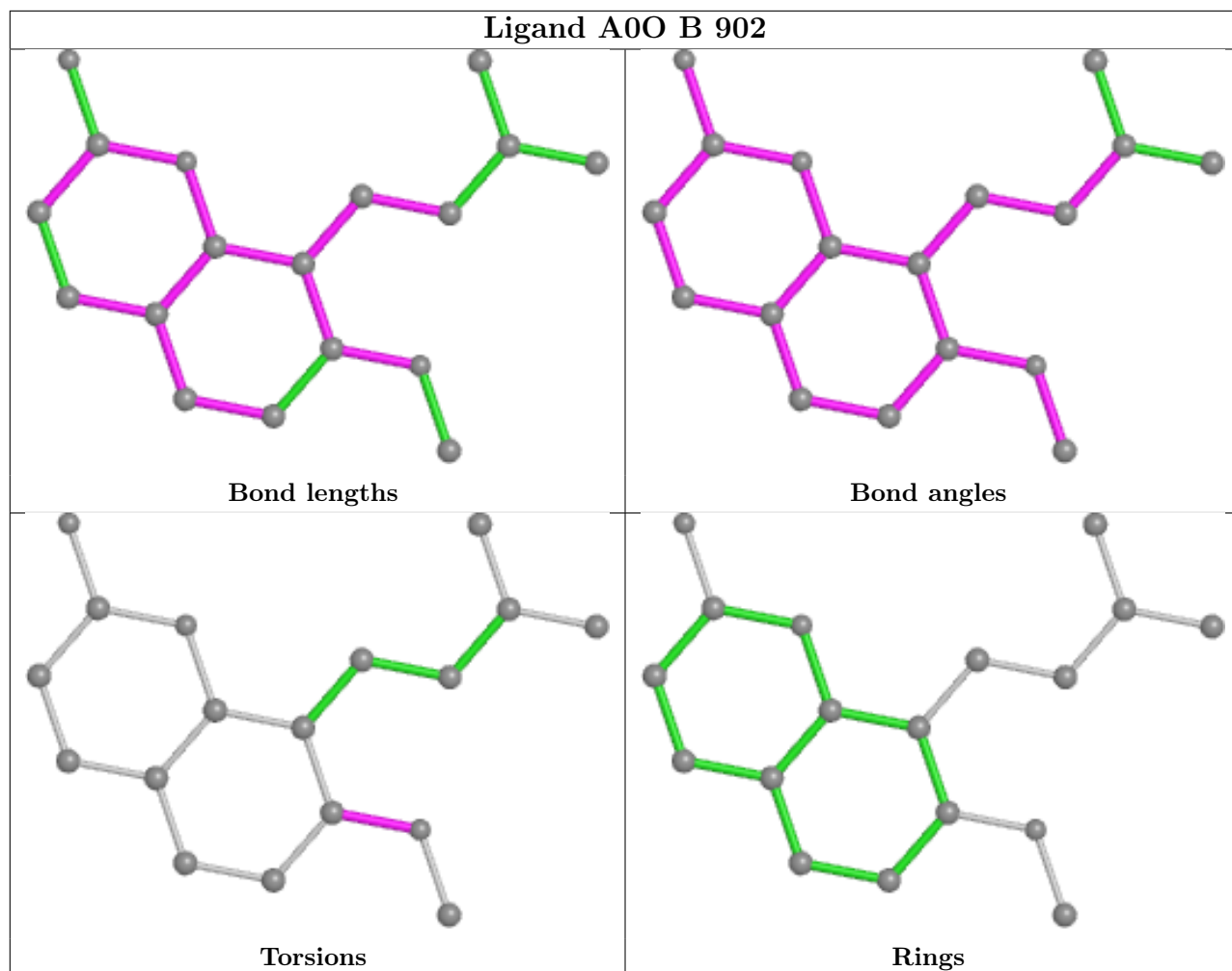
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



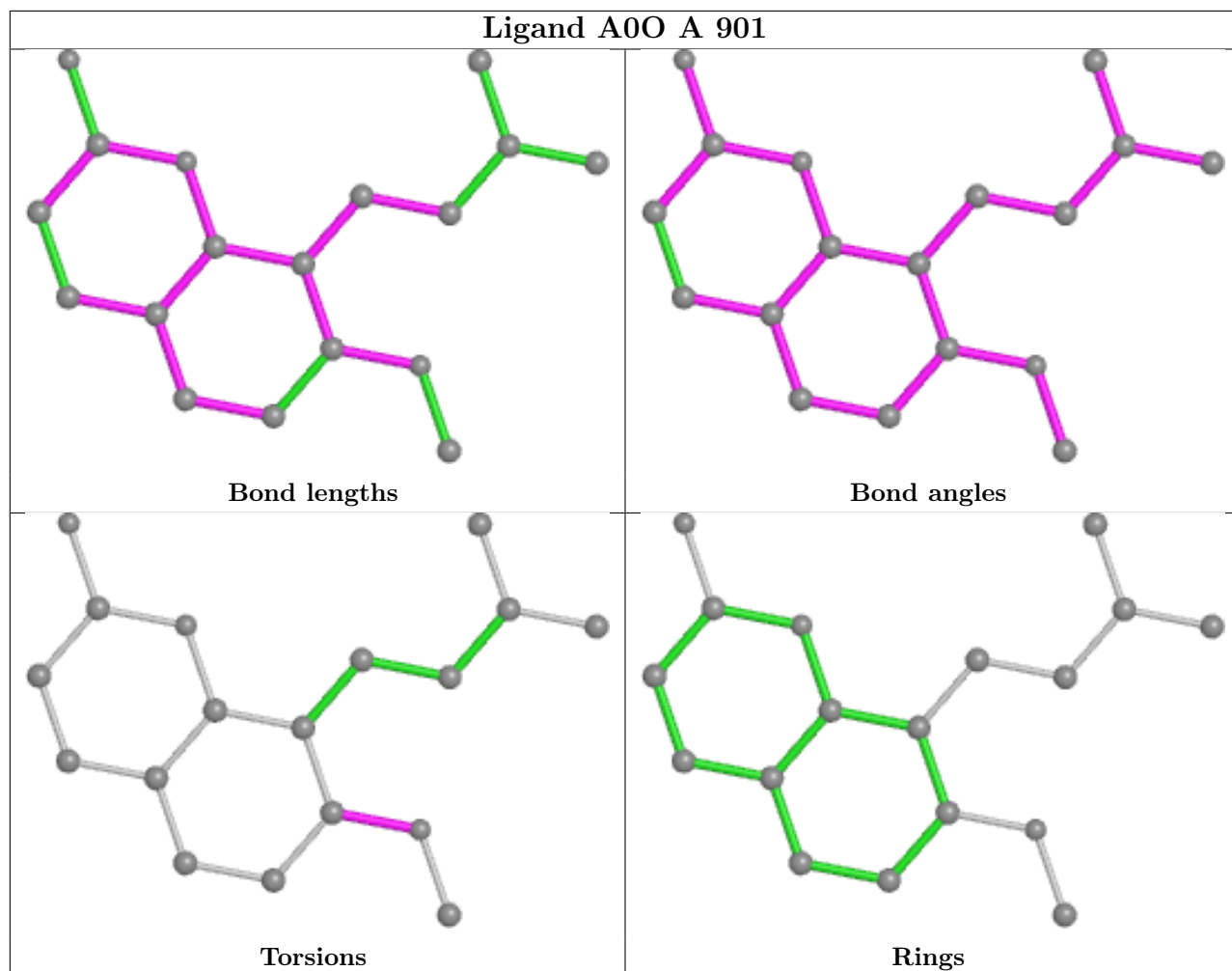


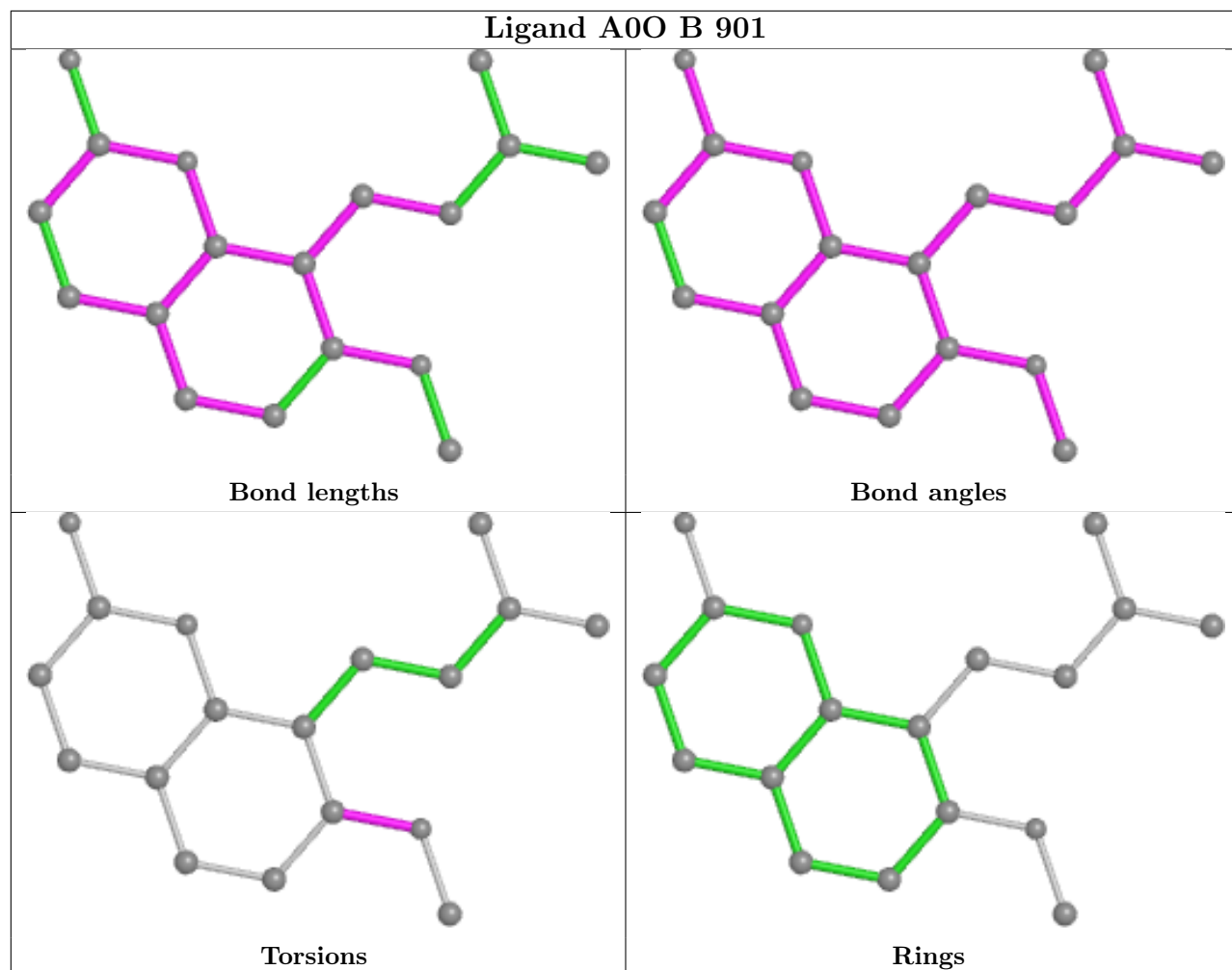


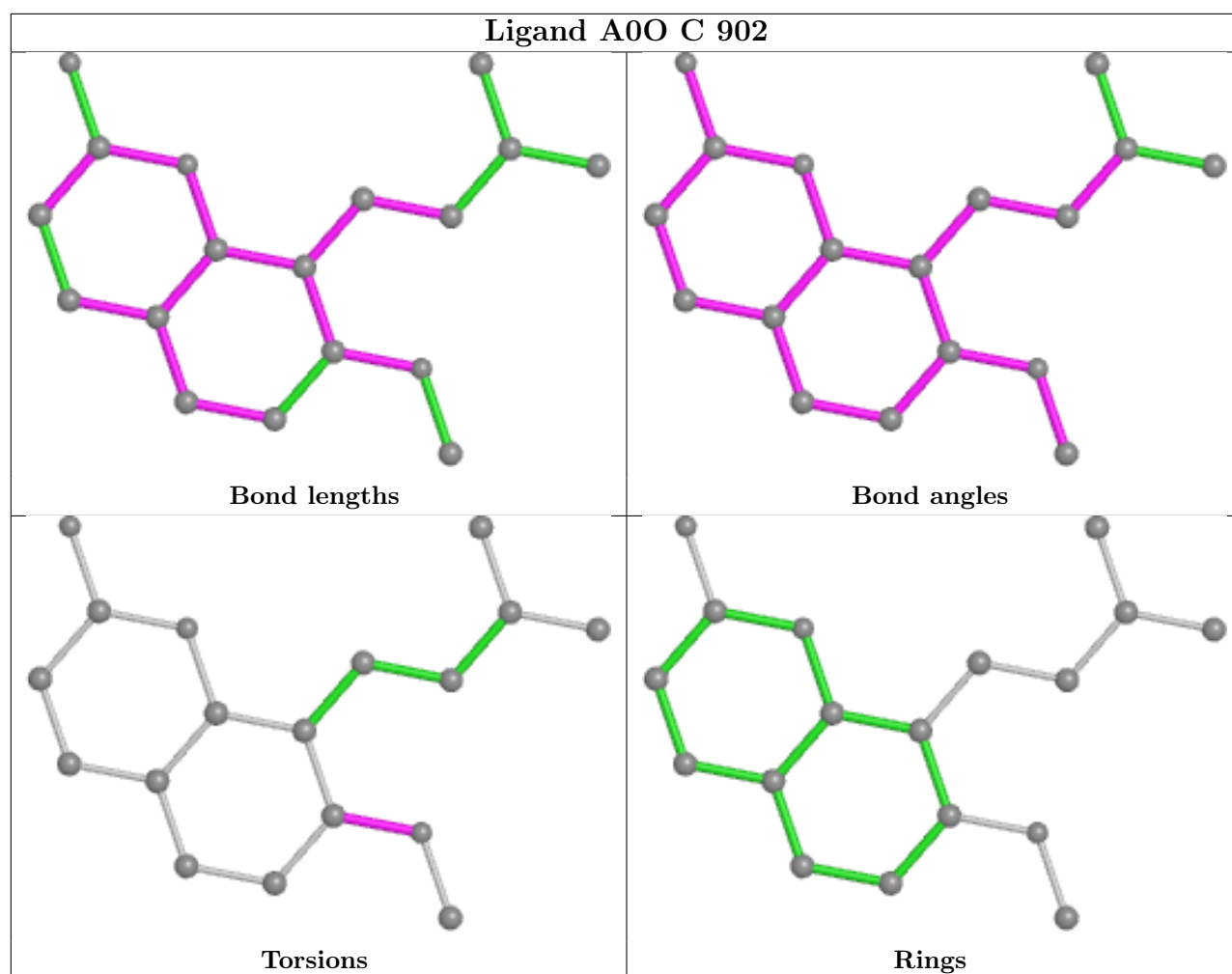












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

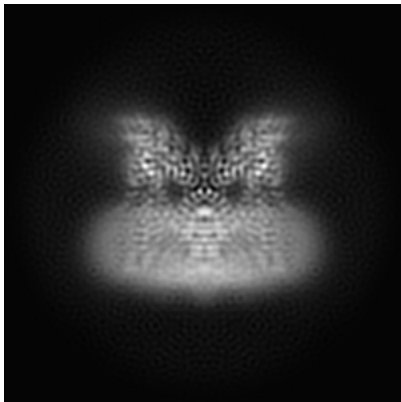
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24385. These allow visual inspection of the internal detail of the map and identification of artifacts.

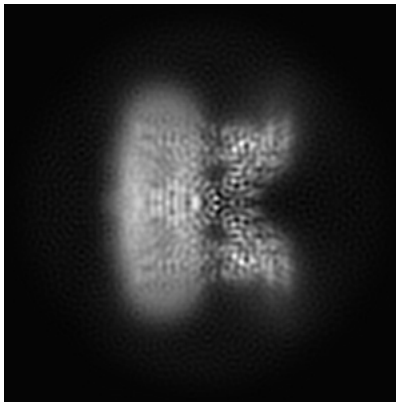
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

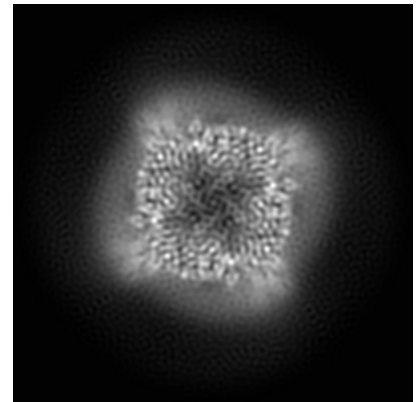
#### 6.1.1 Primary map



X



Y

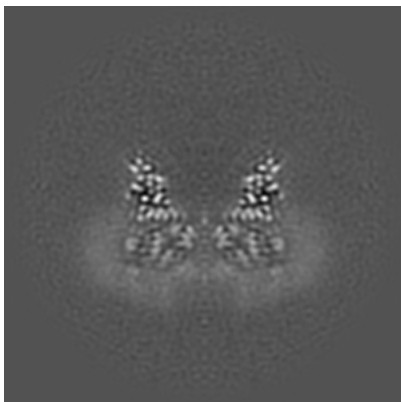


Z

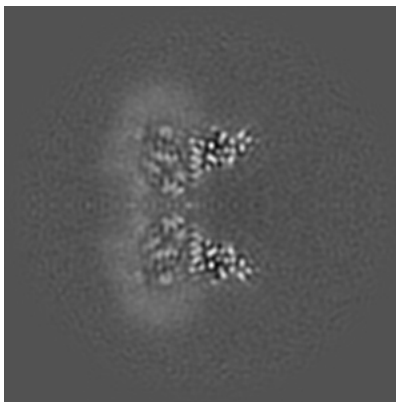
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

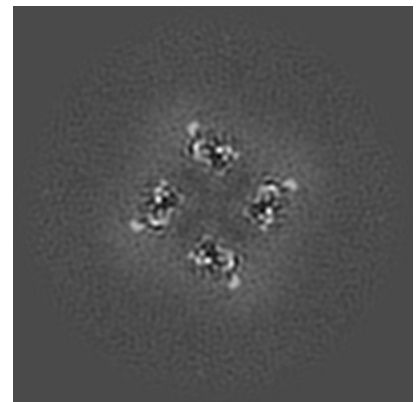
#### 6.2.1 Primary map



X Index: 144



Y Index: 144

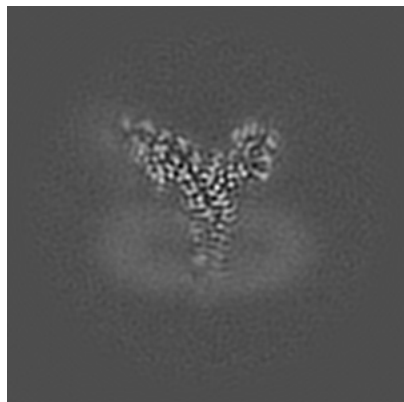


Z Index: 144

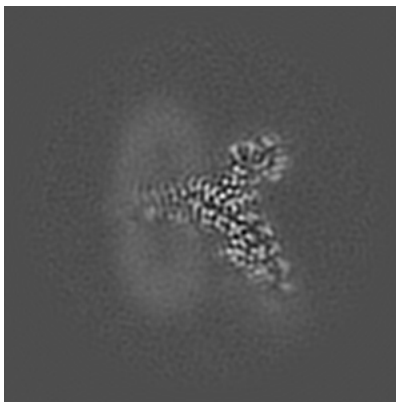
The images above show central slices of the map in three orthogonal directions.

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

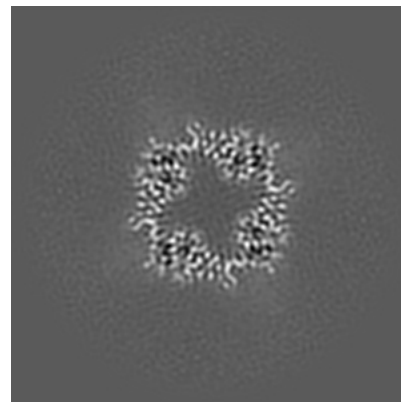
### 6.3.1 Primary map



X Index: 183



Y Index: 105

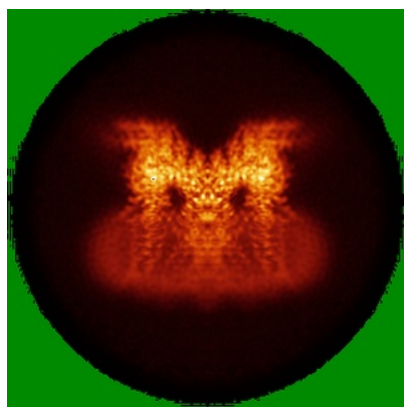


Z Index: 170

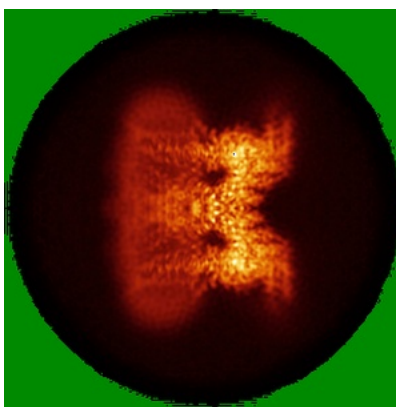
The images above show the largest variance slices of the map in three orthogonal directions.

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

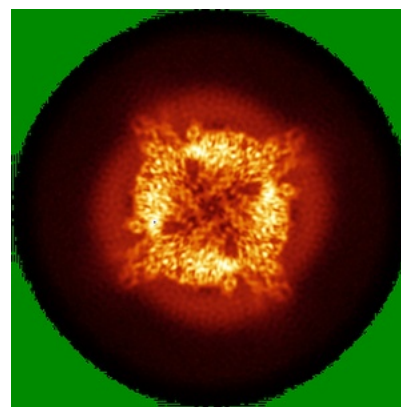
### 6.4.1 Primary map



X



Y



Z

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 0.325. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

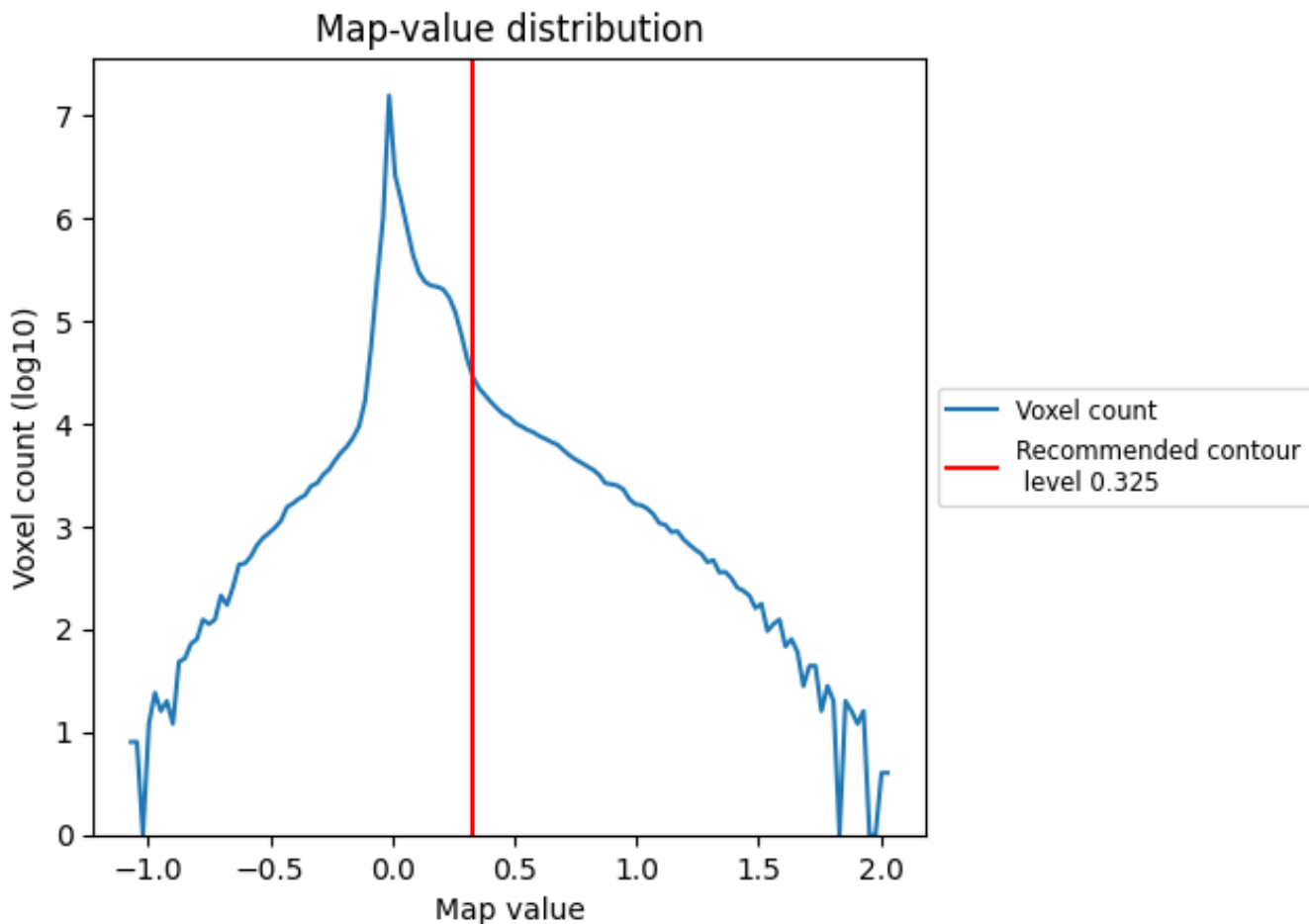
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

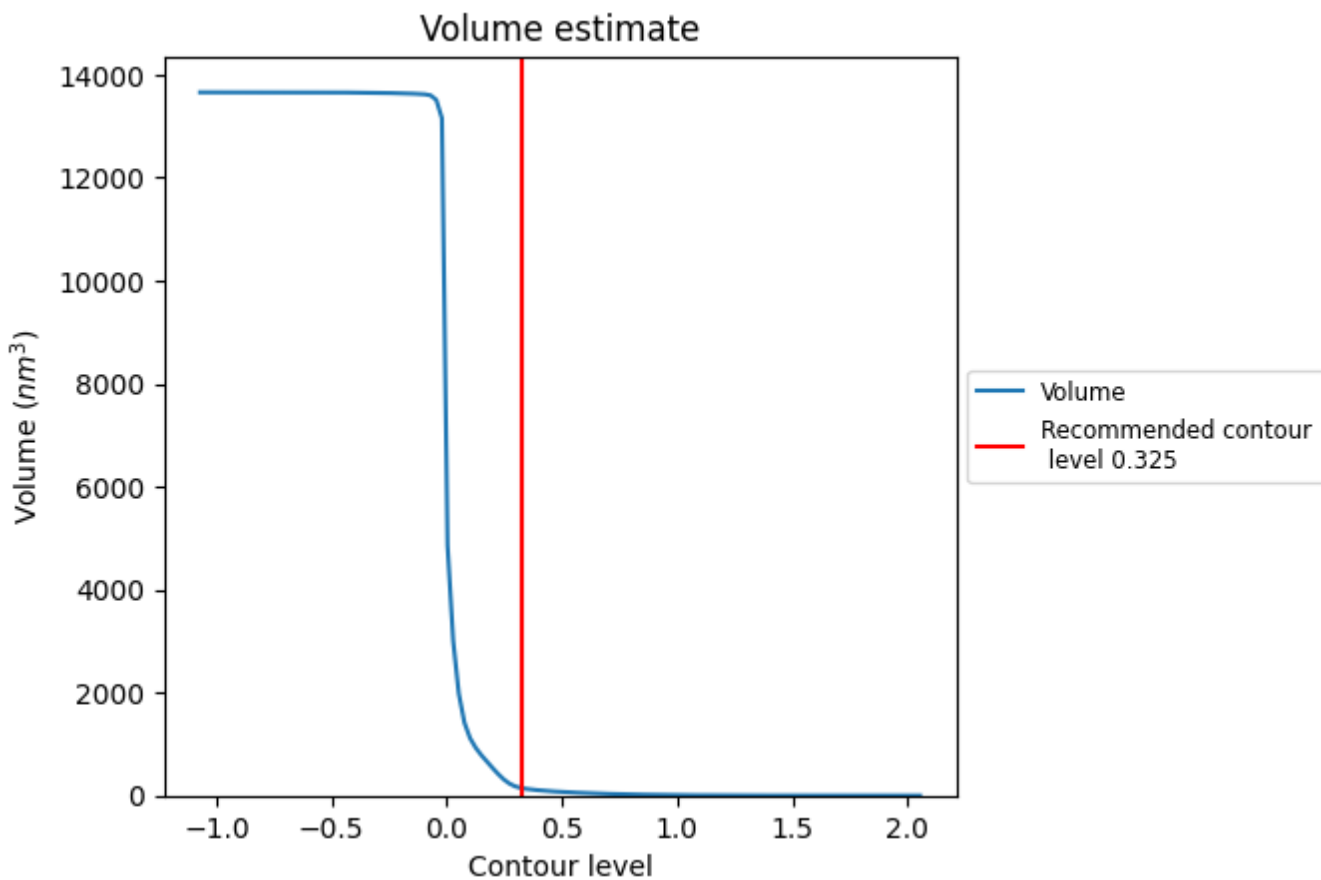
This section contains the results of statistical analysis of the map.

### 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](#)

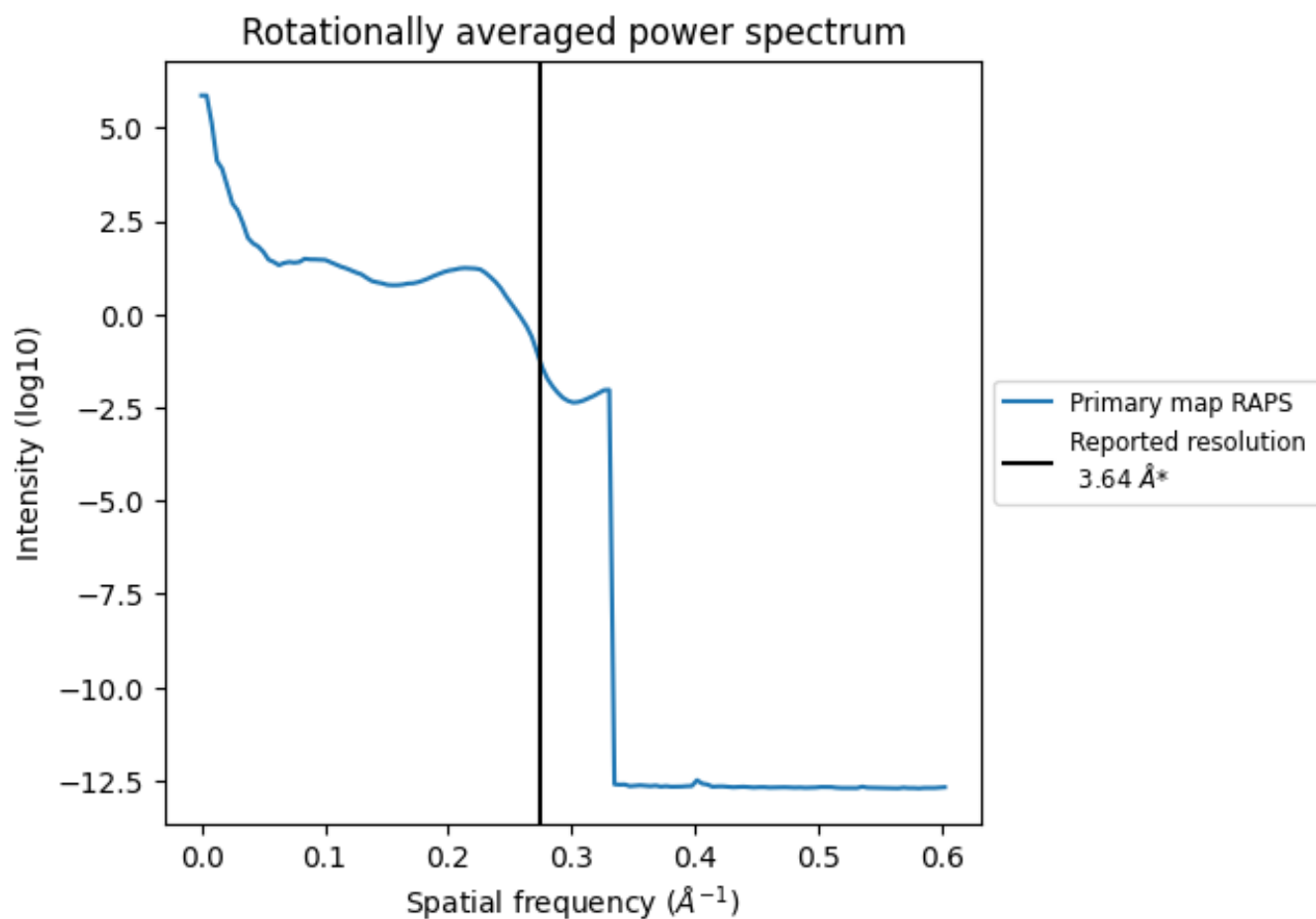


The volume at the recommended contour level is 146 nm<sup>3</sup>; this corresponds to an approximate mass of 131 kDa.

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  $0.275 \text{\AA}^{-1}$

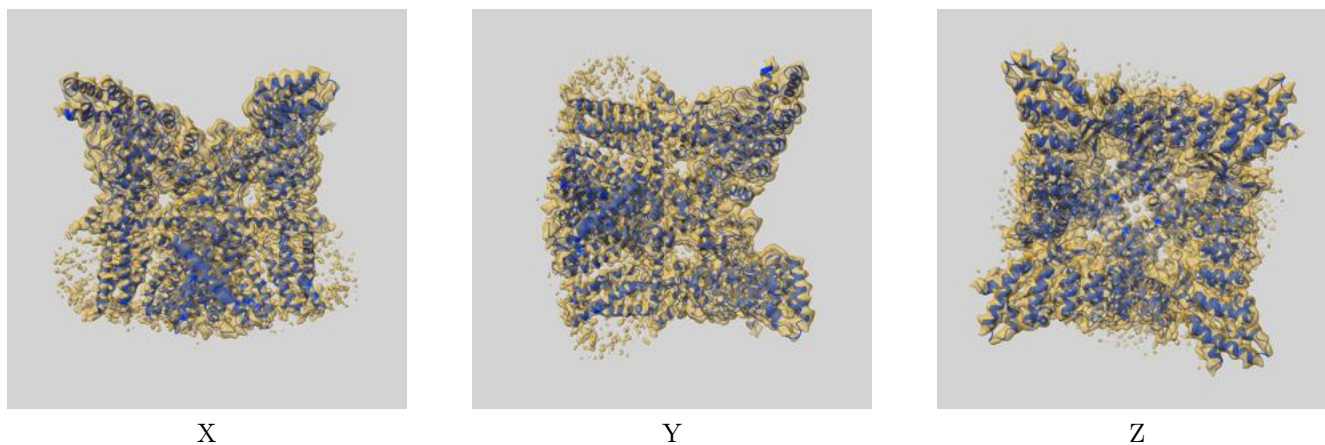
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

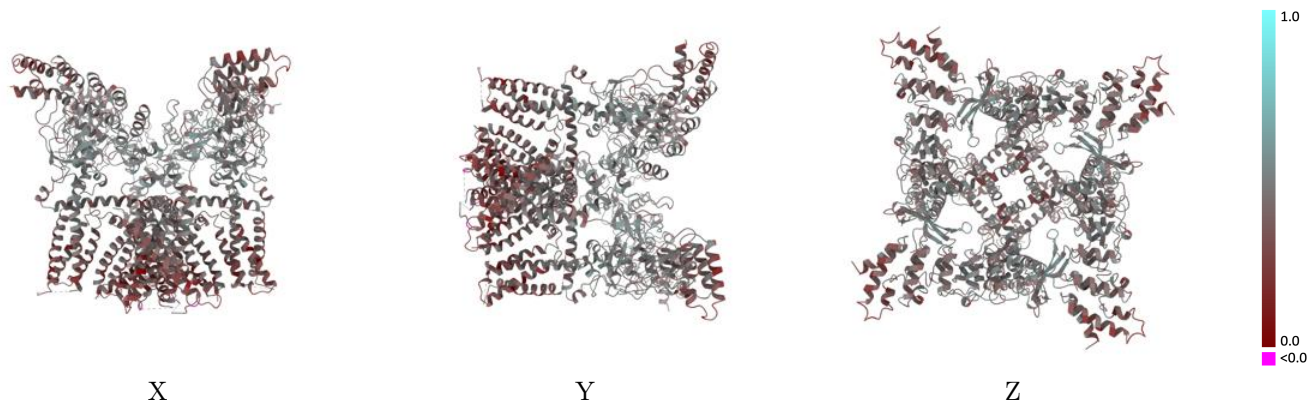
This section contains information regarding the fit between EMDB map EMD-24385 and PDB model 7RAS. Per-residue inclusion information can be found in section 3 on page 8.

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



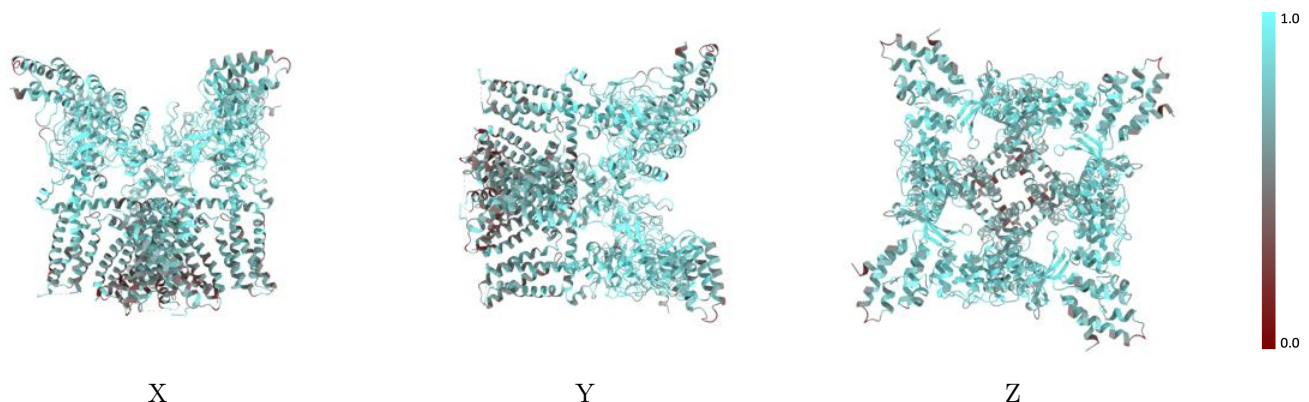
The images above show the 3D surface view of the map at the recommended contour level 0.325 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



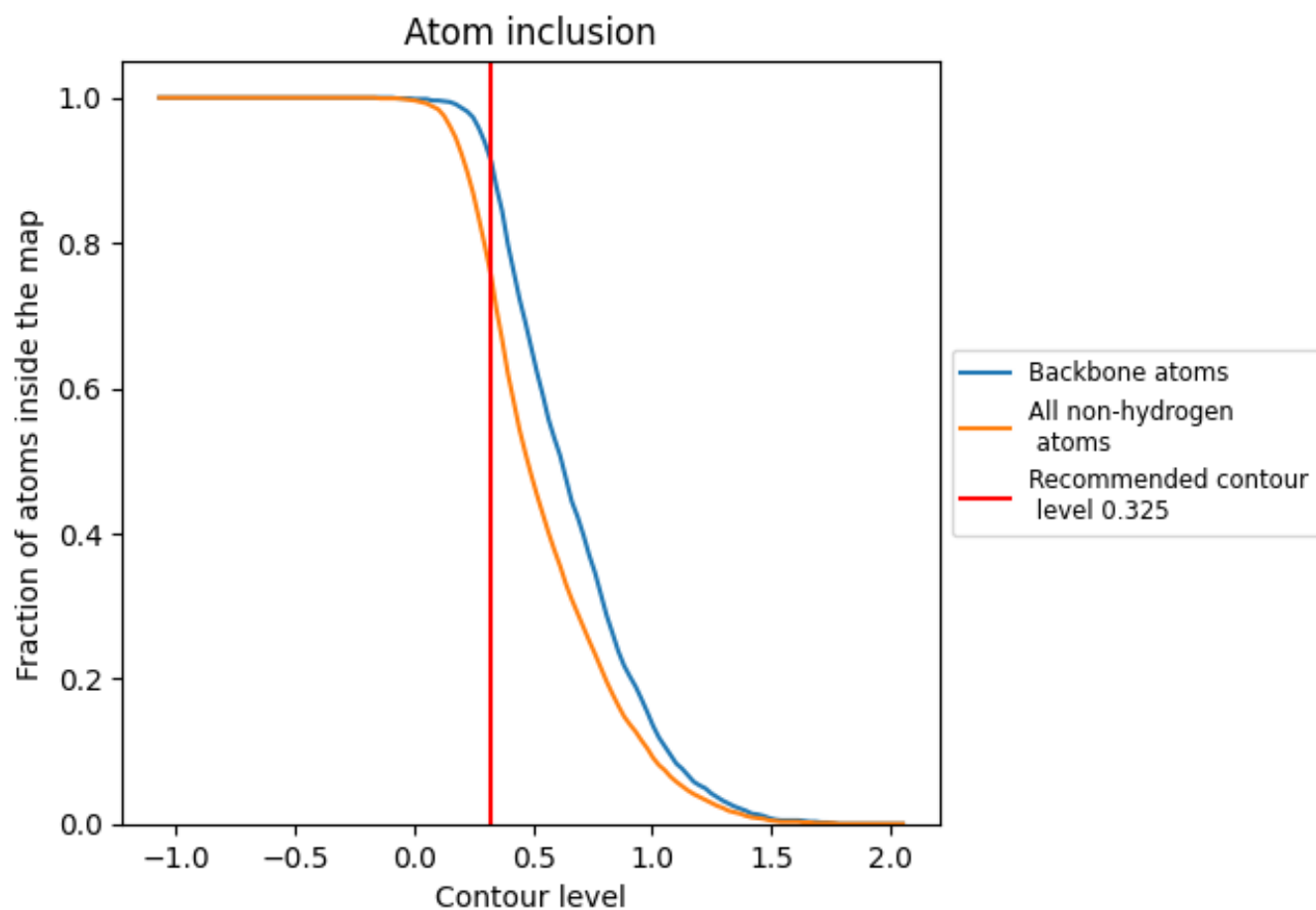
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.325).











## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 75% 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 (0.325) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7520	 0.4130
A	 0.7510	 0.4120
B	 0.7530	 0.4140
C	 0.7520	 0.4130
D	 0.7510	 0.4130

