W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB EM Validation Report ⓘ

Mar 11, 2024 – 07:49 AM EDT

PDB ID	:	6P4J
EMDB ID	:	EMD-20250
Title	:	Mouse norovirus complexed with GCDCA
Authors	:	Smith, T.J.; Smith, T.J.
Deposited on	:	2019-05-27
Resolution	:	3.10 Å(reported)

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

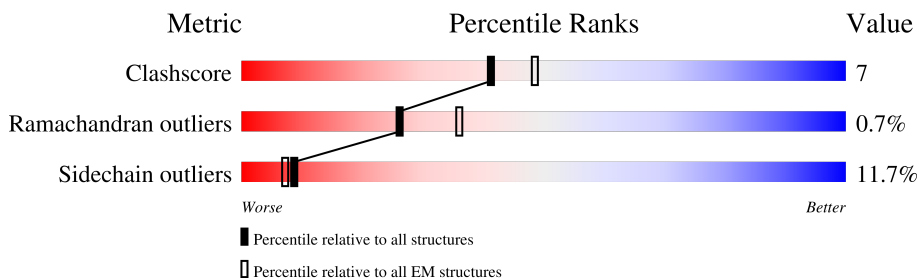|		
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.10 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	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		0.7%
Sidechain outliers		11.7%

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures

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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	516	11% 80% 16% • •
1	B	516	9% 79% 18% • •
1	C	516	6% 78% 16% • •

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:

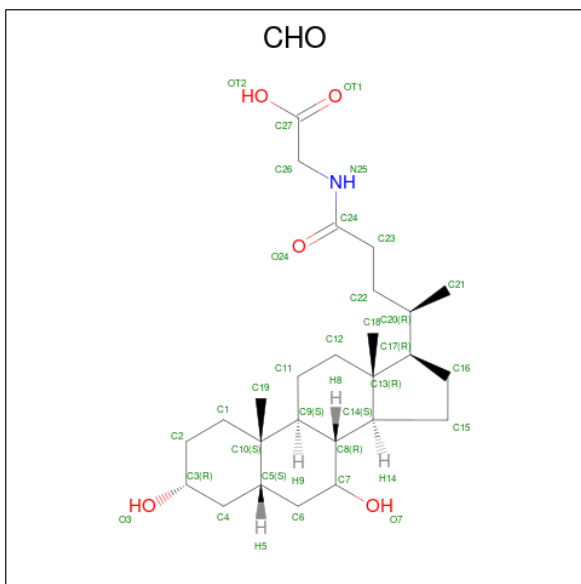| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CHO	B	601	-	X	-	-

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 11945 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 Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	514	Total	C	N	O	S	0	0
			3948	2544	650	738	16		
1	B	513	Total	C	N	O	S	0	0
			3941	2539	649	737	16		
1	C	502	Total	C	N	O	S	0	0
			3864	2493	636	719	16		

- Molecule 2 is GLYCOCHENODEOXYCHOLIC ACID (three-letter code: CHO) (formula: $C_{26}H_{43}NO_5$).

Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			32	26	1	5	
2	A	1	Total	C	N	O	0
			32	26	1	5	
2	B	1	Total	C	N	O	0
			32	26	1	5	

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| Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			32	26	1	5	
2	C	1	Total	C	N	O	0
			32	26	1	5	
2	C	1	Total	C	N	O	0
			32	26	1	5	

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.
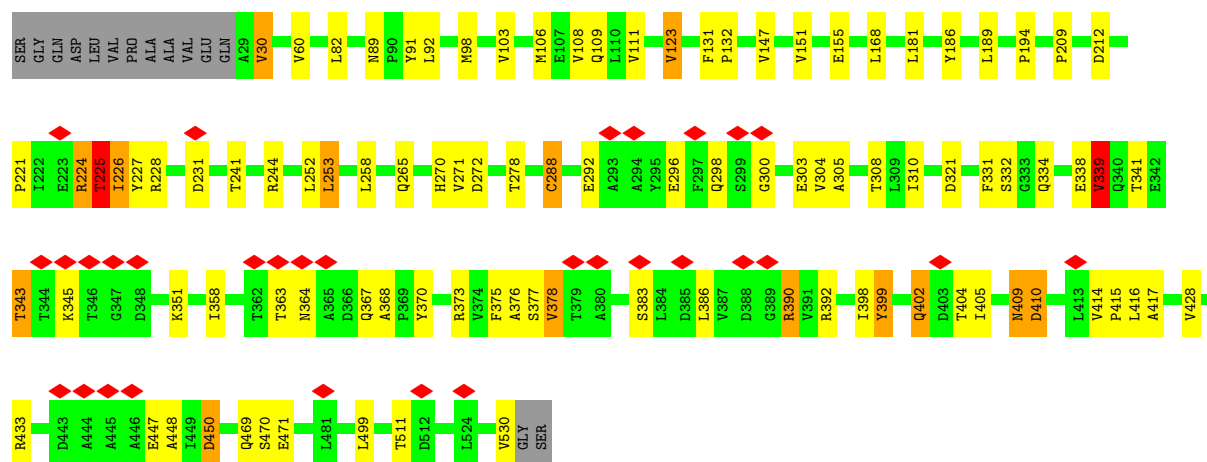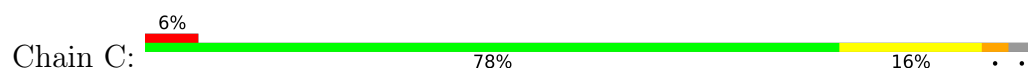
• Molecule 1: Capsid protein

• Molecule 1: Capsid protein

• Molecule 1: Capsid protein

Chain C:

6%

78%

16%
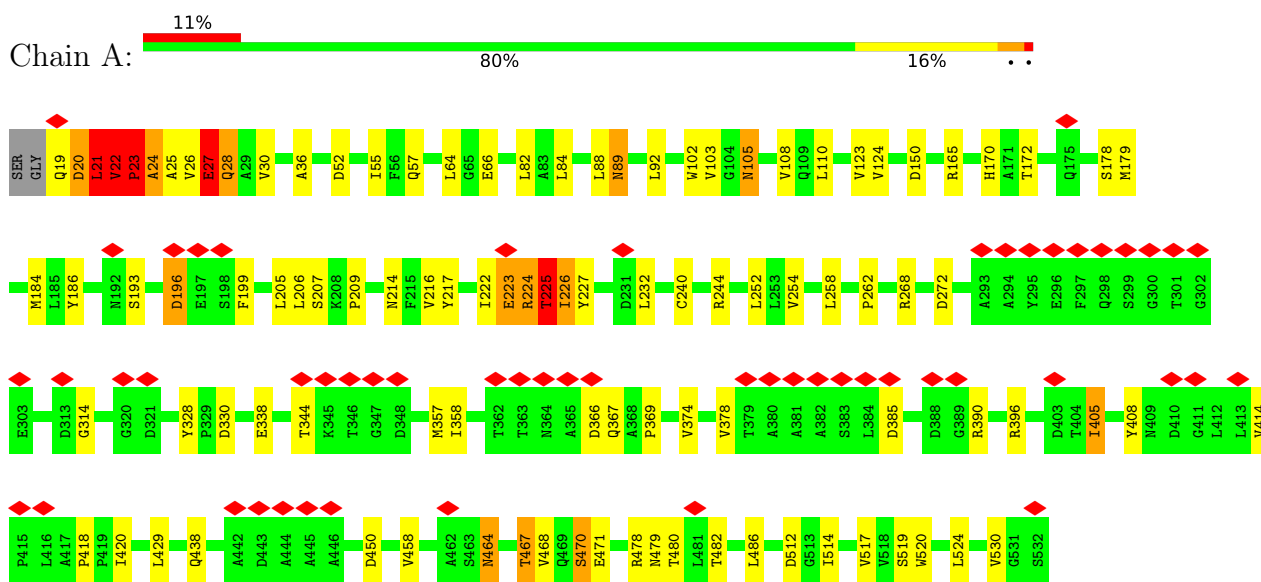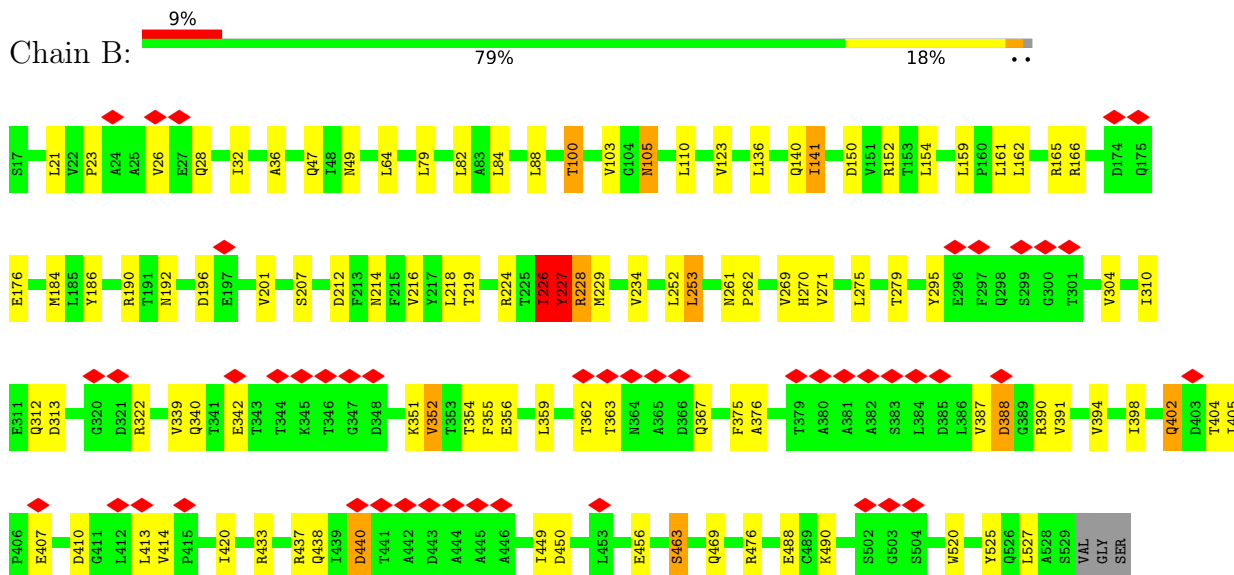
4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28463	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	38	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	OTHER	Depositor
Maximum map value	8.340	Depositor
Minimum map value	-4.068	Depositor
Average map value	0.017	Depositor
Map value standard deviation	0.332	Depositor
Recommended contour level	1.0	Depositor
Map size (Å)	636.01996, 636.01996, 636.01996	wwPDB
Map dimensions	550, 550, 550	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1564, 1.1564, 1.1564	Depositor

5　Model quality ⓘ

5.1　Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CHO

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	0.68	5/4052 (0.1%)	1.55	27/5549 (0.5%)
1	B	0.46	0/4050	0.63	3/5554 (0.1%)
1	C	0.64	3/3972 (0.1%)	0.82	6/5447 (0.1%)
All	All	0.60	8/12074 (0.1%)	1.08	36/16550 (0.2%)

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	1	6
1	B	1	2
1	C	0	3
All	All	2	11

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	224	ARG	C-N	22.96	1.86	1.34
1	A	22	VAL	C-N	20.24	1.72	1.34
1	C	225	THR	C-N	15.62	1.70	1.34
1	A	24	ALA	C-N	-14.05	1.01	1.34
1	A	23	PRO	C-N	12.50	1.62	1.34
1	A	25	ALA	C-N	10.19	1.57	1.34
1	A	226	ILE	C-N	6.03	1.48	1.34
1	C	231	ASP	C-N	-5.24	1.22	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	27	GLU	O-C-N	-61.88	23.70	122.70
1	A	24	ALA	O-C-N	-44.26	51.88	122.70
1	C	224	ARG	O-C-N	32.34	174.44	122.70
1	A	22	VAL	O-C-N	-32.17	59.98	121.10
1	A	22	VAL	C-N-CD	-26.43	62.45	120.60
1	A	224	ARG	CB-CA-C	23.99	158.38	110.40
1	C	224	ARG	CA-C-N	-23.45	65.60	117.20
1	A	223	GLU	N-CA-C	-22.33	50.71	111.00
1	B	227	TYR	N-CA-CB	21.60	149.48	110.60
1	A	23	PRO	O-C-N	19.15	153.34	122.70
1	A	223	GLU	CB-CA-C	18.46	147.33	110.40
1	A	226	ILE	O-C-N	16.82	149.61	122.70
1	A	23	PRO	CA-C-N	-16.16	81.65	117.20
1	A	224	ARG	N-CA-CB	-15.89	82.00	110.60
1	A	23	PRO	C-N-CA	-13.48	88.00	121.70
1	A	226	ILE	CA-C-N	-13.39	87.73	117.20
1	A	21	LEU	CA-C-N	-12.68	89.31	117.20
1	A	21	LEU	C-N-CA	-12.63	90.12	121.70
1	A	225	THR	N-CA-C	-12.30	77.79	111.00
1	C	225	THR	O-C-N	10.64	139.73	122.70
1	C	225	THR	C-N-CA	-10.57	95.28	121.70
1	A	25	ALA	O-C-N	-10.48	105.93	122.70
1	A	226	ILE	C-N-CA	-9.85	97.07	121.70
1	B	226	ILE	N-CA-C	9.84	137.58	111.00
1	C	224	ARG	C-N-CA	-9.16	98.79	121.70
1	A	22	VAL	C-N-CA	9.16	160.46	122.00
1	A	22	VAL	CA-C-N	8.91	142.05	117.10
1	A	21	LEU	O-C-N	8.70	136.62	122.70
1	A	23	PRO	CA-N-CD	-8.58	99.49	111.50
1	B	227	TYR	N-CA-C	-7.52	90.69	111.00
1	A	24	ALA	CA-C-N	7.48	133.66	117.20
1	A	25	ALA	C-N-CA	7.11	139.47	121.70
1	A	224	ARG	N-CA-C	-7.06	91.94	111.00
1	A	25	ALA	CA-C-N	5.90	130.18	117.20
1	C	225	THR	CA-C-N	-5.46	105.19	117.20
1	A	20	ASP	CB-CG-OD2	5.21	122.99	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	223	GLU	CA
1	B	226	ILE	CA

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	PHE	Peptide
1	A	21	LEU	Mainchain
1	A	24	ALA	Mainchain
1	A	27	GLU	Mainchain,Peptide
1	A	458	VAL	Peptide
1	B	226	ILE	Peptide
1	B	227	TYR	Peptide
1	C	131	PHE	Peptide
1	C	30	VAL	Peptide
1	C	339	VAL	Peptide

5.2   Too-close contacts   ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3948	0	3887	70	0
1	B	3941	0	3884	45	0
1	C	3864	0	3812	49	0
2	A	64	0	75	9	0
2	B	64	0	73	3	0
2	C	64	0	74	6	0
All	All	11945	0	11805	175	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 7.

All (175) 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:223:GLU:CA	1:A:224:ARG:C	1.77	1.49
1:C:225:THR:C	1:C:226:ILE:N	1.70	1.45
1:A:223:GLU:HA	1:A:224:ARG:C	1.31	1.42
1:C:224:ARG:CA	1:C:225:THR:N	1.86	1.39
1:C:224:ARG:HA	1:C:225:THR:N	1.40	1.35
1:C:224:ARG:C	1:C:225:THR:N	1.86	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ARG:C	1:A:225:THR:OG1	1.72	1.27
1:A:225:THR:CA	1:A:226:ILE:N	2.02	1.23
1:A:225:THR:C	1:A:226:ILE:N	2.00	1.14
1:A:226:ILE:HG22	1:A:467:THR:CG2	1.78	1.14
1:B:32:ILE:HD13	1:B:162:LEU:HD12	1.27	1.13
1:A:226:ILE:HG22	1:A:467:THR:HG23	1.27	1.12
1:A:224:ARG:O	1:A:225:THR:CB	2.01	1.09
1:A:225:THR:HB	1:A:226:ILE:N	1.68	1.08
1:A:223:GLU:C	1:A:224:ARG:C	2.12	1.06
1:A:225:THR:CB	1:A:226:ILE:N	2.20	1.03
1:A:19:GLN:O	1:A:20:ASP:N	1.98	0.96
1:C:225:THR:C	1:C:226:ILE:CA	2.34	0.94
1:A:19:GLN:C	1:A:20:ASP:N	2.21	0.93
1:A:19:GLN:HB3	1:A:20:ASP:N	1.88	0.89
1:A:26:VAL:O	1:A:27:GLU:HB2	1.70	0.88
1:A:223:GLU:CA	1:A:224:ARG:N	2.37	0.88
1:B:32:ILE:CD1	1:B:162:LEU:HD12	2.02	0.88
1:A:226:ILE:CG2	1:A:467:THR:HG23	2.05	0.87
1:C:225:THR:OG1	1:C:228:ARG:HD2	1.73	0.87
1:A:226:ILE:O	1:A:227:TYR:HB2	1.73	0.86
1:A:226:ILE:CG2	1:A:467:THR:CG2	2.56	0.83
1:C:225:THR:OG1	1:C:228:ARG:CD	2.27	0.83
1:C:224:ARG:C	1:C:225:THR:CA	2.54	0.75
1:A:226:ILE:HG22	1:A:467:THR:HG21	1.67	0.74
1:C:225:THR:C	1:C:226:ILE:HA	2.09	0.73
1:C:225:THR:HB	1:C:227:TYR:H	1.54	0.73
1:A:26:VAL:O	1:A:26:VAL:HG12	1.90	0.70
1:C:390:ARG:HB2	2:C:602:CHO:H112	1.76	0.67
1:C:225:THR:CA	1:C:226:ILE:N	2.59	0.65
1:A:226:ILE:CG2	1:A:467:THR:HG21	2.26	0.65
1:A:19:GLN:CB	1:A:20:ASP:N	2.58	0.65
1:A:223:GLU:HA	1:A:224:ARG:CA	2.26	0.64
1:A:223:GLU:O	1:A:225:THR:HG23	1.97	0.64
1:A:464:ASN:N	1:A:464:ASN:OD1	2.33	0.62
1:A:105:ASN:N	1:A:105:ASN:OD1	2.32	0.62
1:A:23:PRO:HD2	1:A:23:PRO:O	2.01	0.61
1:A:470:SER:OG	1:A:471:GLU:N	2.34	0.61
1:B:105:ASN:OD1	1:B:105:ASN:N	2.33	0.60
1:A:92:LEU:HD11	1:A:209:PRO:HG3	1.83	0.59
1:A:26:VAL:O	1:A:27:GLU:CB	2.44	0.59
1:C:450:ASP:OD1	1:C:450:ASP:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ARG:O	1:A:225:THR:OG1	0.63	0.58
1:C:92:LEU:HD11	1:C:209:PRO:HG3	1.85	0.58
1:A:36:ALA:O	1:A:165:ARG:NH2	2.37	0.58
1:B:351:LYS:NZ	1:B:352:VAL:O	2.37	0.58
1:A:268:ARG:NH1	1:A:418:PRO:O	2.38	0.57
1:C:265:GLN:HE22	1:C:417:ALA:H	1.53	0.56
1:A:21:LEU:O	1:A:22:VAL:C	2.40	0.56
1:C:343:THR:HB	1:C:386:LEU:HD23	1.88	0.56
1:C:225:THR:HG1	1:C:228:ARG:HD2	1.68	0.56
1:A:225:THR:HG22	1:A:226:ILE:O	2.07	0.55
1:C:334:GLN:HB2	1:C:399:TYR:HB3	1.89	0.55
1:B:313:ASP:OD1	1:B:313:ASP:N	2.36	0.55
1:B:64:LEU:HD21	1:B:469:GLN:HB3	1.88	0.54
1:C:304:VAL:HA	1:C:377:SER:HA	1.89	0.54
1:B:224:ARG:NH2	1:B:463:SER:O	2.41	0.54
1:B:390:ARG:HD2	2:B:602:CHO:H41	1.90	0.54
1:B:64:LEU:HD11	1:B:469:GLN:HE21	1.72	0.54
1:B:476:ARG:NH1	1:B:488:GLU:OE1	2.40	0.53
1:A:225:THR:HA	1:A:226:ILE:N	2.13	0.53
1:B:226:ILE:CG2	1:B:226:ILE:O	2.57	0.53
1:C:60:VAL:HG21	1:C:91:TYR:CE2	2.43	0.53
1:B:49:ASN:ND2	1:B:216:VAL:O	2.42	0.53
1:B:36:ALA:O	1:B:165:ARG:NH2	2.42	0.53
1:A:223:GLU:HA	1:A:224:ARG:N	2.16	0.52
1:B:100:THR:O	1:B:100:THR:OG1	2.25	0.52
1:B:136:LEU:HA	1:B:140:GLN:HE21	1.73	0.52
1:B:438:GLN:NE2	1:B:440:ASP:OD2	2.40	0.52
1:C:288:CYS:SG	1:C:392:ARG:NH2	2.80	0.51
1:B:367:GLN:NE2	1:B:375:PHE:O	2.42	0.51
1:B:141:ILE:HD12	1:B:184:MET:HB2	1.92	0.51
1:A:390:ARG:HB3	2:A:602:CHO:H112	1.93	0.51
1:C:253:LEU:HD21	1:C:433:ARG:HG3	1.92	0.51
1:B:490:LYS:HB2	1:B:527:LEU:HD11	1.93	0.51
1:B:261:ASN:ND2	1:B:420:ILE:O	2.44	0.51
1:B:342:GLU:HB2	1:B:387:VAL:HB	1.93	0.51
1:C:410:ASP:OD1	1:C:410:ASP:N	2.41	0.51
1:A:338:GLU:HG3	1:A:396:ARG:HB2	1.93	0.50
1:C:345:LYS:NZ	1:C:383:SER:O	2.42	0.50
1:B:262:PRO:HD2	1:B:420:ILE:HB	1.93	0.50
1:C:292:GLU:HB3	1:C:308:THR:HB	1.93	0.50
1:C:433:ARG:HD2	1:C:448:ALA:HB1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:ASP:N	1:C:212:ASP:OD1	2.44	0.50
1:A:88:LEU:O	1:A:207:SER:OG	2.30	0.50
1:A:385:ASP:OD1	1:A:385:ASP:N	2.42	0.49
1:B:88:LEU:O	1:B:207:SER:OG	2.30	0.49
1:B:437:ARG:N	2:B:601:CHO:H261	2.28	0.49
1:C:367:GLN:NE2	1:C:375:PHE:O	2.46	0.49
1:B:26:VAL:O	1:B:28:GLN:NE2	2.46	0.48
1:B:32:ILE:HD13	1:B:162:LEU:CD1	2.20	0.48
1:C:298:GLN:HG2	1:C:300:GLY:H	1.78	0.48
1:B:269:VAL:HG23	1:B:275:LEU:HG	1.96	0.48
1:A:358:ILE:O	1:A:367:GLN:NE2	2.46	0.48
1:B:47:GLN:HE22	1:B:218:LEU:HB2	1.77	0.48
1:A:82:LEU:HD11	1:A:205:LEU:HD13	1.95	0.48
1:B:212:ASP:N	1:B:212:ASP:OD1	2.45	0.48
1:A:244:ARG:NH1	1:A:450:ASP:O	2.46	0.47
1:A:89:ASN:ND2	1:A:207:SER:O	2.46	0.47
1:B:253:LEU:HD21	1:B:433:ARG:HD2	1.96	0.47
1:A:26:VAL:O	1:A:26:VAL:CG1	2.59	0.47
1:A:226:ILE:O	1:A:227:TYR:CB	2.50	0.47
2:C:602:CHO:H183	2:C:602:CHO:H20	1.80	0.47
1:B:367:GLN:HG2	1:B:375:PHE:HD2	1.80	0.47
1:C:321:ASP:OD1	1:C:321:ASP:N	2.38	0.47
1:A:196:ASP:OD1	1:A:196:ASP:N	2.43	0.47
1:B:32:ILE:CG2	1:B:162:LEU:HD11	2.45	0.47
1:A:369:PRO:HG2	1:A:408:TYR:HA	1.96	0.46
1:C:409:ASN:ND2	1:C:410:ASP:OD1	2.47	0.46
1:A:27:GLU:C	1:A:28:GLN:HG2	2.36	0.46
1:B:84:LEU:HD13	1:B:161:LEU:HG	1.96	0.46
1:C:108:VAL:HG21	1:C:181:LEU:HD11	1.97	0.46
1:C:470:SER:OG	1:C:471:GLU:N	2.48	0.46
1:B:388:ASP:OD1	1:B:388:ASP:N	2.49	0.46
2:C:601:CHO:H162	2:C:601:CHO:H181	1.79	0.46
1:A:519:SER:OG	1:A:520:TRP:N	2.49	0.46
1:A:52:ASP:HB3	1:A:55:ILE:HG13	1.98	0.46
1:B:340:GLN:HA	1:B:352:VAL:HA	1.99	0.45
1:C:305:ALA:HB3	1:C:376:ALA:HB3	1.99	0.45
2:A:601:CHO:H8	2:A:601:CHO:H182	1.65	0.45
1:A:405:ILE:H	1:A:405:ILE:HG13	1.54	0.45
1:C:499:LEU:HD11	1:C:530:VAL:HG21	1.98	0.45
1:A:262:PRO:HG2	1:A:420:ILE:HD12	1.99	0.44
1:C:123:VAL:HG12	1:C:186:TYR:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:602:CHO:H8	2:C:602:CHO:H182	1.58	0.44
1:A:328:TYR:OH	1:A:367:GLN:OE1	2.35	0.44
2:C:602:CHO:H111	2:C:602:CHO:H12	1.47	0.44
1:B:295:TYR:N	1:B:388:ASP:OD2	2.43	0.44
1:A:150:ASP:OD1	1:A:150:ASP:N	2.35	0.44
2:A:601:CHO:H232	2:A:601:CHO:H211	1.82	0.44
1:C:224:ARG:CB	1:C:225:THR:N	2.73	0.44
1:C:303:GLU:HB3	1:C:378:VAL:HB	1.99	0.44
1:C:370:TYR:HE2	1:C:415:PRO:HD2	1.82	0.44
1:A:330:ASP:N	1:A:330:ASP:OD1	2.50	0.43
1:A:225:THR:HB	1:A:226:ILE:CA	2.42	0.43
1:B:490:LYS:NZ	1:B:525:TYR:O	2.42	0.43
1:C:60:VAL:HG21	1:C:91:TYR:HE2	1.82	0.43
1:A:23:PRO:O	1:A:23:PRO:CD	2.67	0.43
1:A:314:GLY:HA2	2:A:602:CHO:H3	1.99	0.43
1:A:480:THR:HB	1:A:514:ILE:HG12	2.00	0.43
1:C:244:ARG:H	1:C:244:ARG:HG2	1.63	0.43
1:B:47:GLN:HE21	1:B:49:ASN:HD21	1.67	0.42
1:C:398:ILE:HD12	1:C:398:ILE:HA	1.89	0.42
2:A:601:CHO:H232	2:A:601:CHO:H261	1.81	0.42
1:C:368:ALA:HB3	1:C:373:ARG:HB2	2.02	0.42
1:B:355:PHE:HB3	1:B:376:ALA:HB1	2.00	0.42
1:C:265:GLN:O	1:C:278:THR:OG1	2.31	0.42
2:A:602:CHO:H12	2:A:602:CHO:H111	1.44	0.42
1:C:332:SER:OG	1:C:402:GLN:NE2	2.53	0.42
1:A:408:TYR:HB2	1:A:414:VAL:HG11	2.01	0.41
1:B:21:LEU:HD22	1:B:152:ARG:HB3	2.02	0.41
1:B:226:ILE:O	1:B:226:ILE:HG22	2.20	0.41
1:A:390:ARG:CB	2:A:602:CHO:H112	2.51	0.41
1:B:402:GLN:HB3	1:B:404:THR:HG23	2.02	0.41
1:A:367:GLN:HG3	1:A:374:VAL:HG22	2.03	0.41
1:C:409:ASN:HD22	1:C:410:ASP:H	1.69	0.41
2:C:601:CHO:H191	2:C:601:CHO:H8	1.74	0.41
1:B:21:LEU:HD12	1:B:154:LEU:HG	2.01	0.41
1:A:102:TRP:HD1	1:A:172:THR:HG22	1.85	0.41
2:A:602:CHO:H182	2:A:602:CHO:H8	1.74	0.41
1:C:303:GLU:O	1:C:378:VAL:N	2.54	0.41
1:A:479:ASN:HB2	1:A:486:LEU:HD23	2.03	0.41
1:B:469:GLN:HB2	1:B:520:TRP:CD2	2.56	0.41
1:A:216:VAL:HG12	1:A:217:TYR:HB2	2.03	0.41
2:A:601:CHO:H8	2:A:601:CHO:H191	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:ARG:H	2:B:601:CHO:H261	1.86	0.40
1:C:98:MET:HG2	1:C:221:PRO:HG3	2.03	0.40
1:C:225:THR:OG1	1:C:228:ARG:CG	2.69	0.40
1:A:438:GLN:HE21	1:A:438:GLN:HB3	1.70	0.40
1:A:165:ARG:HD3	1:A:170:HIS:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	505/516 (98%)	445 (88%)	55 (11%)	5 (1%)	15	49
1	B	511/516 (99%)	463 (91%)	45 (9%)	3 (1%)	25	59
1	C	500/516 (97%)	449 (90%)	48 (10%)	3 (1%)	25	59
All	All	1516/1548 (98%)	1357 (90%)	148 (10%)	11 (1%)	26	57

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	PRO
1	A	28	GLN
1	B	226	ILE
1	B	228	ARG
1	A	27	GLU
1	A	470	SER
1	C	339	VAL
1	C	194	PRO
1	A	22	VAL
1	B	227	TYR
1	C	132	PRO

5.3.2 Protein sidechains ⓘ

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	426/427 (100%)	383 (90%)	43 (10%)	7	28
1	B	425/427 (100%)	369 (87%)	56 (13%)	4	17
1	C	417/427 (98%)	368 (88%)	49 (12%)	5	21
All	All	1268/1281 (99%)	1120 (88%)	148 (12%)	9	22

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	57	GLN
1	A	64	LEU
1	A	66	GLU
1	A	84	LEU
1	A	89	ASN
1	A	103	VAL
1	A	105	ASN
1	A	108	VAL
1	A	110	LEU
1	A	123	VAL
1	A	124	VAL
1	A	178	SER
1	A	179	MET
1	A	184	MET
1	A	186	TYR
1	A	193	SER
1	A	196	ASP
1	A	206	LEU
1	A	214	ASN
1	A	222	ILE
1	A	225	THR
1	A	232	LEU
1	A	240	CYS
1	A	252	LEU
1	A	254	VAL

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Mol	Chain	Res	Type
1	A	258	LEU
1	A	272	ASP
1	A	344	THR
1	A	357	MET
1	A	366	ASP
1	A	378	VAL
1	A	405	ILE
1	A	429	LEU
1	A	464	ASN
1	A	467	THR
1	A	468	VAL
1	A	478	ARG
1	A	482	THR
1	A	512	ASP
1	A	517	VAL
1	A	524	LEU
1	A	530	VAL
1	B	23	PRO
1	B	79	LEU
1	B	82	LEU
1	B	100	THR
1	B	103	VAL
1	B	105	ASN
1	B	110	LEU
1	B	123	VAL
1	B	141	ILE
1	B	150	ASP
1	B	159	LEU
1	B	166	ARG
1	B	176	GLU
1	B	186	TYR
1	B	190	ARG
1	B	192	ASN
1	B	196	ASP
1	B	201	VAL
1	B	214	ASN
1	B	219	THR
1	B	226	ILE
1	B	227	TYR
1	B	228	ARG
1	B	229	MET
1	B	234	VAL

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Mol	Chain	Res	Type
1	B	252	LEU
1	B	253	LEU
1	B	270	HIS
1	B	271	VAL
1	B	279	THR
1	B	304	VAL
1	B	310	ILE
1	B	312	GLN
1	B	322	ARG
1	B	339	VAL
1	B	352	VAL
1	B	354	THR
1	B	356	GLU
1	B	359	LEU
1	B	362	THR
1	B	363	THR
1	B	388	ASP
1	B	391	VAL
1	B	394	VAL
1	B	398	ILE
1	B	402	GLN
1	B	405	ILE
1	B	407	GLU
1	B	410	ASP
1	B	413	LEU
1	B	414	VAL
1	B	440	ASP
1	B	449	ILE
1	B	450	ASP
1	B	456	GLU
1	B	463	SER
1	C	30	VAL
1	C	82	LEU
1	C	89	ASN
1	C	103	VAL
1	C	106	MET
1	C	109	GLN
1	C	111	VAL
1	C	123	VAL
1	C	147	VAL
1	C	151	VAL
1	C	155	GLU

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Mol	Chain	Res	Type
1	C	168	LEU
1	C	189	LEU
1	C	225	THR
1	C	226	ILE
1	C	241	THR
1	C	252	LEU
1	C	253	LEU
1	C	258	LEU
1	C	270	HIS
1	C	271	VAL
1	C	272	ASP
1	C	288	CYS
1	C	296	GLU
1	C	310	ILE
1	C	331	PHE
1	C	338	GLU
1	C	339	VAL
1	C	341	THR
1	C	343	THR
1	C	351	LYS
1	C	358	ILE
1	C	363	THR
1	C	364	ASN
1	C	378	VAL
1	C	390	ARG
1	C	399	TYR
1	C	402	GLN
1	C	404	THR
1	C	405	ILE
1	C	409	ASN
1	C	410	ASP
1	C	414	VAL
1	C	416	LEU
1	C	428	VAL
1	C	447	GLU
1	C	450	ASP
1	C	469	GLN
1	C	511	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	HIS
1	A	214	ASN
1	A	263	GLN
1	A	270	HIS
1	A	298	GLN
1	A	402	GLN
1	A	409	ASN
1	A	438	GLN
1	A	526	GLN
1	B	28	GLN
1	B	33	GLN
1	B	47	GLN
1	B	73	ASN
1	B	140	GLN
1	B	158	GLN
1	B	214	ASN
1	B	312	GLN
1	B	402	GLN
1	B	469	GLN
1	C	57	GLN
1	C	89	ASN
1	C	105	ASN
1	C	109	GLN
1	C	265	GLN
1	C	266	ASN
1	C	298	GLN
1	C	402	GLN
1	C	409	ASN
1	C	484	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	CHO	C	602	-	35,35,35	5.79	18 (51%)	54,54,54	3.67	33 (61%)
2	CHO	B	602	-	35,35,35	6.06	20 (57%)	54,54,54	3.64	27 (50%)
2	CHO	C	601	-	35,35,35	5.90	19 (54%)	54,54,54	3.45	30 (55%)
2	CHO	A	602	-	35,35,35	5.87	19 (54%)	54,54,54	3.53	28 (51%)
2	CHO	B	601	-	35,35,35	5.81	23 (65%)	54,54,54	4.96	36 (66%)
2	CHO	A	601	-	35,35,35	5.82	20 (57%)	54,54,54	3.39	30 (55%)

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	CHO	C	602	-	-	10/14/75/75	0/4/4/4
2	CHO	B	602	-	-	6/14/75/75	0/4/4/4
2	CHO	C	601	-	-	10/14/75/75	0/4/4/4
2	CHO	A	602	-	-	11/14/75/75	0/4/4/4
2	CHO	B	601	-	-	8/14/75/75	1/4/4/4
2	CHO	A	601	-	-	6/14/75/75	0/4/4/4

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	CHO	C12-C13	-17.03	1.23	1.54
2	A	601	CHO	C12-C13	-16.48	1.24	1.54
2	A	602	CHO	C12-C13	-16.16	1.25	1.54
2	B	601	CHO	C12-C13	-16.08	1.25	1.54
2	C	601	CHO	C12-C13	-15.91	1.25	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	CHO	C11-C9	-15.81	1.27	1.53
2	C	602	CHO	C12-C13	-15.60	1.26	1.54
2	C	601	CHO	C13-C17	-15.57	1.25	1.55
2	B	601	CHO	C13-C17	-15.12	1.26	1.55
2	B	602	CHO	C13-C17	-14.86	1.26	1.55
2	A	602	CHO	C13-C17	-14.57	1.27	1.55
2	A	601	CHO	C11-C9	-14.40	1.29	1.53
2	A	602	CHO	C11-C9	-14.39	1.29	1.53
2	C	601	CHO	C11-C9	-14.32	1.29	1.53
2	C	602	CHO	C13-C17	-14.16	1.28	1.55
2	C	602	CHO	C11-C9	-13.78	1.30	1.53
2	B	601	CHO	C11-C9	-13.05	1.31	1.53
2	A	601	CHO	C13-C17	-12.15	1.31	1.55
2	A	601	CHO	C20-C17	10.65	1.73	1.54
2	B	601	CHO	C20-C17	9.51	1.71	1.54
2	C	602	CHO	C16-C15	-9.28	1.28	1.54
2	C	601	CHO	C16-C15	-9.22	1.28	1.54
2	B	601	CHO	C16-C15	-9.18	1.28	1.54
2	B	602	CHO	C20-C17	9.08	1.70	1.54
2	A	602	CHO	C16-C15	-9.03	1.29	1.54
2	A	601	CHO	C16-C15	-8.94	1.29	1.54
2	C	602	CHO	C20-C17	8.93	1.70	1.54
2	B	602	CHO	C8-C14	8.91	1.71	1.53
2	A	602	CHO	C20-C17	8.91	1.70	1.54
2	C	601	CHO	C20-C17	8.64	1.69	1.54
2	B	602	CHO	C16-C15	-8.55	1.30	1.54
2	A	601	CHO	C8-C14	8.36	1.70	1.53
2	A	602	CHO	C8-C14	8.00	1.69	1.53
2	C	601	CHO	C13-C14	-7.38	1.40	1.55
2	C	602	CHO	C24-N25	7.36	1.50	1.33
2	B	601	CHO	C24-N25	7.34	1.50	1.33
2	C	602	CHO	C8-C14	7.34	1.68	1.53
2	C	601	CHO	C24-N25	7.31	1.50	1.33
2	A	602	CHO	C24-N25	7.27	1.49	1.33
2	B	602	CHO	C24-N25	7.21	1.49	1.33
2	C	602	CHO	C13-C14	-7.09	1.41	1.55
2	A	602	CHO	C13-C14	-7.06	1.41	1.55
2	A	601	CHO	C24-N25	7.01	1.49	1.33
2	B	602	CHO	C13-C14	-6.98	1.41	1.55
2	A	602	CHO	C6-C7	6.84	1.64	1.52
2	B	601	CHO	C6-C7	6.76	1.64	1.52
2	B	601	CHO	C8-C14	6.67	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	602	CHO	C6-C7	6.64	1.64	1.52
2	A	601	CHO	C6-C7	6.60	1.64	1.52
2	B	602	CHO	C6-C7	6.58	1.64	1.52
2	C	601	CHO	C8-C14	6.41	1.66	1.53
2	A	601	CHO	C13-C14	-6.27	1.43	1.55
2	C	601	CHO	C6-C7	6.20	1.63	1.52
2	B	601	CHO	C10-C9	5.66	1.66	1.56
2	C	602	CHO	C10-C9	5.65	1.66	1.56
2	B	601	CHO	C13-C14	-5.41	1.44	1.55
2	A	601	CHO	C10-C9	5.41	1.66	1.56
2	C	601	CHO	C10-C9	5.36	1.66	1.56
2	C	601	CHO	C8-C9	-5.25	1.43	1.53
2	B	602	CHO	C8-C9	-5.24	1.43	1.53
2	A	602	CHO	C8-C9	-4.97	1.44	1.53
2	A	602	CHO	C10-C9	4.90	1.65	1.56
2	A	601	CHO	C8-C9	-4.84	1.44	1.53
2	B	602	CHO	C10-C9	4.75	1.64	1.56
2	B	601	CHO	C8-C9	-4.57	1.45	1.53
2	C	602	CHO	C8-C9	-4.54	1.45	1.53
2	A	601	CHO	C12-C11	4.34	1.62	1.53
2	C	602	CHO	C4-C5	4.30	1.60	1.53
2	C	602	CHO	C12-C11	4.14	1.62	1.53
2	A	601	CHO	C4-C5	4.09	1.60	1.53
2	C	601	CHO	C4-C5	4.06	1.60	1.53
2	C	601	CHO	C21-C20	-3.97	1.43	1.53
2	C	602	CHO	C23-C24	3.95	1.58	1.51
2	A	601	CHO	C16-C17	3.91	1.62	1.54
2	B	601	CHO	C4-C5	3.78	1.59	1.53
2	A	602	CHO	C21-C20	-3.75	1.43	1.53
2	B	602	CHO	C21-C20	-3.73	1.44	1.53
2	A	602	CHO	C12-C11	3.66	1.61	1.53
2	C	602	CHO	C21-C20	-3.64	1.44	1.53
2	B	601	CHO	C21-C20	-3.63	1.44	1.53
2	B	601	CHO	C8-C7	3.57	1.59	1.53
2	C	602	CHO	C16-C17	3.51	1.61	1.54
2	A	602	CHO	C23-C24	3.47	1.57	1.51
2	C	601	CHO	C18-C13	3.43	1.60	1.54
2	A	601	CHO	C23-C24	3.43	1.57	1.51
2	C	601	CHO	C23-C24	3.39	1.57	1.51
2	C	601	CHO	C12-C11	3.35	1.60	1.53
2	A	602	CHO	C4-C5	3.35	1.59	1.53
2	B	601	CHO	C23-C24	3.33	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	CHO	C23-C24	3.22	1.57	1.51
2	B	601	CHO	C16-C17	3.20	1.61	1.54
2	B	602	CHO	C12-C11	3.17	1.60	1.53
2	A	602	CHO	C16-C17	3.10	1.60	1.54
2	C	601	CHO	C16-C17	3.08	1.60	1.54
2	B	601	CHO	C18-C13	3.06	1.59	1.54
2	B	601	CHO	C12-C11	3.01	1.59	1.53
2	B	602	CHO	C4-C5	2.92	1.58	1.53
2	C	602	CHO	C18-C13	2.90	1.59	1.54
2	B	602	CHO	C18-C13	2.86	1.59	1.54
2	B	601	CHO	O7-C7	2.84	1.49	1.43
2	A	602	CHO	C18-C13	2.81	1.59	1.54
2	B	602	CHO	C16-C17	2.80	1.60	1.54
2	A	601	CHO	C21-C20	-2.72	1.46	1.53
2	A	601	CHO	C6-C5	-2.59	1.49	1.53
2	B	602	CHO	C6-C5	-2.55	1.49	1.53
2	A	602	CHO	C6-C5	-2.53	1.49	1.53
2	A	601	CHO	C18-C13	2.52	1.58	1.54
2	B	601	CHO	C19-C10	2.45	1.58	1.54
2	C	601	CHO	C26-C27	2.35	1.56	1.51
2	B	601	CHO	C1-C2	2.31	1.58	1.53
2	C	602	CHO	C26-C27	2.22	1.55	1.51
2	B	601	CHO	C26-C27	2.19	1.55	1.51
2	B	602	CHO	O24-C24	-2.17	1.18	1.23
2	A	602	CHO	C26-C27	2.17	1.55	1.51
2	B	601	CHO	O24-C24	-2.16	1.18	1.23
2	B	602	CHO	C26-C27	2.13	1.55	1.51
2	A	601	CHO	O24-C24	-2.11	1.19	1.23
2	C	601	CHO	C8-C7	2.06	1.57	1.53
2	A	601	CHO	C26-C27	2.03	1.55	1.51

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	CHO	C5-C6-C7	-16.97	95.73	114.46
2	B	601	CHO	C14-C8-C7	16.24	133.35	111.81
2	B	602	CHO	C15-C14-C8	9.11	131.07	118.33
2	B	602	CHO	C14-C8-C7	9.01	123.76	111.81
2	B	601	CHO	C1-C2-C3	8.96	121.97	110.47
2	A	602	CHO	C14-C8-C7	8.29	122.80	111.81
2	C	602	CHO	C14-C8-C7	8.05	122.48	111.81
2	C	602	CHO	C1-C2-C3	8.03	120.78	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	CHO	C1-C2-C3	7.68	120.32	110.47
2	B	601	CHO	C6-C5-C10	-7.41	104.79	112.66
2	A	601	CHO	C14-C8-C7	7.34	121.54	111.81
2	B	601	CHO	C9-C8-C7	-7.33	103.11	111.88
2	B	602	CHO	C11-C12-C13	7.15	125.05	112.78
2	B	602	CHO	C11-C9-C10	-7.13	105.70	113.91
2	B	601	CHO	O7-C7-C6	7.13	127.62	109.94
2	B	602	CHO	C4-C3-C2	-7.08	102.10	110.55
2	B	602	CHO	C1-C2-C3	7.07	119.54	110.47
2	C	602	CHO	C12-C13-C17	7.01	127.06	116.57
2	C	601	CHO	C12-C13-C17	6.99	127.03	116.57
2	A	602	CHO	C15-C14-C8	6.94	128.03	118.33
2	C	601	CHO	C11-C12-C13	6.93	124.66	112.78
2	A	601	CHO	C10-C9-C8	-6.90	104.41	111.82
2	A	601	CHO	C15-C14-C8	6.88	127.95	118.33
2	B	601	CHO	C4-C5-C10	6.87	119.95	112.66
2	B	601	CHO	C15-C14-C8	6.85	127.90	118.33
2	C	602	CHO	C18-C13-C12	-6.80	99.86	110.59
2	A	601	CHO	C11-C12-C13	6.69	124.26	112.78
2	C	602	CHO	C11-C12-C13	6.65	124.18	112.78
2	A	602	CHO	C4-C3-C2	-6.62	102.65	110.55
2	A	602	CHO	C11-C12-C13	6.61	124.12	112.78
2	A	601	CHO	C15-C14-C13	6.52	111.70	103.84
2	A	602	CHO	C18-C13-C12	-6.45	100.41	110.59
2	C	601	CHO	C14-C8-C7	6.38	120.26	111.81
2	A	601	CHO	C18-C13-C12	-6.28	100.68	110.59
2	A	602	CHO	C1-C2-C3	6.16	118.38	110.47
2	A	602	CHO	C12-C13-C17	6.16	125.79	116.57
2	B	601	CHO	C18-C13-C12	-6.07	101.00	110.59
2	C	601	CHO	C11-C9-C10	-6.00	107.00	113.91
2	B	601	CHO	C11-C12-C13	5.94	122.97	112.78
2	C	602	CHO	C15-C14-C8	5.93	126.62	118.33
2	C	601	CHO	C21-C20-C17	-5.92	103.85	112.92
2	A	601	CHO	C22-C20-C17	5.85	122.37	110.28
2	A	601	CHO	C12-C13-C17	5.82	125.28	116.57
2	C	602	CHO	C10-C9-C8	-5.66	105.74	111.82
2	C	602	CHO	C4-C5-C10	5.63	118.64	112.66
2	B	602	CHO	C18-C13-C12	-5.56	101.82	110.59
2	C	601	CHO	C18-C13-C12	-5.52	101.86	110.59
2	A	602	CHO	C18-C13-C14	-5.51	101.43	111.71
2	C	602	CHO	C15-C14-C13	5.41	110.36	103.84
2	C	601	CHO	C10-C9-C8	-5.34	106.08	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	602	CHO	C10-C9-C8	-5.34	106.09	111.82
2	B	601	CHO	C12-C13-C17	5.30	124.50	116.57
2	B	602	CHO	C18-C13-C14	-5.26	101.90	111.71
2	C	601	CHO	C4-C5-C10	5.22	118.20	112.66
2	C	602	CHO	C5-C6-C7	5.18	120.17	114.46
2	C	602	CHO	C1-C10-C5	5.12	115.34	107.77
2	B	601	CHO	C15-C14-C13	5.10	109.99	103.84
2	C	602	CHO	C18-C13-C14	-5.10	102.20	111.71
2	C	601	CHO	C18-C13-C14	-5.09	102.22	111.71
2	C	601	CHO	C5-C6-C7	5.05	120.04	114.46
2	A	602	CHO	C11-C9-C10	-5.01	108.14	113.91
2	A	601	CHO	C4-C3-C2	-4.99	104.60	110.55
2	B	602	CHO	C12-C13-C17	4.91	123.93	116.57
2	C	602	CHO	C17-C13-C14	4.89	105.87	100.07
2	A	602	CHO	C22-C20-C17	4.87	120.35	110.28
2	A	601	CHO	C18-C13-C14	-4.82	102.72	111.71
2	B	602	CHO	C14-C8-C9	-4.66	103.31	109.71
2	A	602	CHO	C21-C20-C17	-4.63	105.83	112.92
2	C	602	CHO	C5-C4-C3	4.62	119.54	112.76
2	A	602	CHO	C5-C6-C7	4.59	119.53	114.46
2	B	602	CHO	C22-C20-C17	4.54	119.67	110.28
2	B	601	CHO	C22-C20-C17	4.50	119.59	110.28
2	C	601	CHO	C22-C20-C17	4.50	119.58	110.28
2	B	601	CHO	C11-C9-C8	4.50	119.50	111.25
2	B	601	CHO	C6-C5-C4	4.49	116.36	111.19
2	C	601	CHO	C1-C10-C5	4.46	114.37	107.77
2	A	602	CHO	C17-C13-C14	4.43	105.32	100.07
2	B	601	CHO	C1-C10-C5	4.40	114.28	107.77
2	B	602	CHO	C2-C1-C10	4.39	120.31	112.78
2	B	602	CHO	C21-C20-C17	-4.37	106.23	112.92
2	C	601	CHO	C12-C11-C9	4.35	120.65	113.11
2	B	602	CHO	C12-C13-C14	4.32	113.97	107.27
2	C	601	CHO	C5-C4-C3	4.31	119.09	112.76
2	B	602	CHO	C17-C13-C14	4.31	105.18	100.07
2	B	601	CHO	C1-C10-C9	-4.26	104.66	111.35
2	B	601	CHO	C18-C13-C14	-4.17	103.93	111.71
2	C	602	CHO	C21-C20-C22	-4.10	103.94	110.36
2	B	601	CHO	C2-C1-C10	4.10	119.80	112.78
2	C	602	CHO	C19-C10-C9	-4.09	105.55	111.18
2	C	601	CHO	C19-C10-C9	-4.09	105.55	111.18
2	A	602	CHO	C1-C10-C5	4.01	113.70	107.77
2	C	601	CHO	C21-C20-C22	-3.95	104.18	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	CHO	C11-C9-C8	3.91	118.42	111.25
2	A	602	CHO	C21-C20-C22	-3.90	104.24	110.36
2	B	601	CHO	C21-C20-C17	-3.89	106.97	112.92
2	A	602	CHO	C12-C13-C14	3.88	113.30	107.27
2	A	601	CHO	C13-C17-C20	3.87	125.55	119.49
2	C	602	CHO	C2-C1-C10	3.85	119.38	112.78
2	A	601	CHO	C5-C4-C3	3.84	118.39	112.76
2	B	601	CHO	C17-C13-C14	3.82	104.60	100.07
2	C	601	CHO	C2-C1-C10	3.80	119.30	112.78
2	A	601	CHO	C6-C7-C8	3.79	115.53	111.48
2	B	601	CHO	O7-C7-C8	3.76	117.84	109.43
2	B	601	CHO	C23-C24-N25	3.76	122.75	116.42
2	C	602	CHO	C11-C9-C10	-3.70	109.65	113.91
2	C	602	CHO	C9-C10-C5	3.70	113.77	108.58
2	A	602	CHO	C6-C7-C8	3.69	115.42	111.48
2	C	601	CHO	C9-C10-C5	3.67	113.73	108.58
2	A	602	CHO	C12-C11-C9	3.66	119.46	113.11
2	C	602	CHO	C22-C20-C17	3.66	117.84	110.28
2	B	602	CHO	C6-C5-C4	-3.65	106.99	111.19
2	B	602	CHO	C1-C10-C9	-3.63	105.65	111.35
2	A	601	CHO	C5-C6-C7	3.57	118.40	114.46
2	A	601	CHO	C17-C13-C14	3.50	104.22	100.07
2	C	602	CHO	C12-C11-C9	3.47	119.13	113.11
2	B	601	CHO	C12-C13-C14	3.46	112.64	107.27
2	C	601	CHO	C12-C13-C14	3.44	112.61	107.27
2	B	602	CHO	C1-C10-C5	3.44	112.86	107.77
2	C	601	CHO	C15-C14-C8	3.42	123.11	118.33
2	A	601	CHO	C11-C9-C10	-3.41	109.98	113.91
2	A	602	CHO	C11-C9-C8	3.40	117.49	111.25
2	A	602	CHO	C2-C1-C10	3.39	118.60	112.78
2	B	602	CHO	C6-C7-C8	3.39	115.10	111.48
2	B	601	CHO	C12-C11-C9	3.37	118.95	113.11
2	B	602	CHO	C5-C6-C7	3.36	118.17	114.46
2	A	602	CHO	C15-C14-C13	3.34	107.87	103.84
2	A	601	CHO	C14-C8-C9	-3.33	105.14	109.71
2	B	602	CHO	C23-C24-N25	3.29	121.96	116.42
2	B	602	CHO	C12-C11-C9	3.28	118.81	113.11
2	B	601	CHO	C19-C10-C1	-3.26	103.01	108.26
2	B	601	CHO	C19-C10-C5	3.24	115.86	110.36
2	C	602	CHO	C11-C9-C8	3.23	117.17	111.25
2	A	601	CHO	C9-C10-C5	3.22	113.11	108.58
2	A	602	CHO	C6-C5-C4	-3.18	107.53	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	CHO	C12-C11-C9	3.17	118.60	113.11
2	A	601	CHO	C12-C13-C14	3.15	112.16	107.27
2	C	602	CHO	C21-C20-C17	-3.03	108.29	112.92
2	B	602	CHO	C21-C20-C22	-3.01	105.65	110.36
2	A	602	CHO	C14-C8-C9	-2.99	105.61	109.71
2	A	601	CHO	C6-C5-C4	-2.91	107.83	111.19
2	B	601	CHO	C13-C14-C8	-2.88	110.11	113.98
2	A	601	CHO	C13-C14-C8	-2.86	110.13	113.98
2	B	601	CHO	C10-C9-C8	-2.84	108.77	111.82
2	C	602	CHO	C6-C7-C8	2.83	114.50	111.48
2	B	601	CHO	C6-C7-C8	-2.83	108.46	111.48
2	C	601	CHO	C6-C7-C8	2.80	114.47	111.48
2	A	601	CHO	C1-C10-C9	-2.78	106.98	111.35
2	B	601	CHO	C21-C20-C22	-2.78	106.01	110.36
2	B	602	CHO	C19-C10-C1	-2.76	103.82	108.26
2	A	602	CHO	C1-C10-C9	-2.75	107.03	111.35
2	C	601	CHO	C23-C24-N25	2.74	121.04	116.42
2	A	601	CHO	C9-C8-C7	2.69	115.09	111.88
2	B	601	CHO	C16-C17-C13	2.67	107.06	103.84
2	C	602	CHO	C12-C13-C14	2.65	111.38	107.27
2	B	602	CHO	C16-C17-C20	2.60	116.17	112.15
2	A	601	CHO	C21-C20-C17	-2.52	109.06	112.92
2	C	602	CHO	O7-C7-C6	-2.47	103.83	109.94
2	A	601	CHO	O7-C7-C6	-2.45	103.87	109.94
2	C	601	CHO	C11-C9-C8	2.38	115.62	111.25
2	C	602	CHO	OT2-C27-C26	2.34	120.88	112.74
2	B	601	CHO	C14-C8-C9	-2.32	106.52	109.71
2	C	602	CHO	C6-C5-C4	-2.31	108.53	111.19
2	C	602	CHO	C22-C23-C24	2.30	118.18	113.04
2	B	601	CHO	OT2-C27-C26	2.29	120.69	112.74
2	C	602	CHO	C1-C10-C9	-2.21	107.87	111.35
2	C	601	CHO	C17-C13-C14	2.20	102.68	100.07
2	C	602	CHO	C13-C14-C8	-2.20	111.02	113.98
2	C	601	CHO	O24-C24-N25	-2.20	118.86	123.01
2	C	602	CHO	C18-C13-C17	-2.20	107.61	111.71
2	C	601	CHO	C6-C5-C4	-2.19	108.67	111.19
2	B	602	CHO	O24-C24-N25	-2.19	118.89	123.01
2	A	601	CHO	C19-C10-C9	-2.19	108.17	111.18
2	A	601	CHO	C21-C20-C22	-2.18	106.95	110.36
2	A	601	CHO	C23-C24-N25	2.18	120.09	116.42
2	B	601	CHO	O24-C24-C23	-2.16	118.07	122.02
2	B	602	CHO	C18-C13-C17	-2.15	107.70	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	602	CHO	C18-C13-C17	-2.14	107.73	111.71
2	C	601	CHO	O7-C7-C6	-2.11	104.71	109.94
2	C	602	CHO	O24-C24-N25	-2.11	119.04	123.01
2	A	602	CHO	OT2-C27-C26	2.10	120.03	112.74
2	C	601	CHO	OT2-C27-C26	2.07	119.93	112.74
2	C	601	CHO	C18-C13-C17	-2.05	107.89	111.71
2	B	601	CHO	O24-C24-N25	-2.03	119.17	123.01
2	A	602	CHO	O7-C7-C6	-2.01	104.96	109.94

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	CHO	C13-C17-C20-C22
2	A	602	CHO	C13-C17-C20-C21
2	A	602	CHO	C13-C17-C20-C22
2	A	602	CHO	C16-C17-C20-C21
2	A	602	CHO	C16-C17-C20-C22
2	B	602	CHO	C13-C17-C20-C22
2	B	602	CHO	C16-C17-C20-C22
2	C	601	CHO	C13-C17-C20-C22
2	C	601	CHO	C16-C17-C20-C22
2	C	601	CHO	N25-C26-C27-OT1
2	C	601	CHO	N25-C26-C27-OT2
2	C	602	CHO	C20-C22-C23-C24
2	B	602	CHO	C16-C17-C20-C21
2	C	602	CHO	C16-C17-C20-C21
2	B	602	CHO	C13-C17-C20-C21
2	C	602	CHO	C13-C17-C20-C21
2	B	601	CHO	C13-C17-C20-C22
2	B	601	CHO	C16-C17-C20-C21
2	C	601	CHO	C16-C17-C20-C21
2	A	601	CHO	C13-C17-C20-C21
2	B	601	CHO	C13-C17-C20-C21
2	C	601	CHO	C13-C17-C20-C21
2	A	601	CHO	C16-C17-C20-C22
2	C	602	CHO	C13-C17-C20-C22
2	A	601	CHO	C23-C24-N25-C26
2	A	602	CHO	C23-C24-N25-C26
2	B	601	CHO	C23-C24-N25-C26
2	B	602	CHO	C23-C24-N25-C26
2	C	601	CHO	C23-C24-N25-C26

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Mol	Chain	Res	Type	Atoms
2	C	602	CHO	C23-C24-N25-C26
2	A	601	CHO	C16-C17-C20-C21
2	B	601	CHO	C16-C17-C20-C22
2	C	602	CHO	C16-C17-C20-C22
2	A	602	CHO	C17-C20-C22-C23
2	C	601	CHO	C17-C20-C22-C23
2	A	602	CHO	C21-C20-C22-C23
2	A	601	CHO	O24-C24-N25-C26
2	A	602	CHO	O24-C24-N25-C26
2	B	601	CHO	O24-C24-N25-C26
2	B	602	CHO	O24-C24-N25-C26
2	C	601	CHO	O24-C24-N25-C26
2	C	602	CHO	O24-C24-N25-C26
2	A	602	CHO	N25-C26-C27-OT1
2	C	601	CHO	C21-C20-C22-C23
2	A	602	CHO	N25-C26-C27-OT2
2	B	601	CHO	N25-C26-C27-OT1
2	B	601	CHO	N25-C26-C27-OT2
2	C	602	CHO	N25-C26-C27-OT1
2	C	602	CHO	N25-C26-C27-OT2
2	A	602	CHO	C20-C22-C23-C24
2	C	602	CHO	C27-C26-N25-C24

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	CHO	C10-C5-C6-C7-C8-C9

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	602	CHO	4	0
2	B	602	CHO	1	0
2	C	601	CHO	2	0
2	A	602	CHO	5	0
2	B	601	CHO	2	0
2	A	601	CHO	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 then 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.

Ligand CHO C 602

Bond lengths

Bond angles

Torsions

Rings

Ligand CHO B 602

Bond lengths

Bond angles

Torsions

Rings

Ligand CHO C 601

Bond lengths

Bond angles

Torsions

Rings

Ligand CHO A 602

Bond lengths

Bond angles

Torsions

Rings

Ligand CHO B 601

Bond lengths

Bond angles

Torsions

Rings

Ligand CHO A 601

Bond lengths

Bond angles

Torsions

Rings
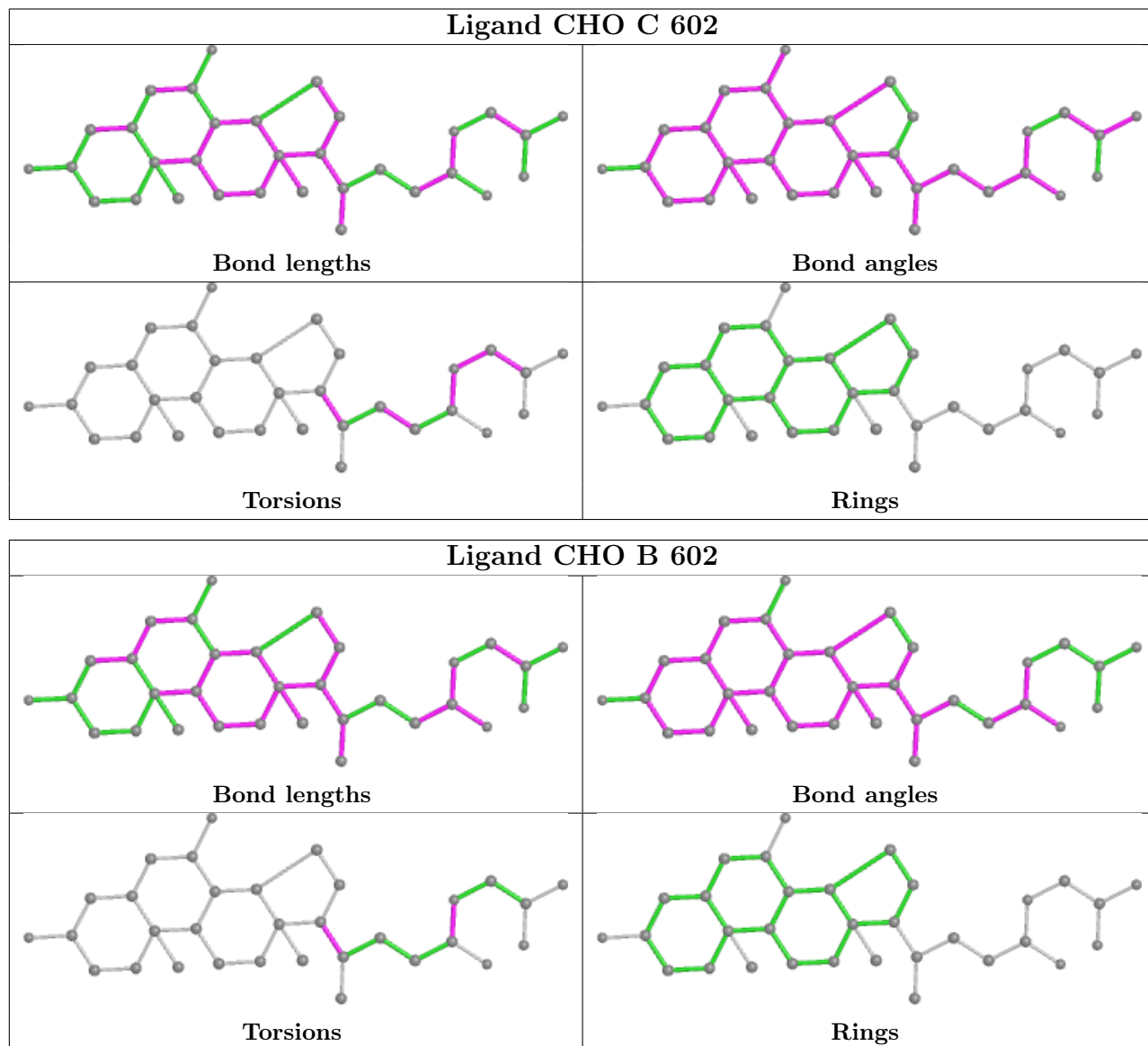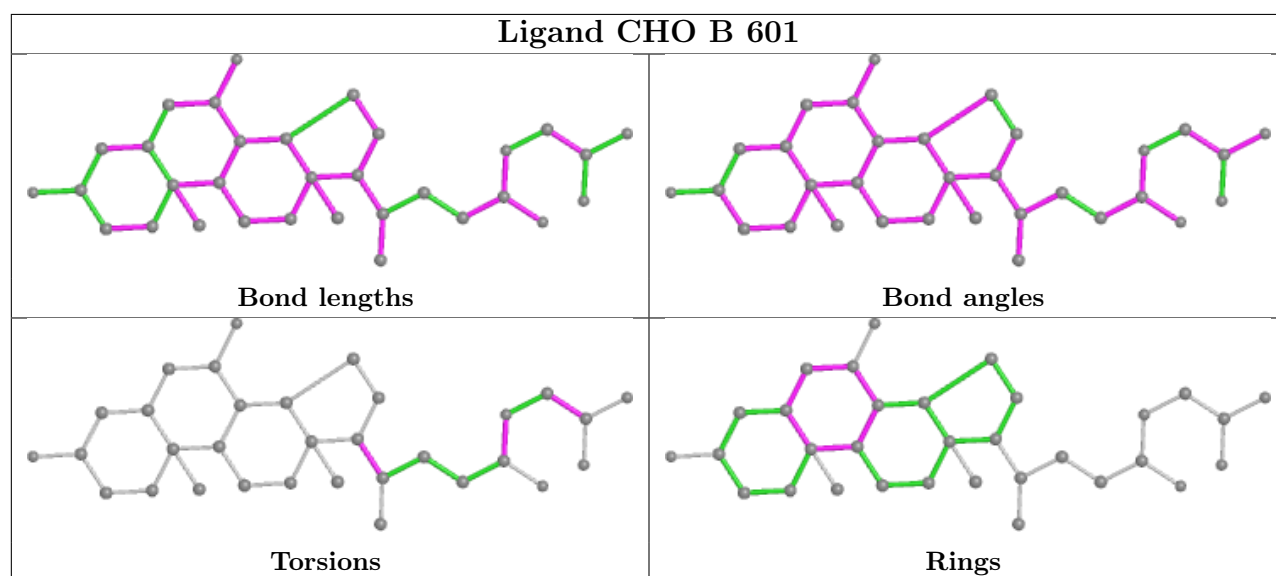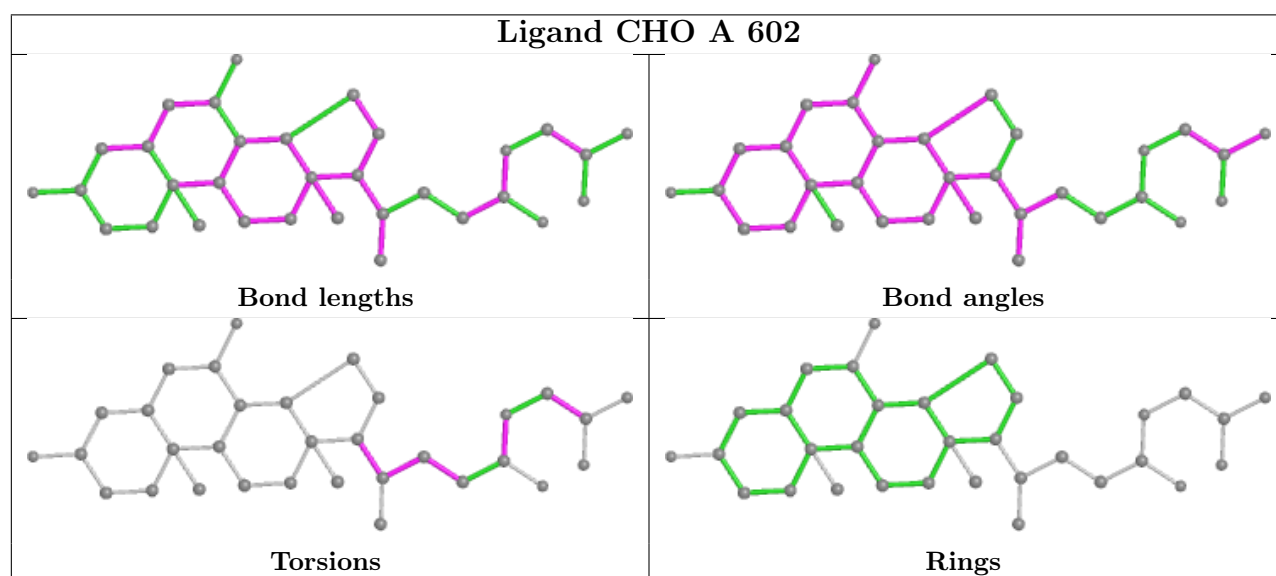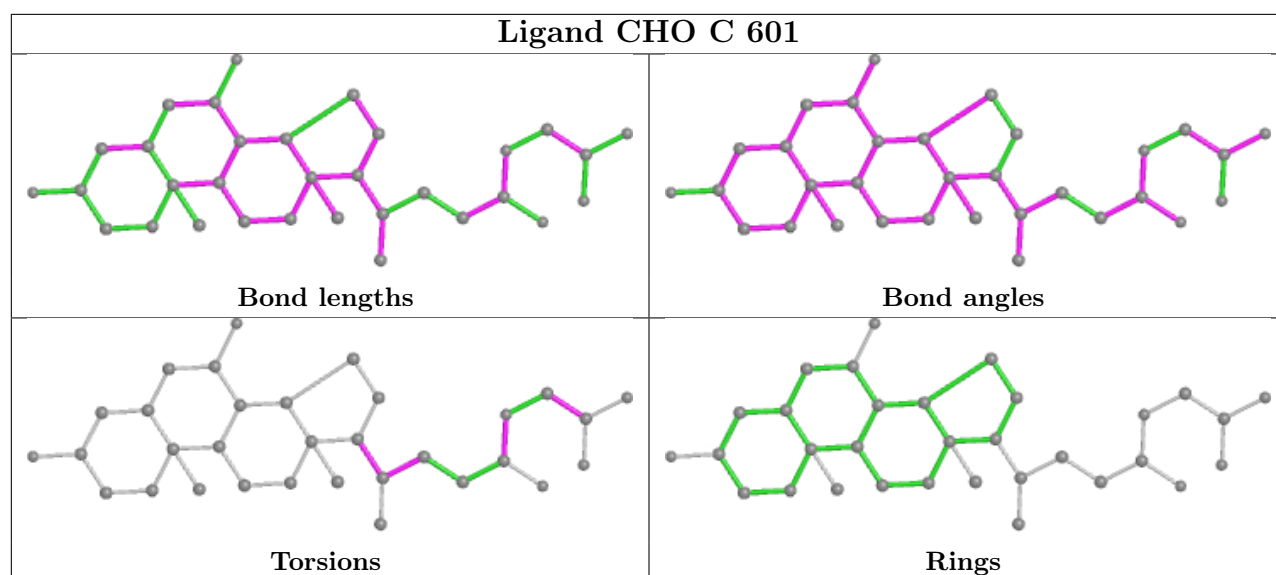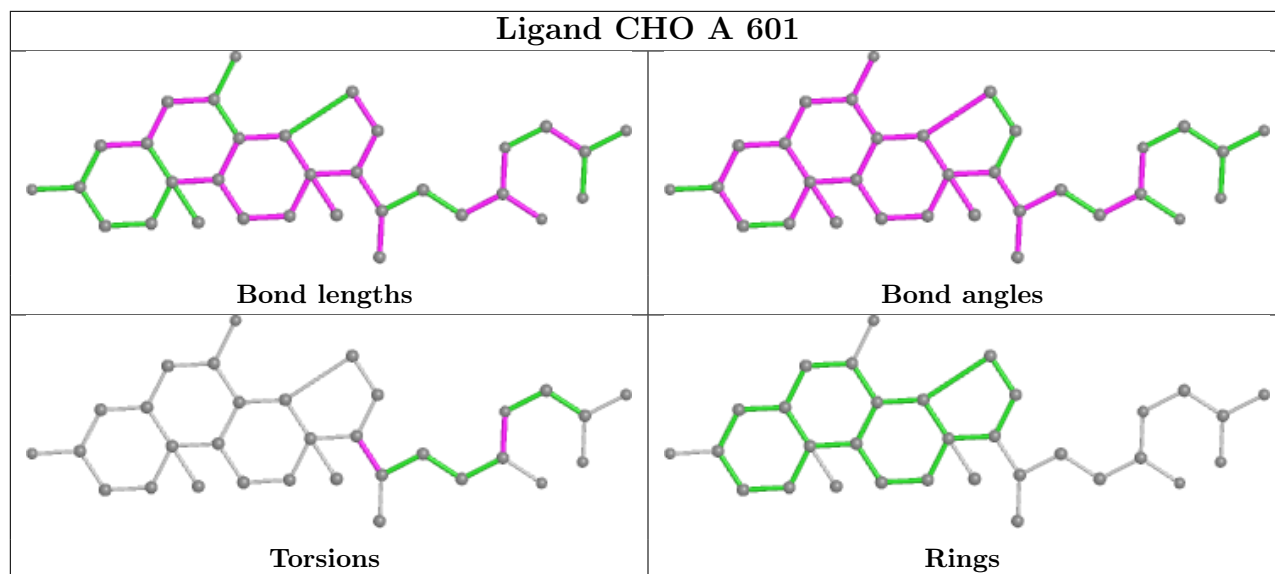
5.7　Other polymers　ⓘ

There are no such residues in this entry.

5.8　Polymer linkage issues　ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	8
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	296:GLU	C	297:PHE	N	5.93
1	A	223:GLU	C	224:ARG	N	2.94
1	A	224:ARG	C	225:THR	N	2.82
1	A	19:GLN	C	20:ASP	N	2.21
1	A	225:THR	C	226:ILE	N	2.00
1	C	224:ARG	C	225:THR	N	1.86
1	A	22:VAL	C	23:PRO	N	1.72
1	C	225:THR	C	226:ILE	N	1.70
1	A	23:PRO	C	24:ALA	N	1.62
1	A	24:ALA	C	25:ALA	N	1.01

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-20250. 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 ⓘ

6.1.1 Primary map

| X | Y | Z |
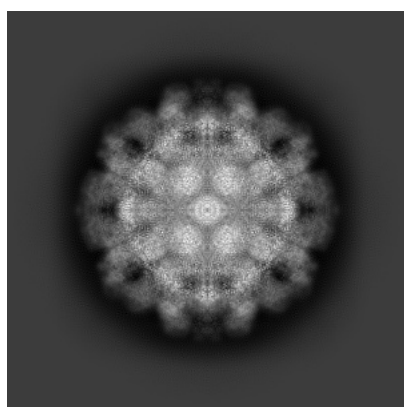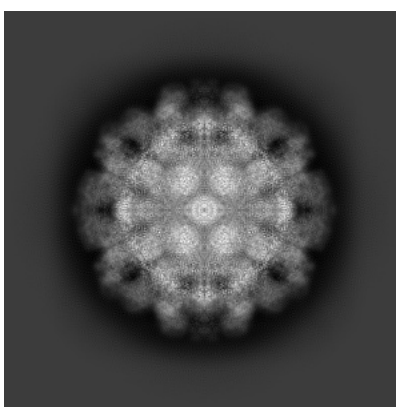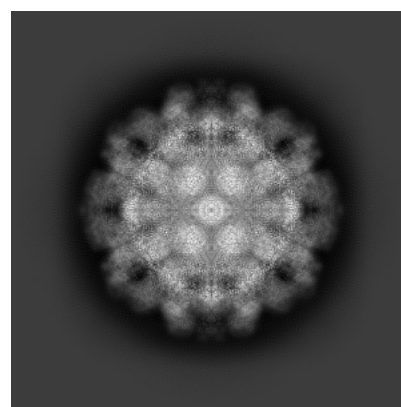
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
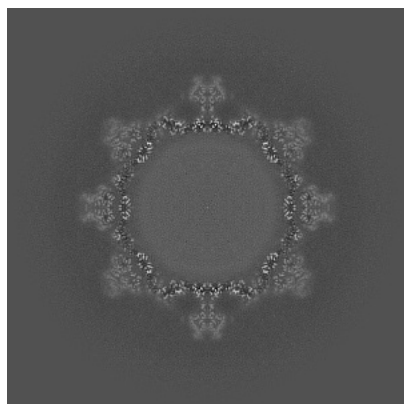
6.2.1 Primary map
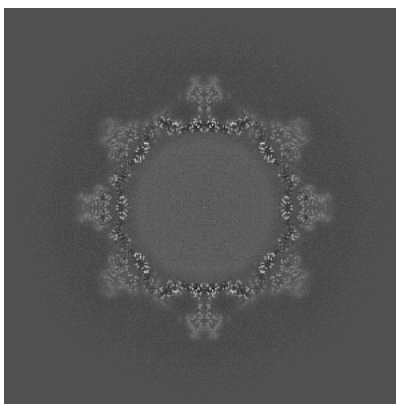
X Index: 275   Y Index: 275   Z Index: 275
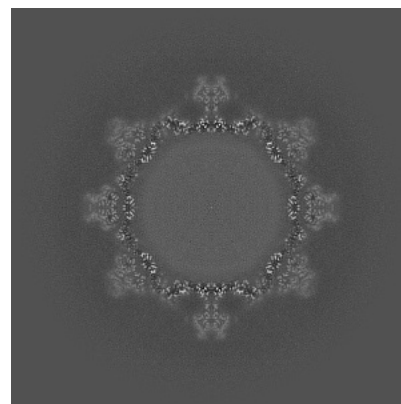
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
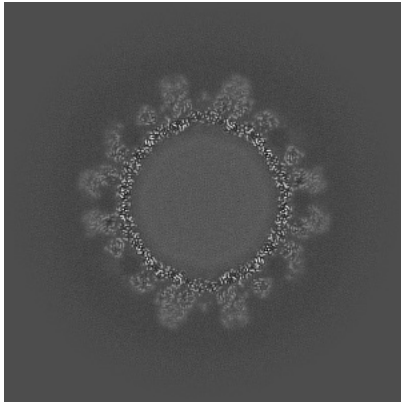
6.3.1 Primary map
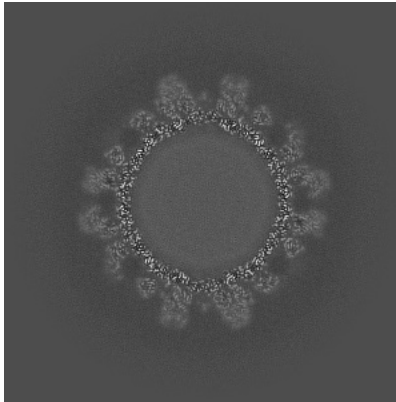
| X Index: 304 | Y Index: 246 | Z Index: 304 |
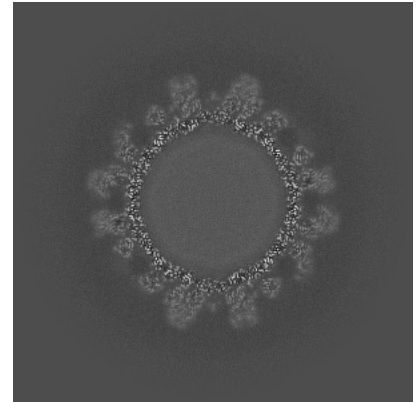
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map

| X | Y | Z |
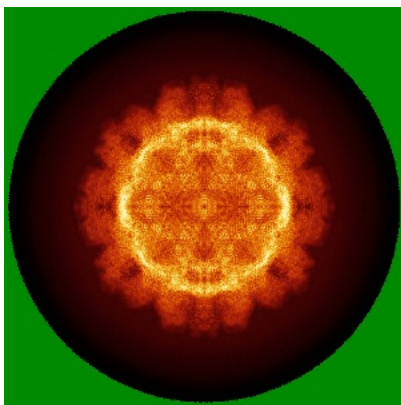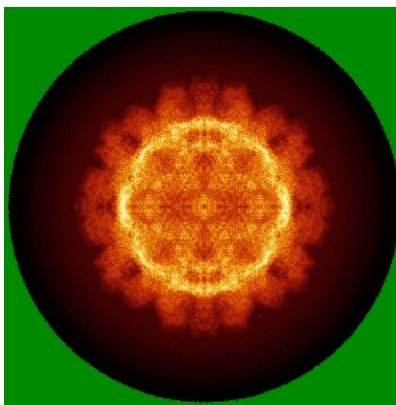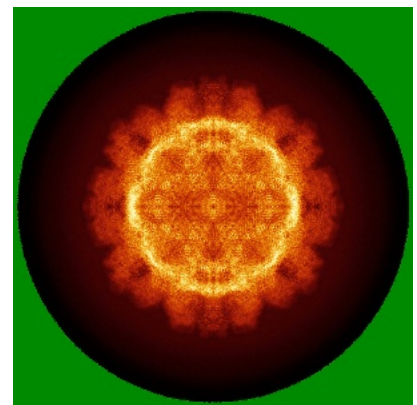
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X	Y	Z
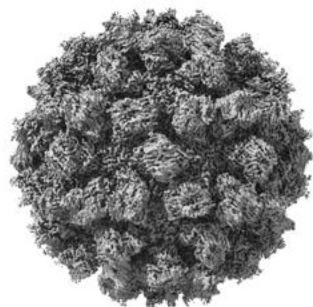
The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 Mask visualisation ⓘ

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

7　Map analysis ⓘ

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

7.1　Map-value distribution ⓘ

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 ⓘ
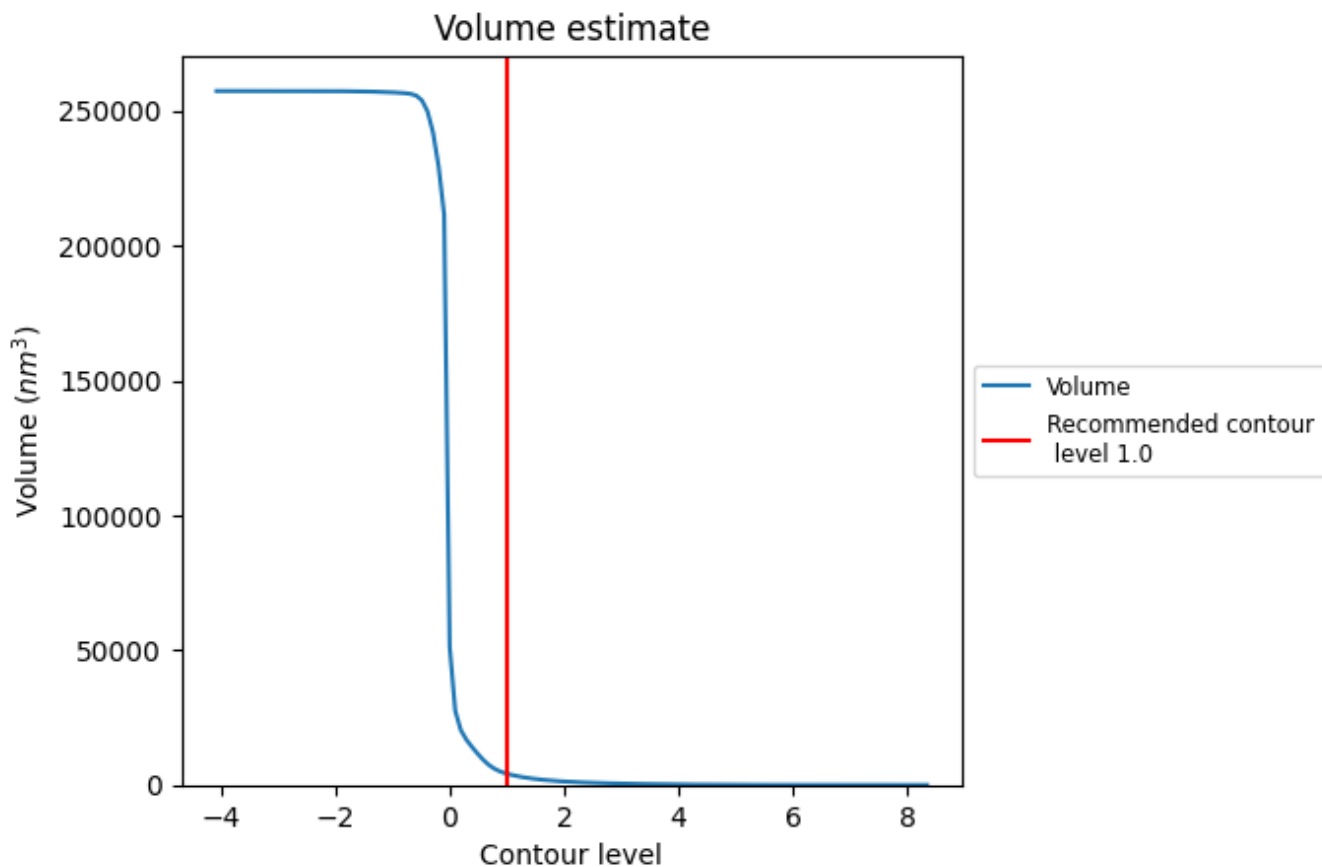
The volume at the recommended contour level is 4184 nm³; this corresponds to an approximate mass of 3779 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3　Rotationally averaged power spectrum ⓘ
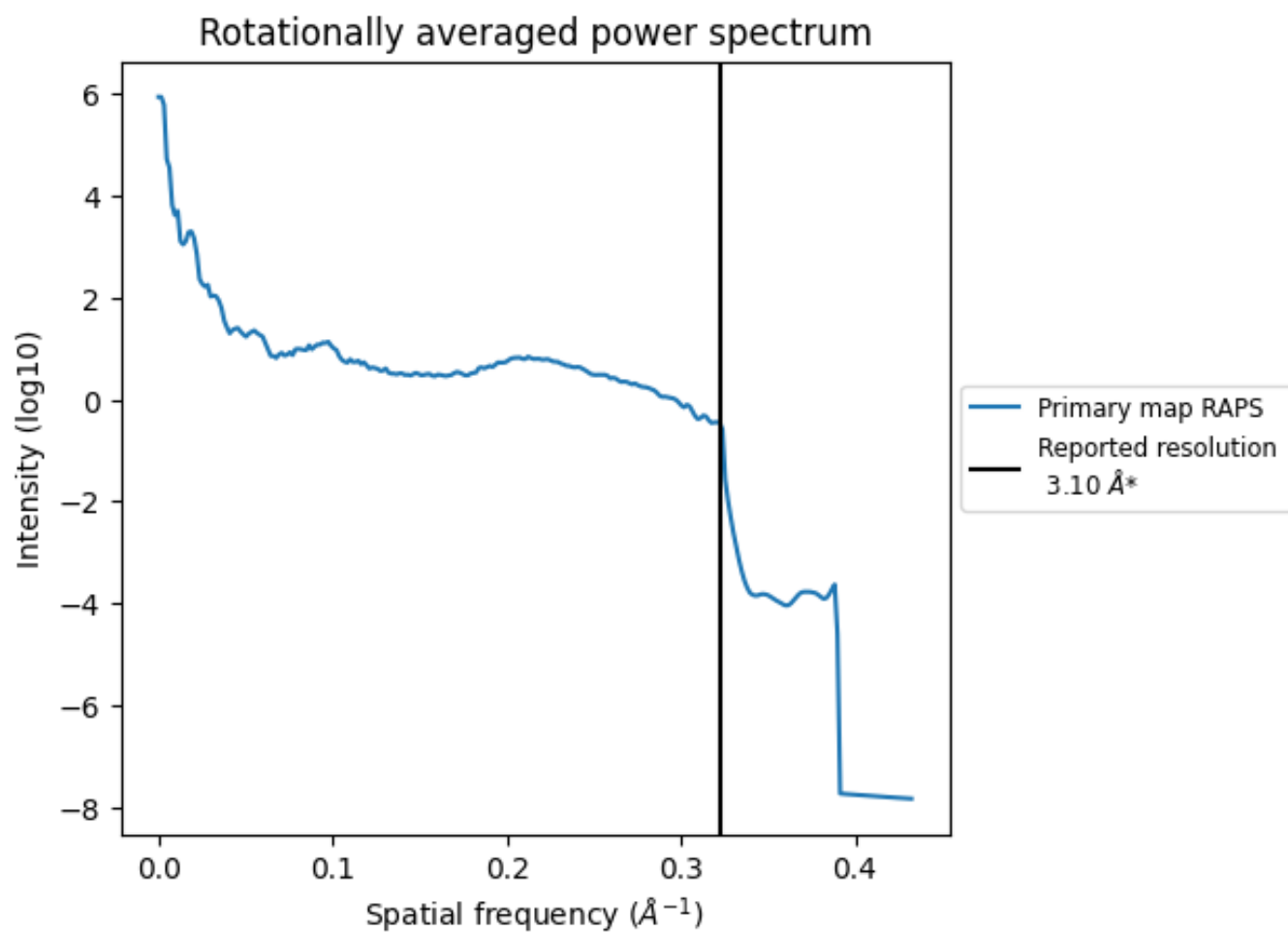
*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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-20250 and PDB model 6P4J. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

9.1.1 Map-model overlay (i)

| X | Y | Z |
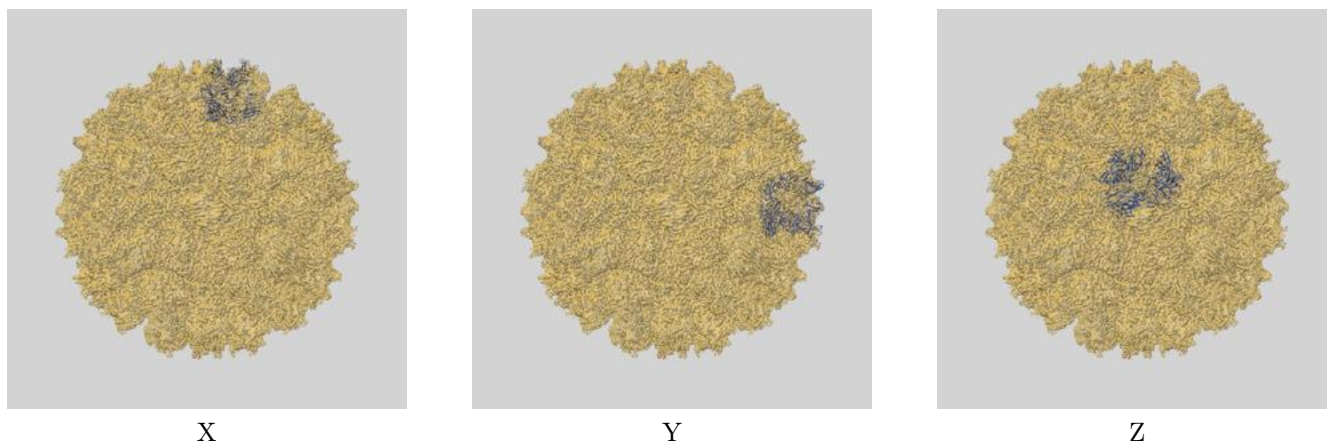
9.1.2 Map-model assembly overlay (i)

| X | Y | Z |
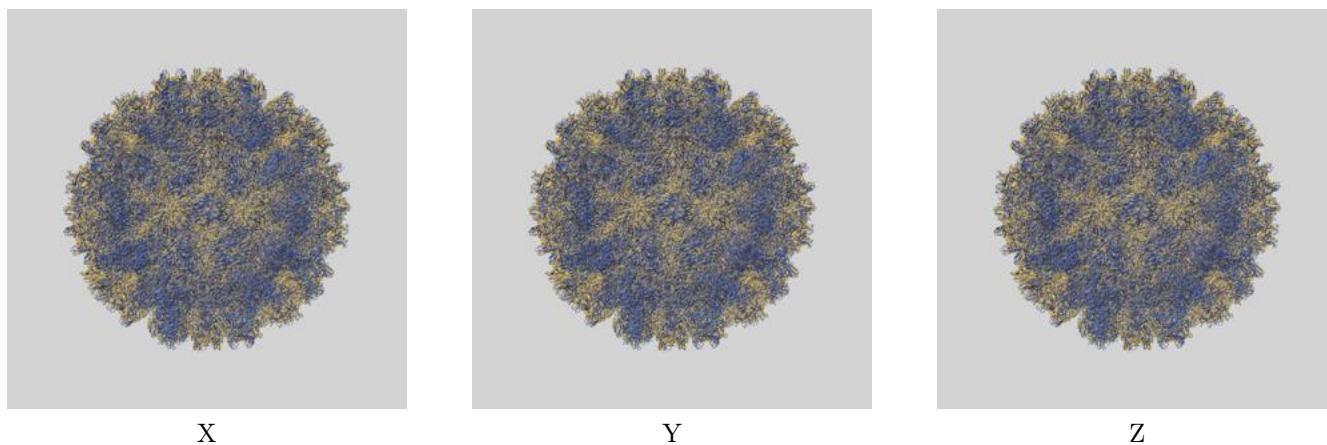
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

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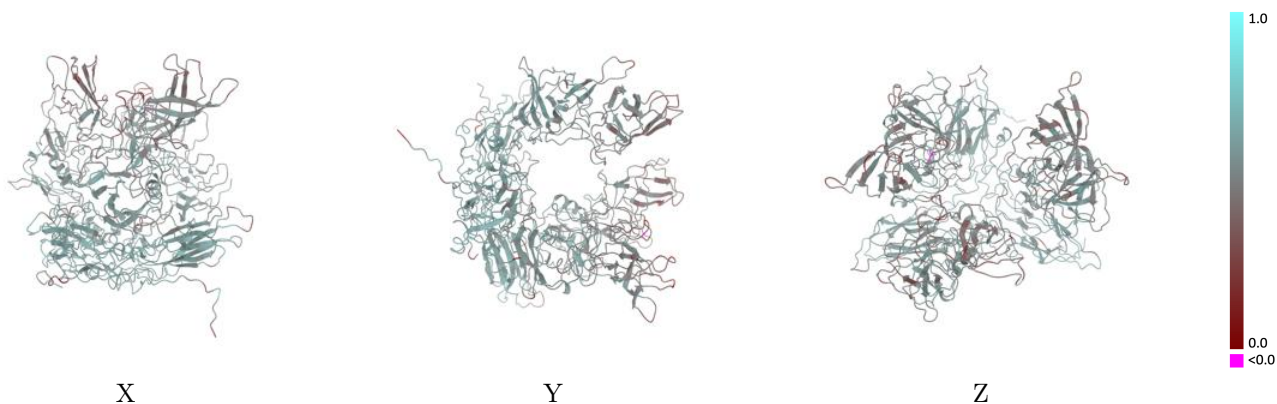
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z
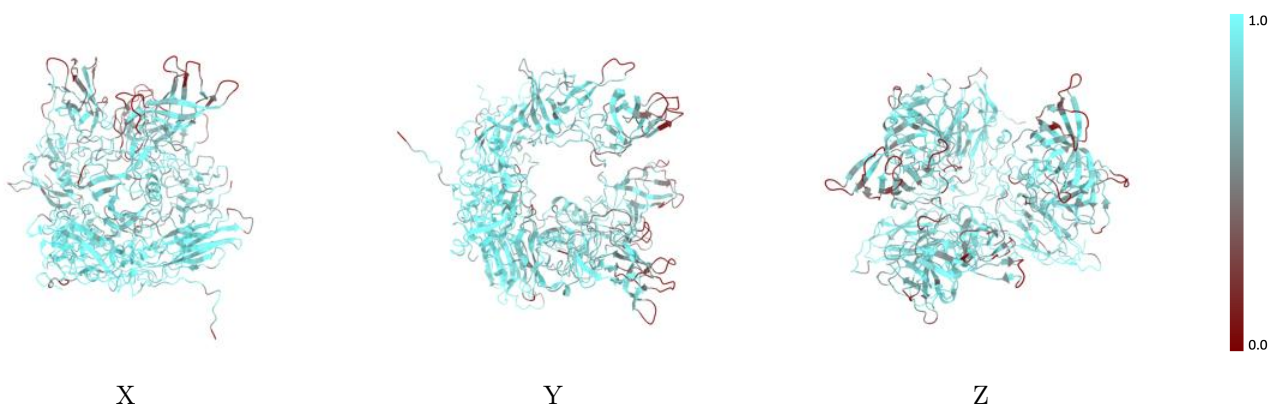
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.0).

9.4 Atom inclusion ⓘ
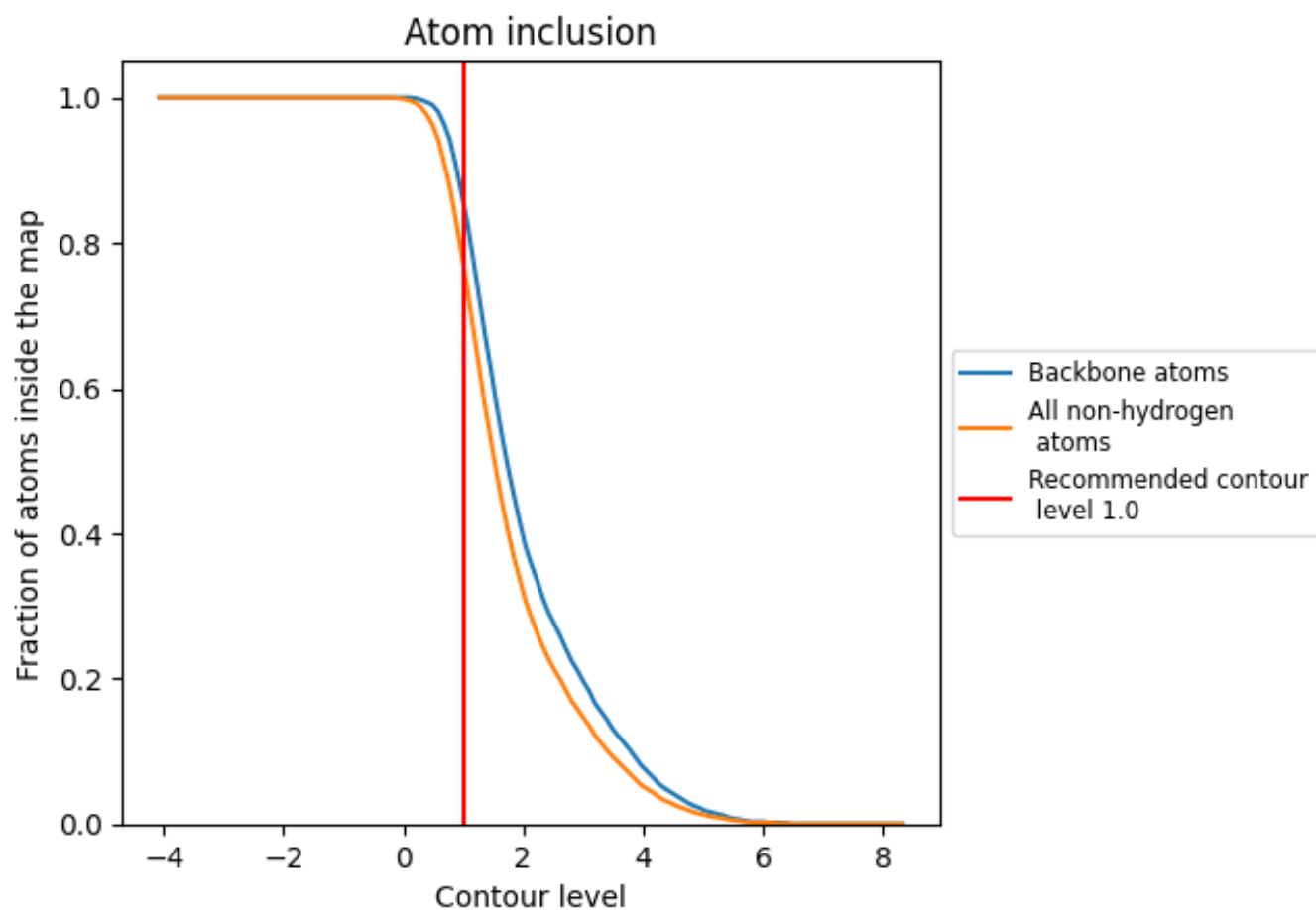
At the recommended contour level, 86% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7730	0.5220
A	0.7520	0.5200
B	0.7750	0.5270
C	0.7930	0.5200

1.0

0.0
<0.0