



## Full wwPDB EM Validation Report ⓘ

May 20, 2026 – 08:01 PM JST

PDB ID : 9WQK / pdb\_00009wqk  
EMDB ID : EMD-66174  
Title : GRM5-Gi Complex Structure  
Authors : Lu, Y.; Wen, T.L.; Shen, Y.Q.; Yang, X.  
Deposited on : 2025-09-11  
Resolution : 3.70 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>.

---

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

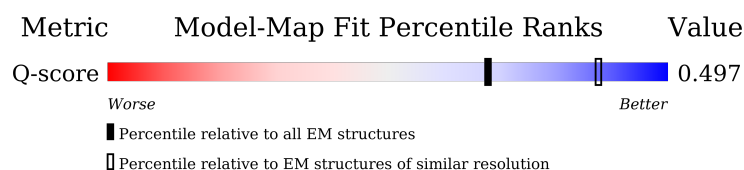
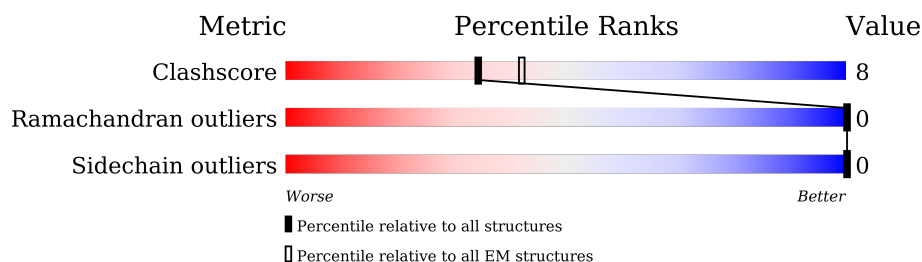
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*




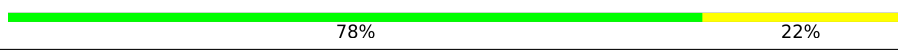
The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 ( 3.20 - 4.20 )

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	X	850	
1	Y	850	
2	A	354	
3	B	340	

*Continued on next page...*

Mol	Chain	Length	Quality of chain
4	G	80	
5	F	260	

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 19277 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 Metabotropic glutamate receptor 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	791	Total	C	N	O	S	0	0
			6211	3988	1038	1126	59		
1	Y	771	Total	C	N	O	S	0	0
			6081	3910	1009	1104	58		

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-10	MET	-	initiating methionine	UNP P41594
X	-9	TRP	-	expression tag	UNP P41594
X	-8	SER	-	expression tag	UNP P41594
X	-7	HIS	-	expression tag	UNP P41594
X	-6	PRO	-	expression tag	UNP P41594
X	-5	GLN	-	expression tag	UNP P41594
X	-4	PHE	-	expression tag	UNP P41594
X	-3	GLU	-	expression tag	UNP P41594
X	-2	LYS	-	expression tag	UNP P41594
X	-1	GLY	-	expression tag	UNP P41594
X	0	GLY	-	expression tag	UNP P41594
X	1	GLY	-	expression tag	UNP P41594
X	2	SER	-	expression tag	UNP P41594
X	3	GLY	-	expression tag	UNP P41594
X	4	GLY	-	expression tag	UNP P41594
X	5	GLY	-	expression tag	UNP P41594
X	6	SER	-	expression tag	UNP P41594
X	7	GLY	-	expression tag	UNP P41594
X	8	GLY	-	expression tag	UNP P41594
X	9	SER	-	expression tag	UNP P41594
X	10	ALA	-	expression tag	UNP P41594
X	11	TRP	-	expression tag	UNP P41594
X	12	SER	-	expression tag	UNP P41594
X	13	HIS	-	expression tag	UNP P41594
X	14	PRO	-	expression tag	UNP P41594
X	15	GLN	-	expression tag	UNP P41594

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
X	16	PHE	-	expression tag	UNP P41594
X	17	GLU	-	expression tag	UNP P41594
X	18	LYS	-	expression tag	UNP P41594
X	19	GLY	-	expression tag	UNP P41594
X	20	SER	-	expression tag	UNP P41594
Y	-10	MET	-	initiating methionine	UNP P41594
Y	-9	TRP	-	expression tag	UNP P41594
Y	-8	SER	-	expression tag	UNP P41594
Y	-7	HIS	-	expression tag	UNP P41594
Y	-6	PRO	-	expression tag	UNP P41594
Y	-5	GLN	-	expression tag	UNP P41594
Y	-4	PHE	-	expression tag	UNP P41594
Y	-3	GLU	-	expression tag	UNP P41594
Y	-2	LYS	-	expression tag	UNP P41594
Y	-1	GLY	-	expression tag	UNP P41594
Y	0	GLY	-	expression tag	UNP P41594
Y	1	GLY	-	expression tag	UNP P41594
Y	2	SER	-	expression tag	UNP P41594
Y	3	GLY	-	expression tag	UNP P41594
Y	4	GLY	-	expression tag	UNP P41594
Y	5	GLY	-	expression tag	UNP P41594
Y	6	SER	-	expression tag	UNP P41594
Y	7	GLY	-	expression tag	UNP P41594
Y	8	GLY	-	expression tag	UNP P41594
Y	9	SER	-	expression tag	UNP P41594
Y	10	ALA	-	expression tag	UNP P41594
Y	11	TRP	-	expression tag	UNP P41594
Y	12	SER	-	expression tag	UNP P41594
Y	13	HIS	-	expression tag	UNP P41594
Y	14	PRO	-	expression tag	UNP P41594
Y	15	GLN	-	expression tag	UNP P41594
Y	16	PHE	-	expression tag	UNP P41594
Y	17	GLU	-	expression tag	UNP P41594
Y	18	LYS	-	expression tag	UNP P41594
Y	19	GLY	-	expression tag	UNP P41594
Y	20	SER	-	expression tag	UNP P41594

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	225	Total	C	N	O	S	0	0
			1778	1128	296	342	12		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ASN	SER	conflict	UNP P63096
A	203	ALA	GLY	conflict	UNP P63096
A	245	ALA	GLU	conflict	UNP P63096
A	326	SER	ALA	conflict	UNP P63096

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	338	Total	C	N	O	S	0	0
			2601	1604	467	509	21		

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	59	Total	C	N	O	S	0	0
			440	276	76	85	3		

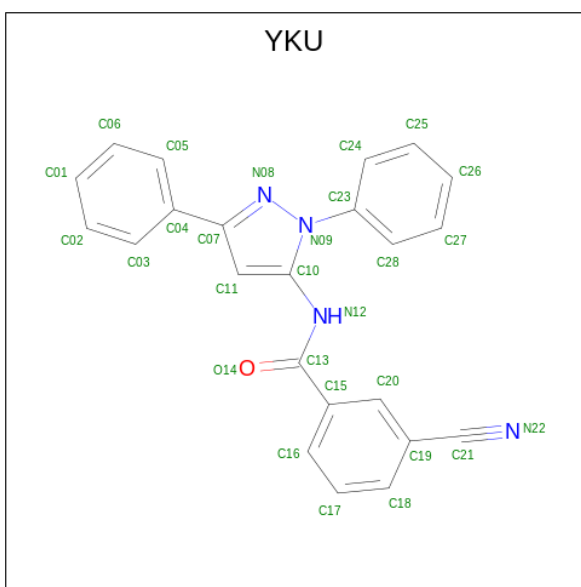
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	72	GLY	-	expression tag	UNP P59768
G	73	SER	-	expression tag	UNP P59768
G	74	ALA	-	expression tag	UNP P59768
G	75	GLY	-	expression tag	UNP P59768
G	76	SER	-	expression tag	UNP P59768
G	77	ALA	-	expression tag	UNP P59768
G	78	GLY	-	expression tag	UNP P59768
G	79	SER	-	expression tag	UNP P59768
G	80	ALA	-	expression tag	UNP P59768

- Molecule 5 is a protein called scFv16.

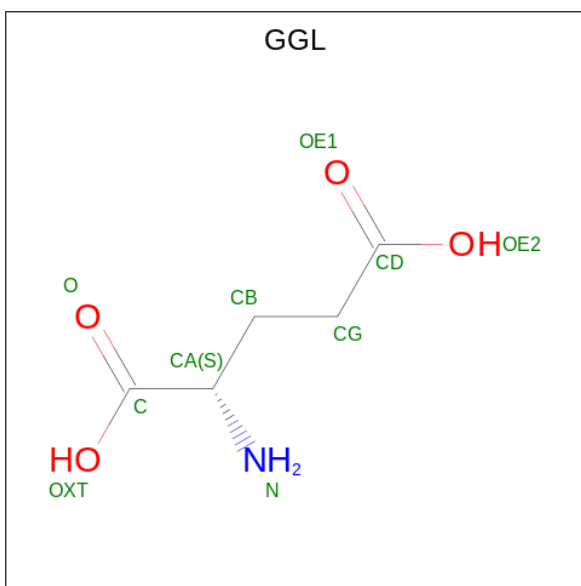
Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	234	Total	C	N	O	S	0	0
			1780	1130	294	346	10		

- Molecule 6 is 3-cyano-N-(1,3-diphenyl-1H-pyrazol-5-yl)benzamide (CCD ID: YKU) (formula: C<sub>23</sub>H<sub>16</sub>N<sub>4</sub>O).



Mol	Chain	Residues	Atoms				AltConf
6	X	1	Total	C	N	O	0
			28	23	4	1	

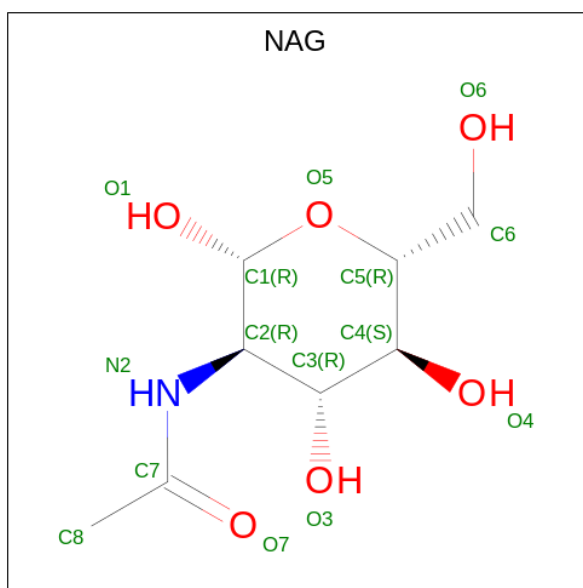
- Molecule 7 is GAMMA-L-GLUTAMIC ACID (CCD ID: GGL) (formula:  $C_5H_9NO_4$ ).



Mol	Chain	Residues	Atoms				AltConf
7	X	1	Total	C	N	O	0
			10	5	1	4	
7	Y	1	Total	C	N	O	0
			10	5	1	4	

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



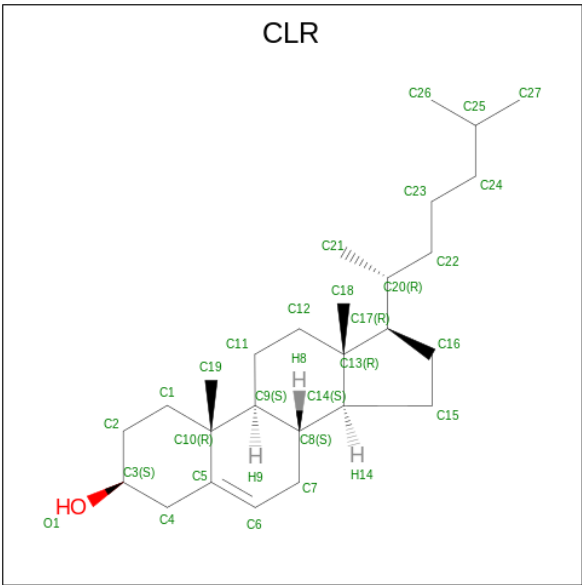
Mol	Chain	Residues	Atoms				AltConf
8	X	1	Total	C	N	O	0
			14	8	1	5	
8	X	1	Total	C	N	O	0
			14	8	1	5	
8	X	1	Total	C	N	O	0
			14	8	1	5	
8	X	1	Total	C	N	O	0
			14	8	1	5	
8	Y	1	Total	C	N	O	0
			14	8	1	5	
8	Y	1	Total	C	N	O	0
			14	8	1	5	
8	Y	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
9	X	1	Total	Cl	0
			1	1	
9	Y	1	Total	Cl	0
			1	1	

- Molecule 10 is CHOLESTEROL (CCD ID: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



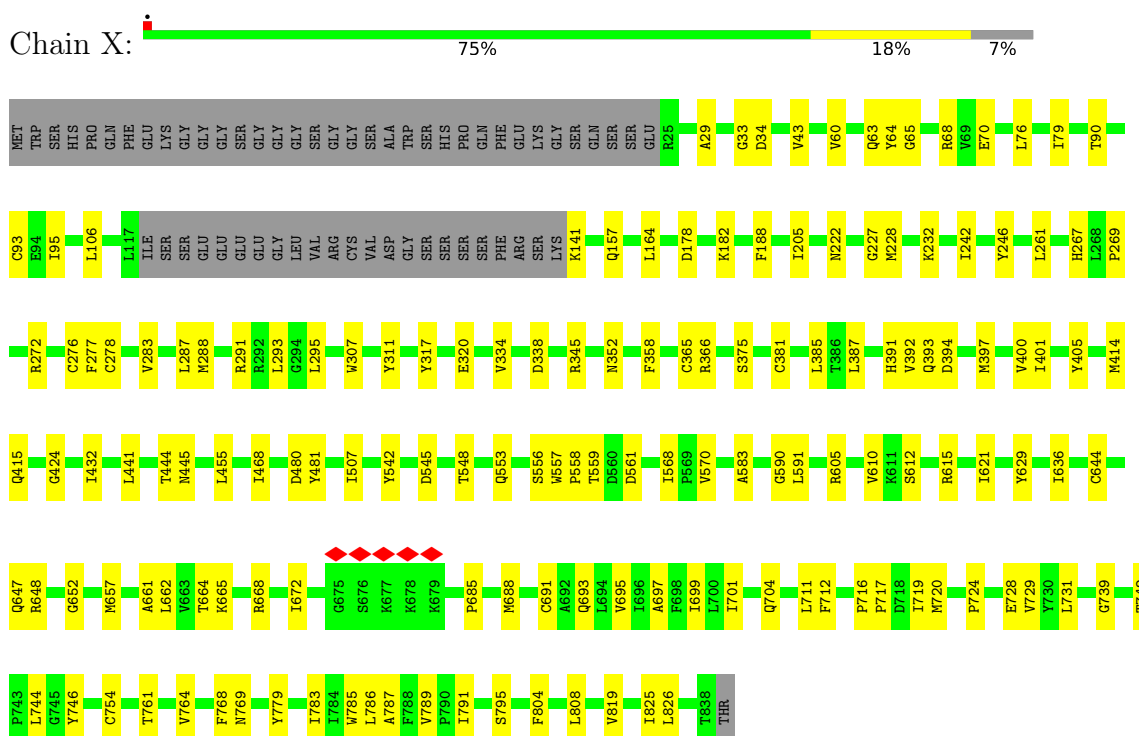


Mol	Chain	Residues	Atoms			AltConf
10	X	1	Total	C	O	0
			28	27	1	
10	X	1	Total	C	O	0
			28	27	1	
10	X	1	Total	C	O	0
			28	27	1	
10	X	1	Total	C	O	0
			28	27	1	
10	Y	1	Total	C	O	0
			28	27	1	
10	Y	1	Total	C	O	0
			28	27	1	
10	Y	1	Total	C	O	0
			28	27	1	
10	Y	1	Total	C	O	0
			28	27	1	

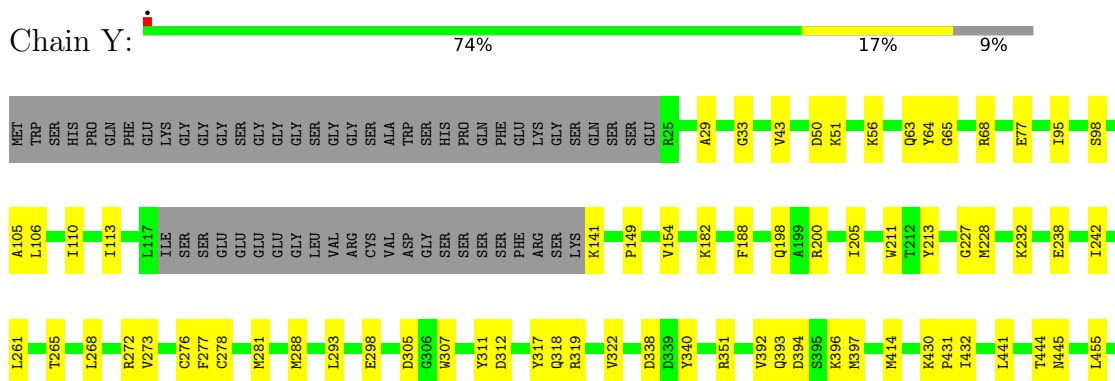
### 3 Residue-property plots [i](#)

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

#### • Molecule 1: Metabotropic glutamate receptor 5

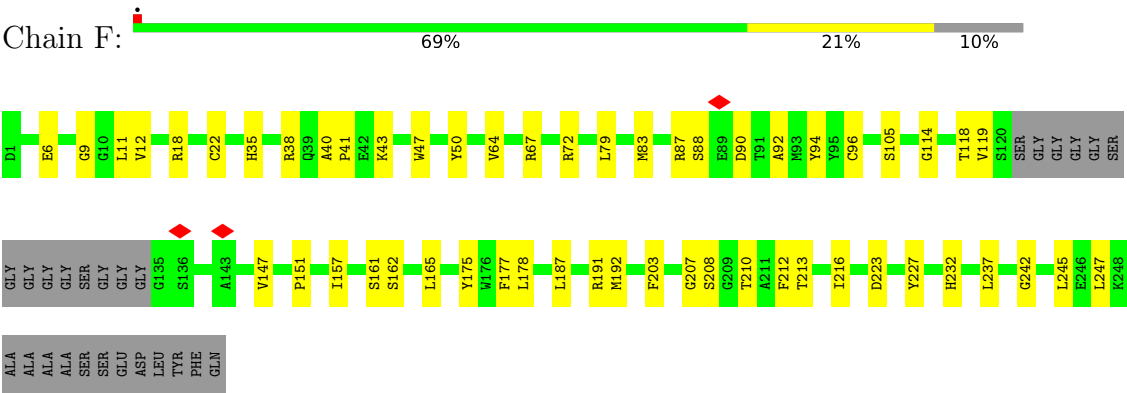


#### • Molecule 1: Metabotropic glutamate receptor 5





● Molecule 5: scFv16



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	161016	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	6000	Depositor
Maximum defocus (nm)	19000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.030	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0027	Depositor
Map size ( $\text{\AA}$ )	357.12, 357.12, 357.12	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.93, 0.93, 0.93	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: CL, GGL, YKU, NAG, CLR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	X	0.23	0/6354	0.29	0/8611
1	Y	0.23	0/6222	0.29	0/8431
2	A	0.14	0/1808	0.27	0/2431
3	B	0.20	0/2648	0.31	0/3589
4	G	0.13	0/446	0.19	0/604
5	F	0.20	0/1824	0.32	0/2475
All	All	0.21	0/19302	0.29	0/26141

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	6211	0	6184	93	0
1	Y	6081	0	6057	90	0
2	A	1778	0	1721	22	0
3	B	2601	0	2505	52	0
4	G	440	0	441	6	0
5	F	1780	0	1705	36	0
6	X	28	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	X	10	0	7	0	0
7	Y	10	0	7	1	0
8	X	56	0	52	0	0
8	Y	56	0	52	1	0
9	X	1	0	0	0	0
9	Y	1	0	0	1	0
10	X	112	0	184	13	0
10	Y	112	0	184	23	0
All	All	19277	0	19099	309	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (309) 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)
5:F:227:TYR:O	5:F:242:GLY:HA2	1.77	0.85
5:F:92:ALA:HB3	5:F:94:TYR:HE1	1.49	0.77
1:X:761:THR:O	1:X:769:ASN:ND2	2.20	0.74
5:F:151:PRO:HG3	5:F:247:LEU:HD22	1.71	0.72
3:B:160:SER:HB3	3:B:190:LEU:HD23	1.73	0.71
1:Y:578:PRO:HB2	10:Y:4410:CLR:H192	1.73	0.70
1:X:365:CYS:SG	1:X:366:ARG:N	2.64	0.70
2:A:251:ASP:OD1	2:A:255:ASN:ND2	2.25	0.70
5:F:9:GLY:O	5:F:18:ARG:NH1	2.25	0.70
1:X:764:VAL:HB	1:X:769:ASN:HB2	1.73	0.69
1:X:652:GLY:O	1:X:704:GLN:NE2	2.26	0.68
1:X:610:VAL:HG12	1:X:615:ARG:HG2	1.78	0.65
1:X:685:PRO:HG2	1:X:688:MET:HG3	1.77	0.65
1:X:785:TRP:HE1	10:X:908:CLR:H213	1.62	0.64
1:X:205:ILE:HD11	1:X:468:ILE:HD12	1.80	0.64
1:Y:635:LEU:HD11	1:Y:651:ILE:HD11	1.79	0.64
5:F:105:SER:O	5:F:191:ARG:NH2	2.29	0.64
1:X:559:THR:OG1	1:X:561:ASP:OD1	2.14	0.64
1:Y:272:ARG:NH1	1:Y:298:GLU:O	2.30	0.64
1:Y:741:VAL:O	1:Y:745:GLY:N	2.31	0.63
1:X:648:ARG:HD2	1:X:712:PHE:HE1	1.63	0.63
1:Y:63:GLN:NE2	1:Y:392:VAL:O	2.27	0.63
5:F:67:ARG:NH2	5:F:90:ASP:OD2	2.31	0.62
3:B:320:VAL:HG22	3:B:327:VAL:HG22	1.80	0.61
2:A:8:GLU:OE2	5:F:175:TYR:OH	2.17	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:579:GLU:HG2	1:Y:580:PRO:HD3	1.83	0.61
3:B:49:ARG:NH1	4:G:61:PHE:O	2.30	0.61
1:Y:668:ARG:NH1	1:Y:688:MET:O	2.34	0.60
1:X:345:ARG:NH1	1:X:385:LEU:O	2.32	0.60
1:Y:662:LEU:HD23	1:Y:778:MET:HE3	1.82	0.60
1:Y:396:LYS:HE3	7:Y:4402:GGL:OE2	2.02	0.59
5:F:227:TYR:O	5:F:242:GLY:CA	2.50	0.59
2:A:241:ASN:HB3	2:A:244:HIS:HD2	1.66	0.59
3:B:45:MET:HB2	3:B:308:LEU:HD21	1.85	0.59
1:X:394:ASP:HB3	1:X:397:MET:HE2	1.85	0.59
1:X:789:VAL:HG12	10:Y:4408:CLR:H193	1.85	0.59
1:X:612:SER:HB2	1:X:768:PHE:HE1	1.67	0.59
5:F:12:VAL:HG21	5:F:18:ARG:HB2	1.83	0.59
1:Y:227:GLY:HA3	1:Y:277:PHE:CE2	2.38	0.58
2:A:250:PHE:HE1	2:A:264:ILE:HG21	1.68	0.58
1:Y:539:GLU:OE1	1:Y:727:ARG:NH2	2.36	0.58
3:B:283:ARG:HB3	4:G:51:LEU:HD11	1.85	0.58
1:Y:33:GLY:O	1:Y:141:LYS:NZ	2.33	0.58
1:X:553:GLN:O	1:X:556:SER:OG	2.18	0.57
1:Y:213:TYR:O	1:Y:509:SER:OG	2.16	0.57
3:B:155:ASN:ND2	3:B:170:ASP:OD1	2.38	0.57
3:B:230:ASN:ND2	3:B:246:ASP:OD1	2.36	0.57
3:B:79:LEU:HB2	3:B:95:LEU:HD21	1.86	0.57
1:X:269:PRO:HB2	1:X:272:ARG:HH21	1.70	0.56
3:B:248:ALA:HB1	3:B:269:ILE:HG22	1.86	0.56
1:X:365:CYS:SG	1:X:381:CYS:N	2.78	0.56
10:X:908:CLR:H231	10:Y:4410:CLR:H161	1.87	0.56
1:X:711:LEU:HD13	1:X:739:GLY:HA2	1.88	0.56
1:Y:338:ASP:OD1	1:Y:393:GLN:NE2	2.33	0.56
1:X:307:TRP:NE1	1:X:481:TYR:OH	2.37	0.55
1:Y:648:ARG:HD2	1:Y:712:PHE:HE1	1.71	0.55
1:Y:394:ASP:HB3	1:Y:397:MET:HE2	1.88	0.55
3:B:25:CYS:O	3:B:259:GLN:NE2	2.39	0.55
1:X:178:ASP:OD2	1:X:222:ASN:ND2	2.31	0.54
2:A:247:MET:SD	2:A:287:TYR:OH	2.55	0.54
1:Y:609:VAL:O	1:Y:613:SER:OG	2.16	0.54
3:B:157:ILE:HG22	3:B:169:TRP:HB2	1.89	0.54
5:F:47:TRP:HZ2	5:F:50:TYR:HB3	1.73	0.54
1:X:228:MET:HG3	1:X:232:LYS:HE3	1.90	0.54
1:Y:553:GLN:O	1:Y:556:SER:OG	2.23	0.54
1:X:311:TYR:OH	1:X:480:ASP:OD1	2.23	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:40:ALA:HB3	5:F:43:LYS:HB2	1.89	0.54
10:X:908:CLR:H193	10:Y:4408:CLR:H21	1.89	0.53
3:B:14:LEU:HD11	4:G:20:LYS:HG3	1.91	0.53
1:X:227:GLY:HA3	1:X:277:PHE:CE1	2.43	0.53
3:B:286:LEU:HD22	3:B:327:VAL:HG11	1.90	0.53
3:B:225:HIS:CE1	3:B:245:SER:HB2	2.43	0.53
1:X:246:TYR:OH	1:X:267:HIS:NE2	2.36	0.53
1:Y:149:PRO:HG3	1:Y:154:VAL:HG12	1.91	0.53
3:B:283:ARG:NE	3:B:298:ASP:OD1	2.40	0.53
2:A:36:LEU:HD13	2:A:222:ILE:HD11	1.90	0.52
3:B:286:LEU:HG	3:B:296:VAL:HG22	1.91	0.52
3:B:180:PHE:HE1	3:B:216:GLY:HA2	1.74	0.52
5:F:208:SER:O	5:F:210:THR:N	2.42	0.52
1:Y:29:ALA:HB3	1:Y:95:ILE:HB	1.92	0.52
2:A:8:GLU:OE1	5:F:191:ARG:NH1	2.43	0.51
2:A:315:ASP:OD1	2:A:315:ASP:N	2.43	0.51
1:X:261:LEU:HD23	1:X:293:LEU:HD22	1.93	0.51
1:Y:265:THR:HG23	1:Y:268:LEU:HD12	1.91	0.51
2:A:348:LEU:HB3	2:A:354:PHE:HB2	1.92	0.51
1:X:29:ALA:HB3	1:X:95:ILE:HB	1.91	0.51
1:X:672:ILE:HD12	2:A:353:LEU:HD12	1.93	0.51
1:X:605:ARG:HB2	1:X:615:ARG:HE	1.76	0.51
2:A:333:GLN:NE2	2:A:337:ASP:OD1	2.43	0.51
1:X:605:ARG:HB2	1:X:615:ARG:HH21	1.76	0.51
1:Y:654:SER:HB2	1:Y:655:PRO:HD3	1.93	0.51
1:Y:725:SER:OG	1:Y:728:GLU:OE1	2.22	0.51
3:B:271:CYS:HB2	3:B:290:ASP:HB2	1.92	0.51
3:B:15:LYS:HE3	4:G:19:LEU:HD11	1.93	0.51
3:B:279:SER:OG	4:G:48:ASP:OD2	2.25	0.51
1:X:664:THR:OG1	1:X:693:GLN:OE1	2.28	0.50
1:Y:228:MET:HG3	1:Y:232:LYS:HE3	1.93	0.50
1:X:288:MET:HG2	1:X:317:TYR:CZ	2.46	0.50
1:Y:556:SER:HB2	1:Y:565:CYS:HB3	1.94	0.50
2:A:210:LYS:HA	2:A:213:HIS:CD2	2.45	0.50
5:F:178:LEU:HD13	5:F:227:TYR:CZ	2.47	0.50
1:Y:50:ASP:N	1:Y:50:ASP:OD1	2.42	0.50
1:X:724:PRO:HG2	1:X:728:GLU:HG2	1.94	0.50
1:X:819:VAL:HG11	10:X:910:CLR:H14	1.92	0.50
1:X:182:LYS:NZ	1:X:188:PHE:O	2.43	0.50
1:X:662:LEU:HD22	1:X:754:CYS:SG	2.51	0.49
1:Y:182:LYS:NZ	1:Y:188:PHE:O	2.44	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:644:CYS:HA	1:Y:647:GLN:HG2	1.94	0.49
3:B:124:TYR:CE2	3:B:135:VAL:HG22	2.47	0.49
4:G:28:ILE:HD12	4:G:32:LYS:HB3	1.94	0.49
1:Y:319:ARG:NH2	1:Y:477:ASP:OD1	2.45	0.49
3:B:68:ARG:HE	3:B:83:ASP:CG	2.20	0.49
1:X:783:ILE:HD11	1:Y:784:ILE:HA	1.94	0.49
2:A:27:GLY:HA3	3:B:55:LEU:HD13	1.94	0.49
2:A:283:LEU:HD11	2:A:303:ILE:HD11	1.94	0.49
1:X:70:GLU:OE2	1:X:352:ASN:ND2	2.34	0.49
1:X:63:GLN:NE2	1:X:392:VAL:O	2.38	0.49
1:X:590:GLY:HA3	1:X:629:TYR:CZ	2.48	0.49
3:B:245:SER:OG	3:B:246:ASP:N	2.45	0.49
1:X:291:ARG:NH2	1:X:320:GLU:OE1	2.46	0.49
1:X:791:ILE:O	1:X:795:SER:OG	2.28	0.49
5:F:6:GLU:OE2	5:F:96:CYS:N	2.42	0.49
5:F:35:HIS:ND1	5:F:50:TYR:HB2	2.28	0.49
1:Y:586:PHE:HZ	1:Y:811:THR:HG21	1.77	0.48
3:B:232:ILE:HG13	3:B:243:THR:HG22	1.96	0.48
5:F:38:ARG:HH12	5:F:64:VAL:HG11	1.78	0.48
1:X:415:GLN:NE2	1:X:424:GLY:O	2.36	0.48
3:B:30:LEU:HD23	3:B:262:MET:HE2	1.95	0.48
5:F:67:ARG:NH1	5:F:87:ARG:HG3	2.29	0.48
1:Y:198:GLN:OE1	1:Y:305:ASP:N	2.44	0.48
1:X:664:THR:HG21	1:X:697:ALA:HB2	1.96	0.48
1:X:621:ILE:HG13	1:X:661:ALA:HB3	1.96	0.48
1:X:744:LEU:HD13	1:X:785:TRP:HZ3	1.79	0.48
1:Y:525:LYS:HE3	1:Y:525:LYS:HB2	1.61	0.48
3:B:180:PHE:HB3	3:B:211:TRP:CE3	2.49	0.47
5:F:94:TYR:O	5:F:114:GLY:HA2	2.14	0.47
1:Y:578:PRO:O	1:Y:581:ILE:HG22	2.15	0.47
1:X:691:CYS:O	1:X:695:VAL:HG23	2.15	0.47
3:B:68:ARG:O	3:B:84:SER:OG	2.23	0.47
1:Y:307:TRP:NE1	1:Y:481:TYR:OH	2.43	0.47
5:F:203:PHE:CD1	5:F:216:ILE:HG12	2.49	0.47
1:X:43:VAL:HA	1:X:65:GLY:HA3	1.96	0.47
1:Y:232:LYS:HG2	1:Y:242:ILE:HD12	1.97	0.47
1:Y:792:TYR:CE1	1:Y:798:LYS:HB3	2.49	0.47
10:Y:4401:CLR:H222	10:Y:4401:CLR:H162	1.70	0.47
1:Y:545:ASP:OD1	1:Y:545:ASP:N	2.48	0.47
1:Y:625:ILE:HD13	1:Y:814:LEU:HB2	1.96	0.47
1:Y:825:ILE:HG22	1:Y:826:LEU:HD23	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:233:VAL:HA	2:A:241:ASN:HA	1.97	0.47
1:Y:211:TRP:CD2	1:Y:273:VAL:HG21	2.49	0.47
1:Y:662:LEU:HD13	1:Y:817:MET:HE3	1.96	0.47
3:B:63:TRP:CD2	3:B:321:THR:HG22	2.50	0.47
1:X:64:TYR:O	1:X:68:ARG:HD2	2.15	0.46
1:X:764:VAL:HG11	1:X:768:PHE:HB2	1.97	0.46
5:F:232:HIS:HA	5:F:237:LEU:HD22	1.97	0.46
1:Y:110:ILE:HA	1:Y:113:ILE:HG12	1.97	0.46
1:Y:276:CYS:HB3	1:Y:278:CYS:SG	2.55	0.46
1:Y:445:ASN:HB2	1:Y:455:LEU:HB3	1.96	0.46
1:X:34:ASP:N	1:X:90:THR:O	2.49	0.46
1:Y:312:ASP:N	1:Y:312:ASP:OD1	2.49	0.46
1:X:583:ALA:HB3	1:X:636:ILE:HD11	1.98	0.46
1:X:711:LEU:HD11	1:X:742:THR:HB	1.98	0.46
5:F:22:CYS:HB3	5:F:79:LEU:HB3	1.98	0.46
1:X:366:ARG:HH12	1:X:375:SER:HA	1.80	0.46
1:X:695:VAL:O	1:X:699:ILE:HG13	2.16	0.46
5:F:223:ASP:O	5:F:227:TYR:OH	2.23	0.46
3:B:321:THR:OG1	3:B:323:ASP:OD1	2.31	0.45
1:Y:51:LYS:HD3	1:Y:56:LYS:HD3	1.97	0.45
5:F:147:VAL:HB	5:F:245:LEU:HD23	1.98	0.45
1:X:719:ILE:HD12	1:X:731:LEU:HD11	1.99	0.45
5:F:6:GLU:N	5:F:6:GLU:OE1	2.49	0.45
5:F:11:LEU:HA	5:F:118:THR:HB	1.97	0.45
1:X:106:LEU:HD13	1:X:157:GLN:HG3	1.98	0.45
10:X:910:CLR:H222	10:X:910:CLR:H162	1.76	0.45
10:X:911:CLR:H232	10:X:911:CLR:H211	1.68	0.45
1:Y:645:TYR:CE1	1:Y:717:PRO:HG2	2.52	0.45
2:A:34:VAL:HG11	2:A:339:VAL:HG11	1.97	0.45
1:Y:200:ARG:HH22	1:Y:238:GLU:HG3	1.81	0.45
1:Y:777:THR:HG21	1:Y:817:MET:SD	2.57	0.45
3:B:68:ARG:NE	3:B:83:ASP:OD1	2.38	0.45
2:A:208:ARG:HG3	2:A:211:TRP:CH2	2.51	0.45
10:X:908:CLR:H222	10:X:908:CLR:H162	1.80	0.45
1:Y:288:MET:HG2	1:Y:317:TYR:CZ	2.51	0.45
1:X:33:GLY:O	1:X:141:LYS:NZ	2.38	0.45
1:Y:815:GLY:HA3	10:Y:4409:CLR:H151	1.99	0.45
1:X:68:ARG:HG2	1:X:400:VAL:HG21	1.99	0.44
5:F:165:LEU:HD12	5:F:212:PHE:CZ	2.52	0.44
1:X:338:ASP:OD1	1:X:393:GLN:NE2	2.50	0.44
1:Y:506:ILE:HD13	8:Y:4404:NAG:H81	1.98	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:788:PHE:HB2	10:Y:4408:CLR:H263	2.00	0.44
3:B:211:TRP:CZ3	3:B:218:CYS:HB2	2.53	0.44
1:X:441:LEU:O	1:X:444:THR:HG22	2.18	0.44
1:Y:43:VAL:HA	1:Y:65:GLY:HA3	1.99	0.44
1:Y:579:GLU:CG	1:Y:580:PRO:HD3	2.47	0.44
10:Y:4410:CLR:H222	10:Y:4410:CLR:H162	1.76	0.44
10:Y:4401:CLR:H272	10:Y:4401:CLR:H232	1.76	0.44
3:B:212:ASP:HB3	3:B:215:GLU:HB3	1.99	0.44
1:Y:281:MET:HG2	9:Y:4407:CL:CL	2.55	0.44
1:X:334:VAL:HG21	1:X:401:ILE:HD12	1.99	0.44
3:B:137:ARG:HH21	3:B:174:GLY:HA3	1.83	0.44
3:B:222:PHE:HE1	3:B:258:ASP:HA	1.82	0.44
1:X:804:PHE:O	1:X:808:LEU:HB2	2.18	0.44
1:X:76:LEU:CD1	1:X:93:CYS:HB3	2.49	0.43
1:X:716:PRO:HA	1:X:717:PRO:HD3	1.87	0.43
10:X:911:CLR:H183	10:X:911:CLR:H20	1.74	0.43
10:Y:4410:CLR:H232	10:Y:4410:CLR:H211	1.70	0.43
3:B:180:PHE:CE1	3:B:216:GLY:HA2	2.52	0.43
3:B:290:ASP:HA	3:B:314:ARG:HG3	1.99	0.43
10:X:908:CLR:H183	10:X:908:CLR:H20	1.74	0.43
1:Y:414:MET:HE1	1:Y:432:ILE:HG23	1.99	0.43
5:F:88:SER:HA	5:F:119:VAL:HG11	1.99	0.43
1:X:60:VAL:HG11	1:X:358:PHE:HA	2.00	0.43
1:Y:600:VAL:HG11	1:Y:822:VAL:HG22	2.00	0.43
10:Y:4409:CLR:H222	10:Y:4409:CLR:H162	1.45	0.43
3:B:254:ASP:OD1	3:B:257:ALA:N	2.29	0.43
5:F:72:ARG:HB3	5:F:79:LEU:HD12	2.01	0.43
1:X:557:TRP:HB2	1:X:568:ILE:HD11	2.01	0.43
1:X:414:MET:HE1	1:X:432:ILE:HG23	2.00	0.43
1:Y:98:SER:HB2	1:Y:105:ALA:HB2	2.01	0.43
3:B:225:HIS:ND1	3:B:245:SER:HB2	2.34	0.43
5:F:40:ALA:HB1	5:F:41:PRO:HD2	2.00	0.43
5:F:67:ARG:HH12	5:F:87:ARG:H	1.67	0.43
1:X:164:LEU:HD11	1:Y:106:LEU:HB3	2.01	0.43
10:Y:4408:CLR:H193	10:Y:4408:CLR:H111	1.81	0.43
2:A:33:GLU:HG2	2:A:195:HIS:HB2	2.00	0.43
3:B:183:HIS:CD2	3:B:211:TRP:HZ2	2.35	0.43
1:X:612:SER:HB2	1:X:768:PHE:CE1	2.51	0.43
1:Y:621:ILE:HG13	1:Y:661:ALA:HB3	2.01	0.43
2:A:250:PHE:HZ	2:A:319:ILE:HD13	1.84	0.43
10:Y:4409:CLR:H183	10:Y:4409:CLR:H20	1.71	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:295:LEU:HD23	1:X:295:LEU:HA	1.90	0.43
1:X:79:ILE:HD11	1:X:405:TYR:CD1	2.54	0.42
1:X:779:TYR:OH	1:Y:784:ILE:HG13	2.18	0.42
1:Y:441:LEU:O	1:Y:444:THR:HG22	2.19	0.42
2:A:208:ARG:HG2	2:A:212:ILE:CG2	2.49	0.42
5:F:83:MET:SD	5:F:94:TYR:HE2	2.42	0.42
1:X:545:ASP:OD1	1:X:548:THR:N	2.52	0.42
1:Y:704:GLN:HE21	1:Y:708:ILE:HG13	1.83	0.42
1:Y:575:TRP:H	1:Y:575:TRP:CD1	2.37	0.42
1:Y:663:VAL:HG22	1:Y:754:CYS:HB2	2.00	0.42
3:B:78:LYS:HA	3:B:78:LYS:HD3	1.70	0.42
5:F:157:ILE:O	5:F:213:THR:HA	2.19	0.42
1:X:76:LEU:HD12	1:X:93:CYS:HB3	2.02	0.42
1:Y:311:TYR:OH	1:Y:480:ASP:OD1	2.26	0.42
5:F:177:PHE:HD1	5:F:187:LEU:HA	1.85	0.42
1:Y:625:ILE:HG23	1:Y:810:ALA:HB1	2.02	0.42
1:X:272:ARG:HG3	1:X:507:ILE:HD11	2.00	0.42
1:Y:808:LEU:HA	1:Y:811:THR:HG22	2.02	0.42
10:Y:4408:CLR:H222	10:Y:4408:CLR:H162	1.66	0.42
3:B:51:LEU:HB2	3:B:336:LEU:HB2	2.00	0.42
2:A:184:ILE:HD13	3:B:99:TRP:CD1	2.54	0.42
3:B:152:LEU:HD23	3:B:152:LEU:HA	1.89	0.42
3:B:215:GLU:HG2	3:B:217:MET:H	1.85	0.42
10:X:909:CLR:H111	10:X:909:CLR:H193	1.80	0.42
3:B:159:THR:OG1	3:B:169:TRP:NE1	2.39	0.42
1:X:657:MET:HA	1:X:701:ILE:HG12	2.02	0.42
1:X:79:ILE:HD11	1:X:405:TYR:HD1	1.84	0.41
1:X:283:VAL:O	1:X:287:LEU:HG	2.20	0.41
1:X:825:ILE:HG22	1:X:826:LEU:HD23	2.02	0.41
1:Y:261:LEU:HD23	1:Y:293:LEU:HD12	2.01	0.41
1:Y:787:ALA:O	1:Y:790:PRO:HD2	2.20	0.41
1:Y:808:LEU:HA	1:Y:808:LEU:HD12	1.93	0.41
1:Y:469:MET:HE3	1:Y:481:TYR:HB3	2.02	0.41
1:Y:808:LEU:HD13	10:Y:4410:CLR:H271	2.01	0.41
10:Y:4409:CLR:H193	10:Y:4409:CLR:H111	1.81	0.41
10:Y:4410:CLR:H183	10:Y:4410:CLR:H20	1.70	0.41
1:X:665:LYS:O	1:X:668:ARG:HG2	2.21	0.41
1:Y:64:TYR:O	1:Y:68:ARG:HD2	2.20	0.41
1:Y:205:ILE:HD11	1:Y:468:ILE:HD12	2.01	0.41
3:B:58:ILE:O	3:B:316:SER:OG	2.24	0.41
1:X:704:GLN:HB2	1:X:746:TYR:CE2	2.55	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:340:TYR:OH	1:Y:351:ARG:NH2	2.53	0.41
1:Y:815:GLY:O	1:Y:819:VAL:HB	2.19	0.41
10:Y:4401:CLR:H183	10:Y:4401:CLR:H20	1.70	0.41
3:B:82:TRP:CH2	3:B:89:LYS:HE3	2.55	0.41
10:X:909:CLR:H162	10:X:909:CLR:H222	1.82	0.41
1:Y:77:GLU:CD	1:Y:351:ARG:HH12	2.27	0.41
1:X:387:LEU:O	1:X:391:HIS:HB2	2.21	0.41
1:X:445:ASN:HB2	1:X:455:LEU:HB3	2.02	0.41
1:X:570:VAL:HG13	1:X:729:VAL:HG12	2.03	0.41
5:F:192:MET:HG2	5:F:207:GLY:HA3	2.02	0.41
1:X:720:MET:HE3	1:X:720:MET:HB2	1.98	0.41
5:F:161:SER:OG	5:F:162:SER:N	2.53	0.41
1:X:542:TYR:HB3	1:X:558:PRO:HB3	2.02	0.41
1:X:644:CYS:HA	1:X:647:GLN:HG2	2.02	0.41
1:X:672:ILE:HG13	1:X:688:MET:HE2	2.02	0.41
1:X:787:ALA:HA	1:Y:791:ILE:HD11	2.02	0.41
1:Y:430:LYS:HA	1:Y:431:PRO:HA	1.97	0.41
3:B:47:THR:HG21	3:B:337:LYS:HD3	2.03	0.41
10:X:911:CLR:H222	10:X:911:CLR:H162	1.84	0.41
1:Y:472:LYS:HE3	1:Y:474:MET:SD	2.61	0.41
1:Y:502:LYS:HB2	1:Y:505:ASN:OD1	2.20	0.41
10:Y:4401:CLR:H232	10:Y:4401:CLR:H211	1.66	0.41
1:X:232:LYS:HG2	1:X:242:ILE:HD12	2.03	0.40
1:X:786:LEU:HD13	10:Y:4408:CLR:H211	2.03	0.40
1:Y:508:ARG:NH2	1:Y:513:GLU:OE1	2.53	0.40
1:Y:577:ASP:HB2	1:Y:580:PRO:HG2	2.02	0.40
1:X:591:LEU:HD23	1:X:591:LEU:HA	1.84	0.40
1:Y:800:ILE:HG23	10:Y:4408:CLR:H151	2.03	0.40
10:Y:4410:CLR:H232	10:Y:4410:CLR:H272	1.82	0.40
3:B:149:CYS:HB3	3:B:159:THR:HG22	2.04	0.40
1:X:276:CYS:HB3	1:X:278:CYS:SG	2.62	0.40
1:Y:318:GLN:O	1:Y:322:VAL:HG23	2.21	0.40
1:Y:723:TYR:HD1	1:Y:729:VAL:HG22	1.87	0.40
2:A:253:ILE:HD13	2:A:253:ILE:HA	1.92	0.40
3:B:251:ARG:NH1	3:B:263:THR:OG1	2.54	0.40
10:X:909:CLR:H12	10:Y:4401:CLR:H193	2.04	0.40
1:Y:573:LEU:HD23	1:Y:573:LEU:HA	1.96	0.40
3:B:118:ASP:N	3:B:118:ASP:OD1	2.54	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	X	787/850 (93%)	762 (97%)	25 (3%)	0	100	100
1	Y	765/850 (90%)	744 (97%)	21 (3%)	0	100	100
2	A	221/354 (62%)	217 (98%)	4 (2%)	0	100	100
3	B	336/340 (99%)	324 (96%)	12 (4%)	0	100	100
4	G	57/80 (71%)	57 (100%)	0	0	100	100
5	F	230/260 (88%)	216 (94%)	14 (6%)	0	100	100
All	All	2396/2734 (88%)	2320 (97%)	76 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	X	681/735 (93%)	681 (100%)	0	100	100
1	Y	670/735 (91%)	670 (100%)	0	100	100
2	A	189/305 (62%)	189 (100%)	0	100	100
3	B	281/283 (99%)	281 (100%)	0	100	100
4	G	45/61 (74%)	45 (100%)	0	100	100
5	F	194/209 (93%)	194 (100%)	0	100	100
All	All	2060/2328 (88%)	2060 (100%)	0	100	100



There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	350	HIS
1	X	412	HIS
1	Y	166	ASN
1	Y	667	ASN
2	A	331	ASN
3	B	293	ASN
5	F	39	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
8	NAG	Y	4405	1	14,14,15	0.24	0	17,19,21	0.52	0
8	NAG	X	906	1	14,14,15	0.16	0	17,19,21	0.52	0
8	NAG	X	904	1	14,14,15	0.51	0	17,19,21	0.43	0
10	CLR	X	911	-	31,31,31	1.19	3 (9%)	48,48,48	1.68	11 (22%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	Y	4403	1	14,14,15	0.19	0	17,19,21	0.40	0
7	GGL	Y	4402	-	8,9,9	1.03	0	10,11,11	1.23	0
10	CLR	Y	4409	-	31,31,31	1.13	3 (9%)	48,48,48	1.62	12 (25%)
8	NAG	Y	4404	1	14,14,15	0.20	0	17,19,21	0.48	0
10	CLR	X	908	-	31,31,31	1.16	3 (9%)	48,48,48	1.65	11 (22%)
10	CLR	X	910	-	31,31,31	1.10	3 (9%)	48,48,48	1.60	13 (27%)
6	YKU	X	901	-	31,31,31	1.88	6 (19%)	40,42,42	1.82	9 (22%)
8	NAG	Y	4406	1	14,14,15	0.38	0	17,19,21	0.36	0
10	CLR	Y	4410	-	31,31,31	1.16	3 (9%)	48,48,48	1.71	12 (25%)
7	GGL	X	902	-	8,9,9	1.02	0	10,11,11	1.19	0
8	NAG	X	903	1	14,14,15	0.20	0	17,19,21	0.37	0
10	CLR	Y	4401	-	31,31,31	1.16	3 (9%)	48,48,48	1.72	12 (25%)
10	CLR	Y	4408	-	31,31,31	1.19	3 (9%)	48,48,48	1.79	13 (27%)
8	NAG	X	905	1	14,14,15	0.39	0	17,19,21	0.33	0
10	CLR	X	909	-	31,31,31	1.18	3 (9%)	48,48,48	1.67	13 (27%)

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
8	NAG	Y	4405	1	-	4/6/23/26	0/1/1/1
8	NAG	X	906	1	-	3/6/23/26	0/1/1/1
8	NAG	X	904	1	-	2/6/23/26	0/1/1/1
10	CLR	X	911	-	-	5/10/68/68	0/4/4/4
8	NAG	Y	4403	1	-	3/6/23/26	0/1/1/1
7	GGL	Y	4402	-	-	6/9/9/9	-
10	CLR	Y	4409	-	-	5/10/68/68	0/4/4/4
8	NAG	Y	4404	1	-	2/6/23/26	0/1/1/1
10	CLR	X	908	-	-	4/10/68/68	0/4/4/4
10	CLR	X	910	-	-	2/10/68/68	0/4/4/4
6	YKU	X	901	-	-	0/18/18/18	0/4/4/4
8	NAG	Y	4406	1	-	2/6/23/26	0/1/1/1
10	CLR	Y	4410	-	-	4/10/68/68	0/4/4/4
7	GGL	X	902	-	-	1/9/9/9	-
8	NAG	X	903	1	-	3/6/23/26	0/1/1/1
10	CLR	Y	4401	-	-	6/10/68/68	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLR	Y	4408	-	-	4/10/68/68	0/4/4/4
8	NAG	X	905	1	-	1/6/23/26	0/1/1/1
10	CLR	X	909	-	-	5/10/68/68	0/4/4/4

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	X	901	YKU	C10-N09	-5.53	1.31	1.36
6	X	901	YKU	C10-N12	4.65	1.45	1.39
6	X	901	YKU	C13-N12	4.28	1.45	1.37
6	X	901	YKU	C19-C21	3.84	1.53	1.44
10	X	911	CLR	C13-C17	-3.42	1.48	1.55
10	Y	4408	CLR	C13-C17	-3.40	1.48	1.55
10	Y	4410	CLR	C13-C17	-3.23	1.48	1.55
10	Y	4401	CLR	C13-C17	-3.21	1.48	1.55
6	X	901	YKU	C04-C07	3.21	1.52	1.47
10	Y	4409	CLR	C13-C17	-3.18	1.48	1.55
10	X	908	CLR	C13-C17	-3.16	1.49	1.55
10	X	909	CLR	C13-C17	-3.15	1.49	1.55
10	Y	4410	CLR	C16-C15	3.07	1.62	1.54
10	X	911	CLR	C16-C15	3.07	1.62	1.54
10	X	908	CLR	C16-C15	3.03	1.62	1.54
10	Y	4409	CLR	C16-C15	3.03	1.62	1.54
10	X	910	CLR	C16-C15	3.01	1.62	1.54
10	Y	4401	CLR	C16-C15	3.00	1.62	1.54
10	Y	4408	CLR	C16-C15	2.99	1.62	1.54
10	X	909	CLR	C16-C15	2.96	1.62	1.54
10	X	910	CLR	C13-C17	-2.89	1.49	1.55
10	Y	4401	CLR	C7-C6	2.46	1.55	1.50
6	X	901	YKU	O14-C13	-2.43	1.18	1.23
10	X	908	CLR	C7-C6	2.38	1.55	1.50
10	X	909	CLR	C7-C6	2.36	1.55	1.50
10	X	910	CLR	C7-C6	2.34	1.55	1.50
10	X	911	CLR	C7-C6	2.34	1.55	1.50
10	Y	4410	CLR	C7-C6	2.31	1.55	1.50
10	Y	4409	CLR	C7-C6	2.29	1.55	1.50
10	Y	4408	CLR	C7-C6	2.26	1.55	1.50

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Y	4408	CLR	C13-C17-C20	-5.16	111.40	119.49

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Y	4401	CLR	C13-C17-C20	-5.00	111.66	119.49
6	X	901	YKU	C11-C10-N12	-4.95	124.64	132.66
10	X	911	CLR	C13-C17-C20	-4.88	111.84	119.49
10	Y	4410	CLR	C13-C17-C20	-4.83	111.92	119.49
10	Y	4409	CLR	C13-C17-C20	-4.71	112.11	119.49
6	X	901	YKU	N12-C10-N09	4.64	128.06	120.11
10	X	908	CLR	C13-C17-C20	-4.54	112.37	119.49
6	X	901	YKU	C04-C07-N08	4.12	125.69	120.39
6	X	901	YKU	C07-N08-N09	4.07	107.21	104.79
10	Y	4408	CLR	C10-C9-C8	-3.80	107.03	112.73
10	X	909	CLR	C13-C17-C20	-3.68	113.72	119.49
10	X	910	CLR	C13-C17-C20	-3.58	113.88	119.49
10	Y	4410	CLR	C13-C14-C8	-3.56	109.10	114.38
10	Y	4410	CLR	C11-C9-C10	-3.46	108.53	113.08
10	X	911	CLR	C21-C20-C17	-3.34	107.81	112.92
10	Y	4401	CLR	C13-C14-C8	-3.28	109.53	114.38
6	X	901	YKU	C11-C07-N08	-3.25	107.68	111.14
10	Y	4408	CLR	C11-C12-C13	-3.25	107.21	112.78
10	X	909	CLR	C4-C5-C10	3.21	120.69	116.42
10	X	911	CLR	C11-C9-C10	-3.17	108.91	113.08
6	X	901	YKU	C23-N09-C10	-3.17	126.67	129.78
10	X	910	CLR	C16-C15-C14	-3.16	98.87	105.13
10	Y	4401	CLR	C11-C9-C10	-3.11	108.98	113.08
10	Y	4409	CLR	C13-C14-C8	-3.10	109.80	114.38
10	X	909	CLR	C3-C4-C5	-3.09	106.78	112.03
10	Y	4408	CLR	C15-C14-C8	-3.09	113.99	119.08
10	Y	4408	CLR	C4-C5-C10	3.08	120.52	116.42
10	Y	4401	CLR	C17-C13-C14	3.08	103.72	100.07
10	Y	4410	CLR	C3-C4-C5	-3.07	106.82	112.03
10	X	909	CLR	C16-C15-C14	-3.06	99.06	105.13
10	X	910	CLR	C13-C14-C8	-3.05	109.87	114.38
10	Y	4409	CLR	C3-C4-C5	-3.02	106.90	112.03
10	X	909	CLR	C11-C9-C10	-2.99	109.14	113.08
10	X	910	CLR	C3-C4-C5	-2.99	106.96	112.03
10	X	911	CLR	C11-C12-C13	-2.97	107.69	112.78
10	X	911	CLR	C3-C4-C5	-2.96	107.01	112.03
6	X	901	YKU	C15-C13-N12	2.95	120.64	116.24
10	Y	4410	CLR	C17-C13-C14	2.95	103.56	100.07
10	X	908	CLR	C11-C9-C10	-2.94	109.21	113.08
10	Y	4401	CLR	C16-C15-C14	-2.92	99.34	105.13
10	X	908	CLR	C4-C5-C10	2.90	120.27	116.42
10	X	908	CLR	C10-C9-C8	-2.86	108.45	112.73

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Y	4409	CLR	C16-C15-C14	-2.81	99.56	105.13
10	Y	4401	CLR	C3-C4-C5	-2.80	107.27	112.03
10	X	908	CLR	C16-C15-C14	-2.80	99.58	105.13
10	X	908	CLR	C11-C12-C13	-2.79	107.99	112.78
10	Y	4408	CLR	C11-C9-C10	-2.79	109.41	113.08
6	X	901	YKU	C23-N09-N08	2.78	122.89	118.69
10	X	911	CLR	C13-C14-C8	-2.77	110.28	114.38
10	Y	4408	CLR	C16-C15-C14	-2.77	99.64	105.13
10	X	908	CLR	C13-C14-C8	-2.77	110.28	114.38
10	Y	4408	CLR	C13-C14-C8	-2.76	110.30	114.38
10	Y	4401	CLR	C10-C9-C8	-2.75	108.61	112.73
10	X	910	CLR	C17-C13-C14	2.75	103.33	100.07
10	X	910	CLR	C11-C9-C10	-2.73	109.48	113.08
10	Y	4409	CLR	C11-C9-C10	-2.70	109.53	113.08
10	X	909	CLR	C15-C14-C8	-2.70	114.64	119.08
10	Y	4401	CLR	C11-C12-C13	-2.67	108.20	112.78
10	Y	4410	CLR	C10-C9-C8	-2.65	108.76	112.73
10	X	911	CLR	C16-C15-C14	-2.64	99.90	105.13
10	X	908	CLR	C15-C14-C8	-2.64	114.74	119.08
10	X	911	CLR	C10-C9-C8	-2.63	108.79	112.73
10	Y	4410	CLR	C16-C15-C14	-2.63	99.93	105.13
10	X	908	CLR	C17-C13-C14	2.62	103.18	100.07
10	X	908	CLR	C3-C4-C5	-2.62	107.59	112.03
10	X	909	CLR	C13-C14-C8	-2.61	110.51	114.38
10	Y	4401	CLR	C4-C5-C10	2.59	119.86	116.42
10	X	911	CLR	C15-C14-C8	-2.58	114.83	119.08
10	Y	4410	CLR	C15-C14-C8	-2.57	114.85	119.08
10	Y	4408	CLR	C21-C20-C17	-2.54	109.03	112.92
10	Y	4408	CLR	C17-C13-C14	2.54	103.08	100.07
10	Y	4410	CLR	C11-C12-C13	-2.51	108.48	112.78
10	X	910	CLR	C4-C5-C10	2.51	119.75	116.42
10	Y	4409	CLR	C15-C14-C8	-2.49	114.98	119.08
10	X	909	CLR	C19-C10-C9	-2.48	108.73	111.68
10	X	911	CLR	C4-C5-C10	2.45	119.67	116.42
10	X	909	CLR	C11-C12-C13	-2.44	108.60	112.78
10	Y	4401	CLR	C15-C14-C8	-2.43	115.08	119.08
10	X	910	CLR	C14-C8-C9	-2.41	105.86	109.09
10	Y	4410	CLR	C19-C10-C9	-2.41	108.81	111.68
10	Y	4409	CLR	C4-C5-C10	2.40	119.61	116.42
10	Y	4408	CLR	C3-C4-C5	-2.40	107.96	112.03
10	Y	4410	CLR	C4-C5-C10	2.32	119.51	116.42
10	Y	4409	CLR	C11-C12-C13	-2.31	108.82	112.78

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	909	CLR	C10-C9-C8	-2.29	109.31	112.73
10	Y	4409	CLR	C17-C13-C14	2.28	102.78	100.07
10	X	909	CLR	C4-C5-C6	-2.27	117.33	120.61
10	X	910	CLR	C16-C17-C20	-2.24	108.68	112.15
10	Y	4409	CLR	C21-C20-C17	-2.18	109.58	112.92
10	Y	4408	CLR	C4-C5-C6	-2.18	117.47	120.61
10	X	910	CLR	C11-C12-C13	-2.17	109.06	112.78
10	Y	4408	CLR	C7-C8-C9	-2.16	107.10	109.71
10	X	911	CLR	C19-C10-C9	-2.15	109.11	111.68
10	X	910	CLR	C4-C5-C6	-2.15	117.51	120.61
10	Y	4401	CLR	C21-C20-C17	-2.14	109.64	112.92
10	X	910	CLR	C15-C14-C8	-2.12	115.58	119.08
10	Y	4409	CLR	C4-C5-C6	-2.12	117.55	120.61
10	X	909	CLR	C21-C20-C17	-2.12	109.68	112.92
10	Y	4410	CLR	C21-C20-C17	-2.11	109.69	112.92
10	Y	4401	CLR	C19-C10-C9	-2.10	109.18	111.68
10	X	909	CLR	C16-C17-C20	-2.08	108.92	112.15
10	X	910	CLR	C23-C22-C20	-2.08	109.05	115.03
10	X	908	CLR	C4-C5-C6	-2.06	117.64	120.61
10	Y	4409	CLR	C14-C8-C9	-2.03	106.37	109.09
6	X	901	YKU	O14-C13-N12	-2.01	119.27	122.26

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	X	911	CLR	C13-C17-C20-C21
10	Y	4408	CLR	C13-C17-C20-C21
8	X	906	NAG	C4-C5-C6-O6
10	X	911	CLR	C16-C17-C20-C21
10	Y	4401	CLR	C13-C17-C20-C21
10	Y	4409	CLR	C13-C17-C20-C21
10	Y	4410	CLR	C13-C17-C20-C21
8	Y	4404	NAG	O5-C5-C6-O6
10	Y	4401	CLR	C16-C17-C20-C21
10	Y	4408	CLR	C16-C17-C20-C21
10	Y	4409	CLR	C16-C17-C20-C21
10	X	908	CLR	C13-C17-C20-C21
10	X	911	CLR	C13-C17-C20-C22
10	Y	4401	CLR	C13-C17-C20-C22
10	Y	4408	CLR	C13-C17-C20-C22
10	Y	4409	CLR	C13-C17-C20-C22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
10	Y	4410	CLR	C13-C17-C20-C22
8	X	906	NAG	O5-C5-C6-O6
10	Y	4410	CLR	C16-C17-C20-C21
10	X	911	CLR	C16-C17-C20-C22
10	Y	4408	CLR	C16-C17-C20-C22
8	Y	4406	NAG	O5-C5-C6-O6
8	Y	4405	NAG	O5-C5-C6-O6
8	Y	4404	NAG	C4-C5-C6-O6
10	X	908	CLR	C13-C17-C20-C22
8	Y	4405	NAG	C4-C5-C6-O6
10	Y	4409	CLR	C20-C22-C23-C24
8	Y	4406	NAG	C4-C5-C6-O6
8	X	903	NAG	C8-C7-N2-C2
8	X	903	NAG	O7-C7-N2-C2
8	Y	4403	NAG	C8-C7-N2-C2
8	Y	4403	NAG	O7-C7-N2-C2
8	Y	4405	NAG	C8-C7-N2-C2
8	Y	4405	NAG	O7-C7-N2-C2
10	X	909	CLR	C20-C22-C23-C24
10	Y	4409	CLR	C16-C17-C20-C22
8	X	904	NAG	C4-C5-C6-O6
10	X	908	CLR	C16-C17-C20-C21
10	Y	4410	CLR	C16-C17-C20-C22
10	Y	4401	CLR	C16-C17-C20-C22
8	X	903	NAG	O5-C5-C6-O6
8	X	904	NAG	O5-C5-C6-O6
8	X	905	NAG	O5-C5-C6-O6
10	X	909	CLR	C13-C17-C20-C21
8	Y	4403	NAG	O5-C5-C6-O6
10	X	908	CLR	C16-C17-C20-C22
7	X	902	GGL	CA-CB-CG-CD
10	Y	4401	CLR	C20-C22-C23-C24
10	X	909	CLR	C23-C24-C25-C27
7	Y	4402	GGL	O-C-CA-CB
10	X	910	CLR	C13-C17-C20-C21
7	Y	4402	GGL	CA-CB-CG-CD
10	Y	4401	CLR	C22-C23-C24-C25
10	X	909	CLR	C16-C17-C20-C21
7	Y	4402	GGL	OXT-C-CA-CB
8	X	906	NAG	C3-C2-N2-C7
10	X	909	CLR	C13-C17-C20-C22
10	X	910	CLR	C20-C22-C23-C24

*Continued on next page...*

*Continued from previous page...*

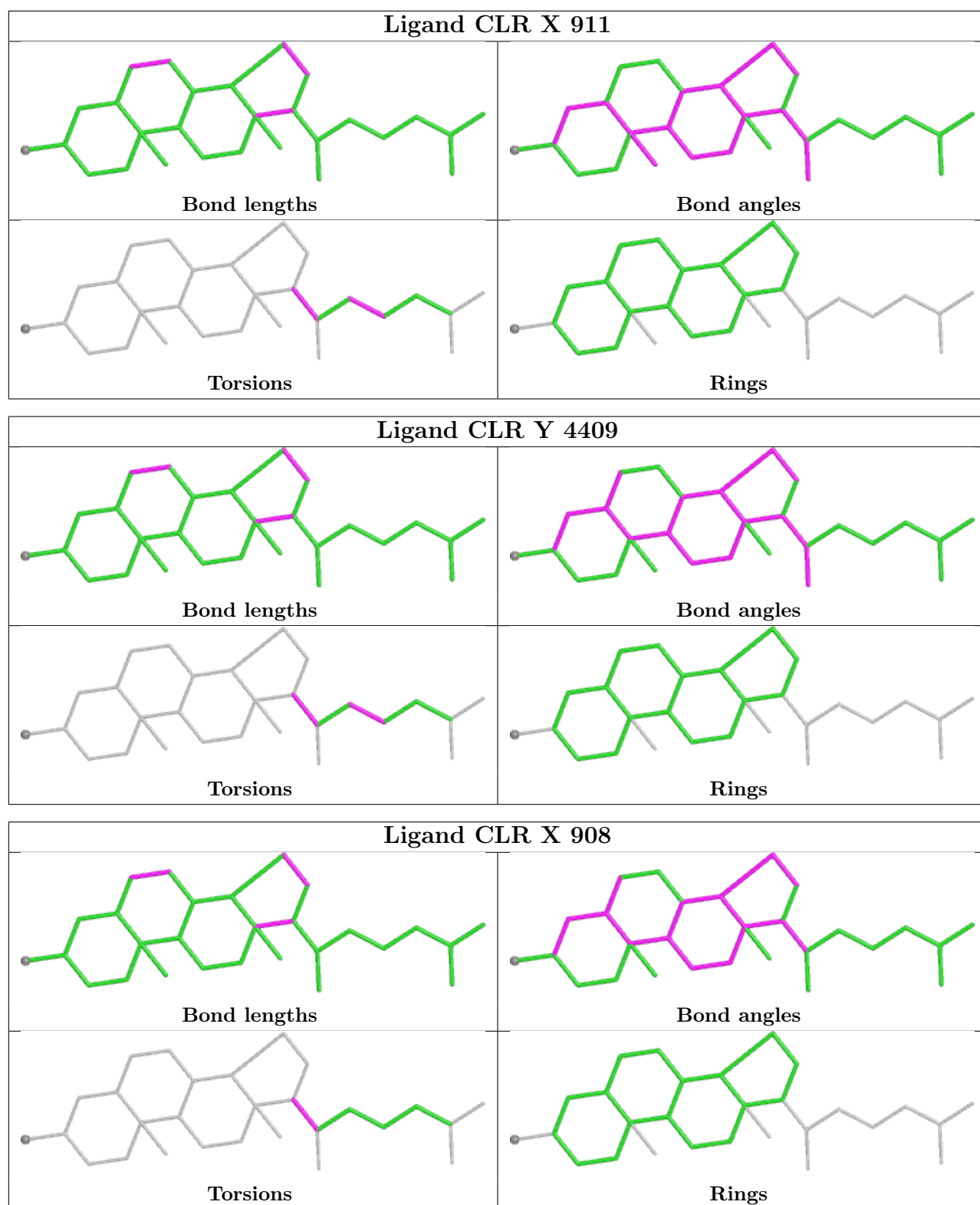
Mol	Chain	Res	Type	Atoms
7	Y	4402	GGL	OE2-CD-CG-CB
7	Y	4402	GGL	C-CA-CB-CG
7	Y	4402	GGL	OE1-CD-CG-CB
10	X	911	CLR	C20-C22-C23-C24

There are no ring outliers.

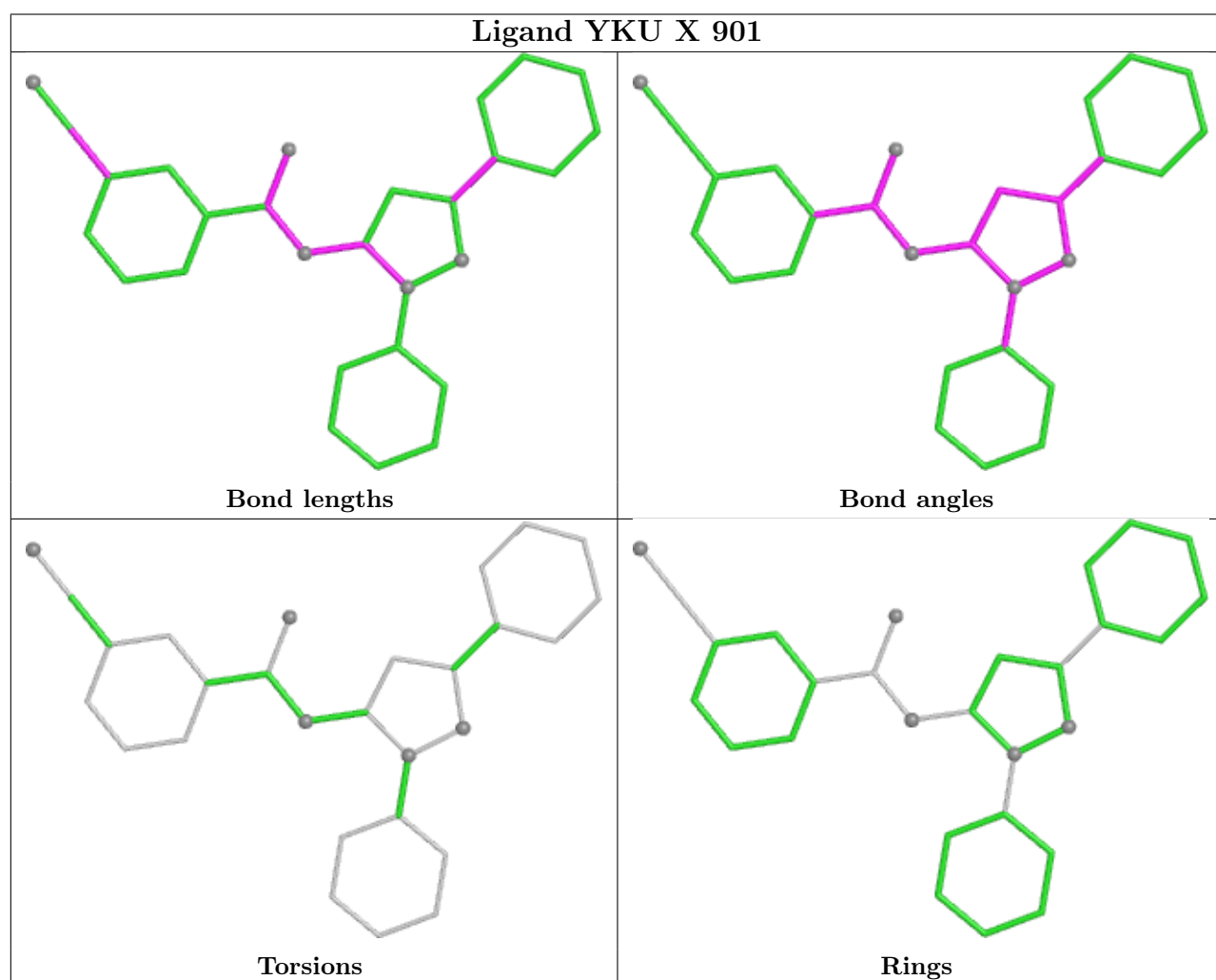
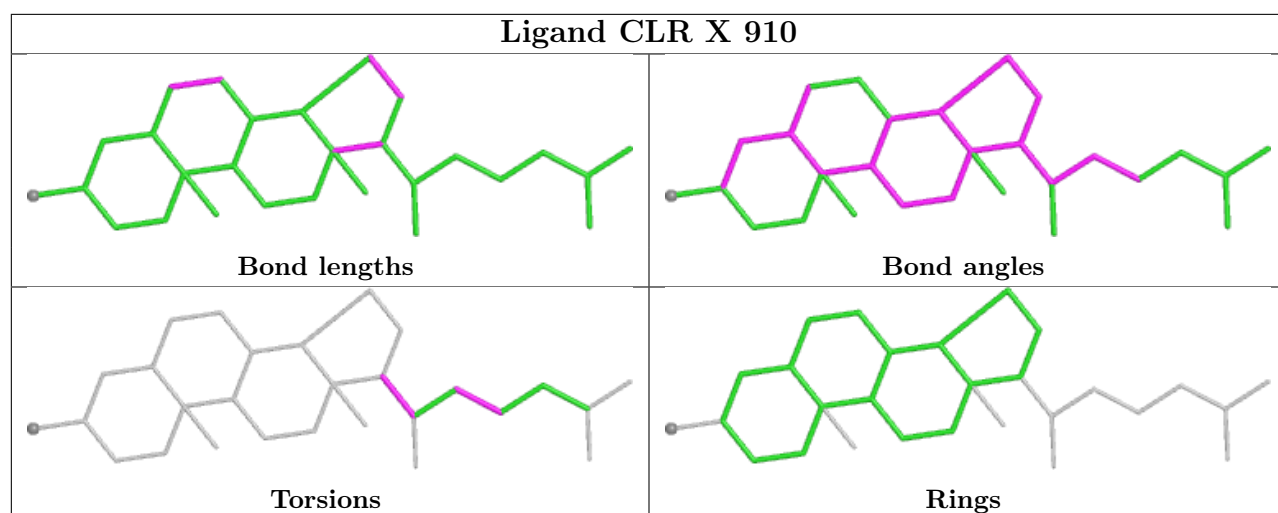
10 monomers are involved in 35 short contacts:

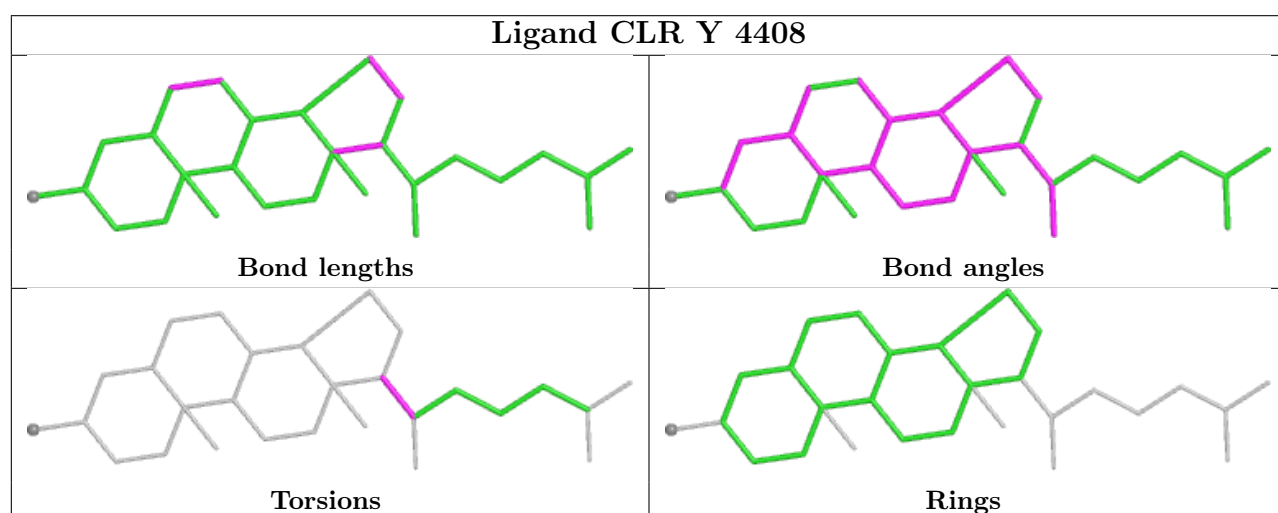
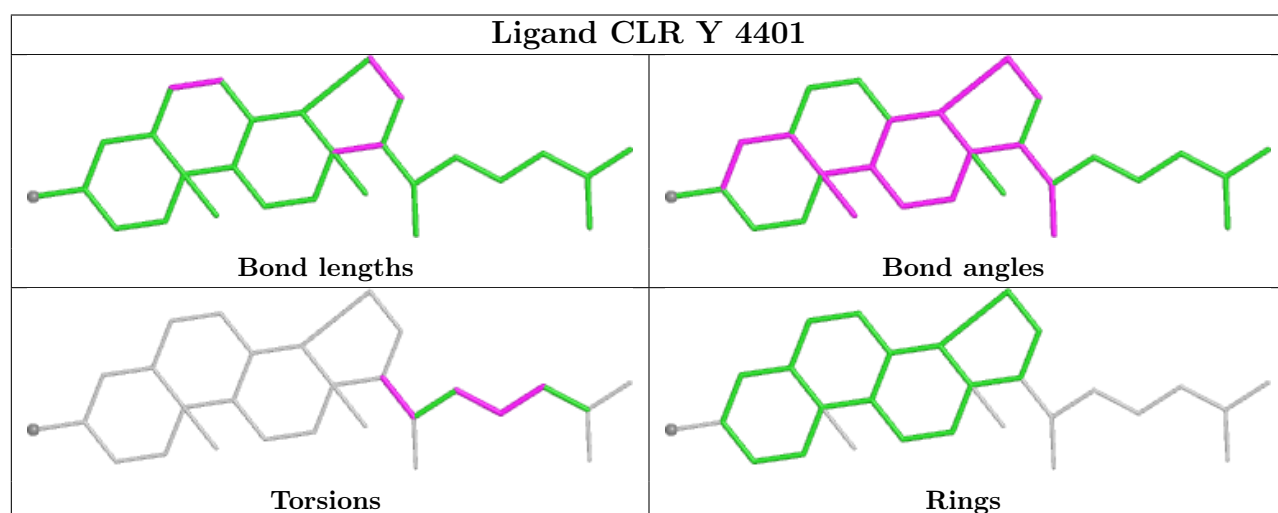
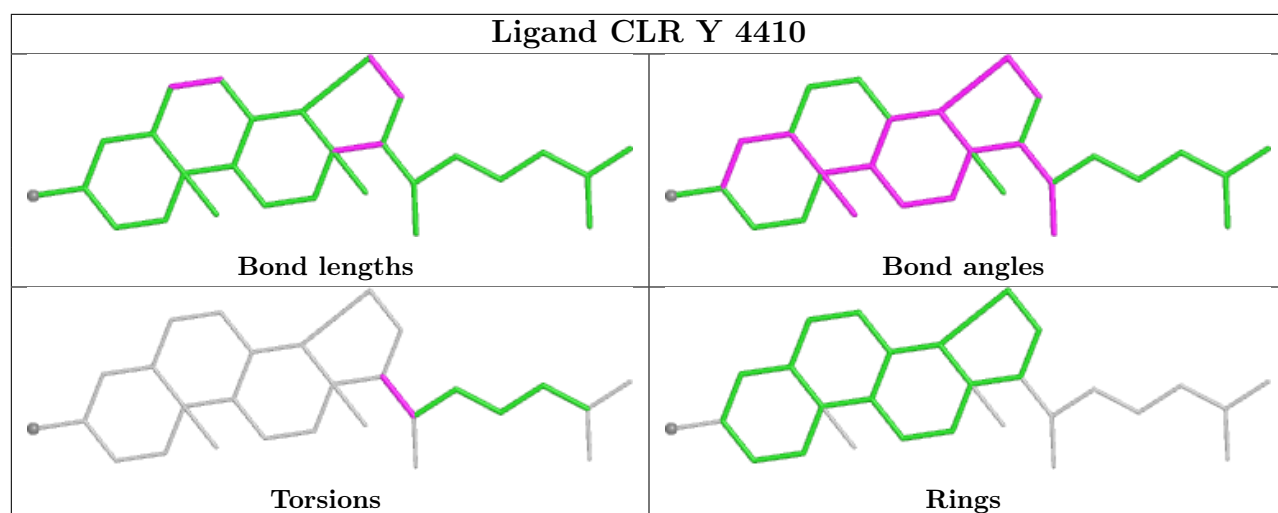
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	X	911	CLR	3	0
7	Y	4402	GGL	1	0
10	Y	4409	CLR	4	0
8	Y	4404	NAG	1	0
10	X	908	CLR	5	0
10	X	910	CLR	2	0
10	Y	4410	CLR	7	0
10	Y	4401	CLR	5	0
10	Y	4408	CLR	7	0
10	X	909	CLR	3	0

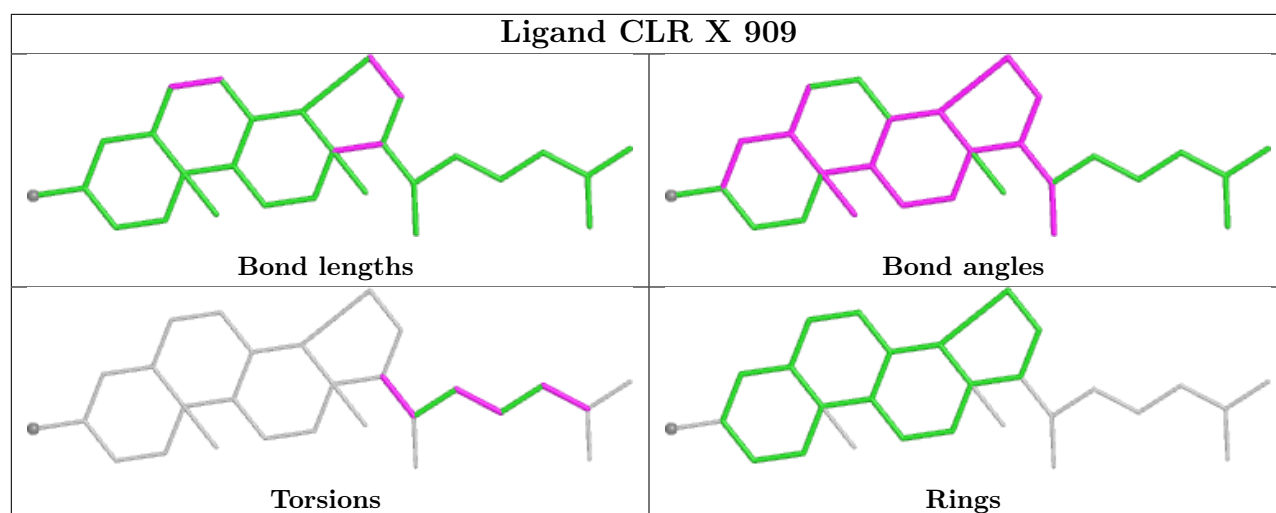
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

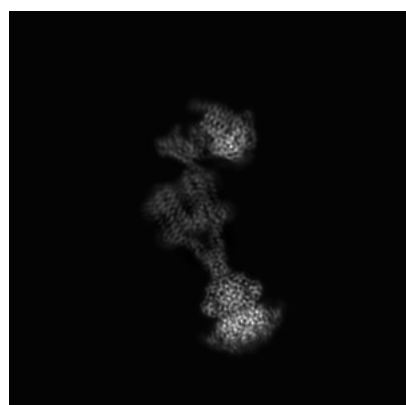
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66174. These allow visual inspection of the internal detail of the map and identification of artifacts.

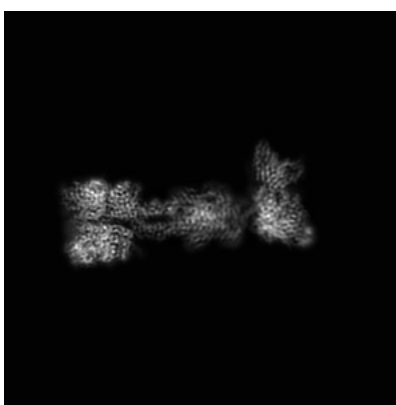
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

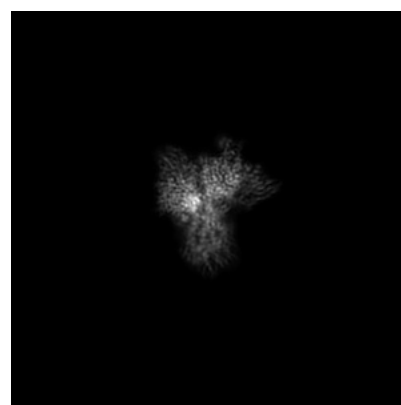
#### 6.1.1 Primary map



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: 192



Y Index: 192

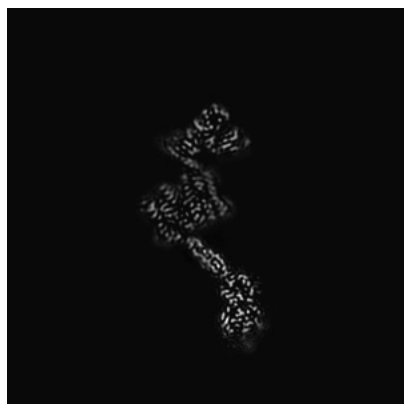


Z Index: 192

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

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

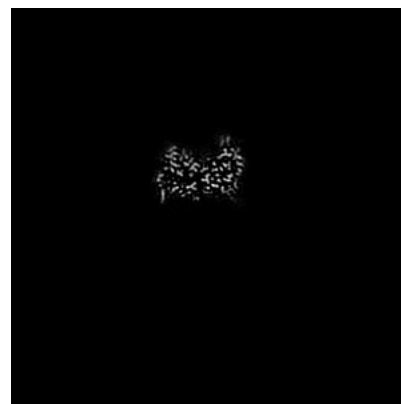
### 6.3.1 Primary map



X Index: 189



Y Index: 212

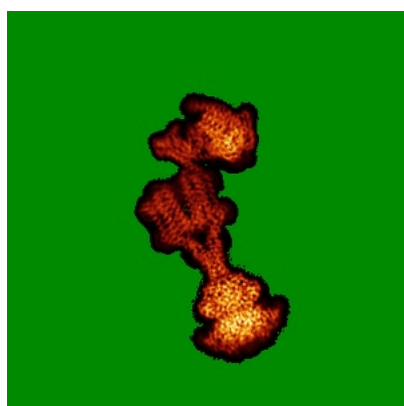


Z Index: 84

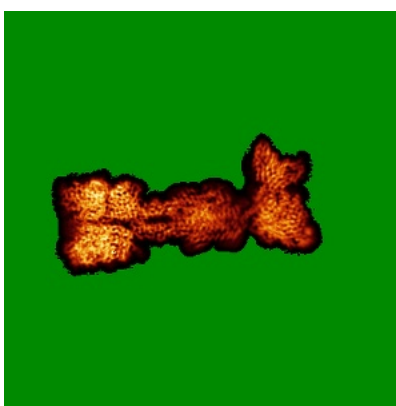
The images above show the largest variance slices of the map in three orthogonal directions.

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

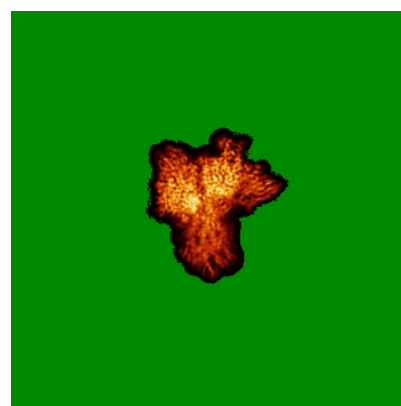
### 6.4.1 Primary map



X



Y

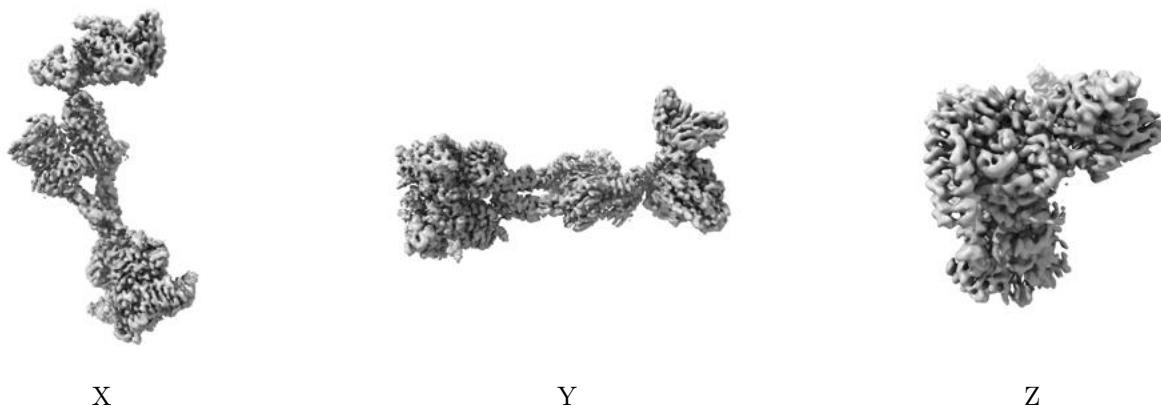


Z

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 0.0027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

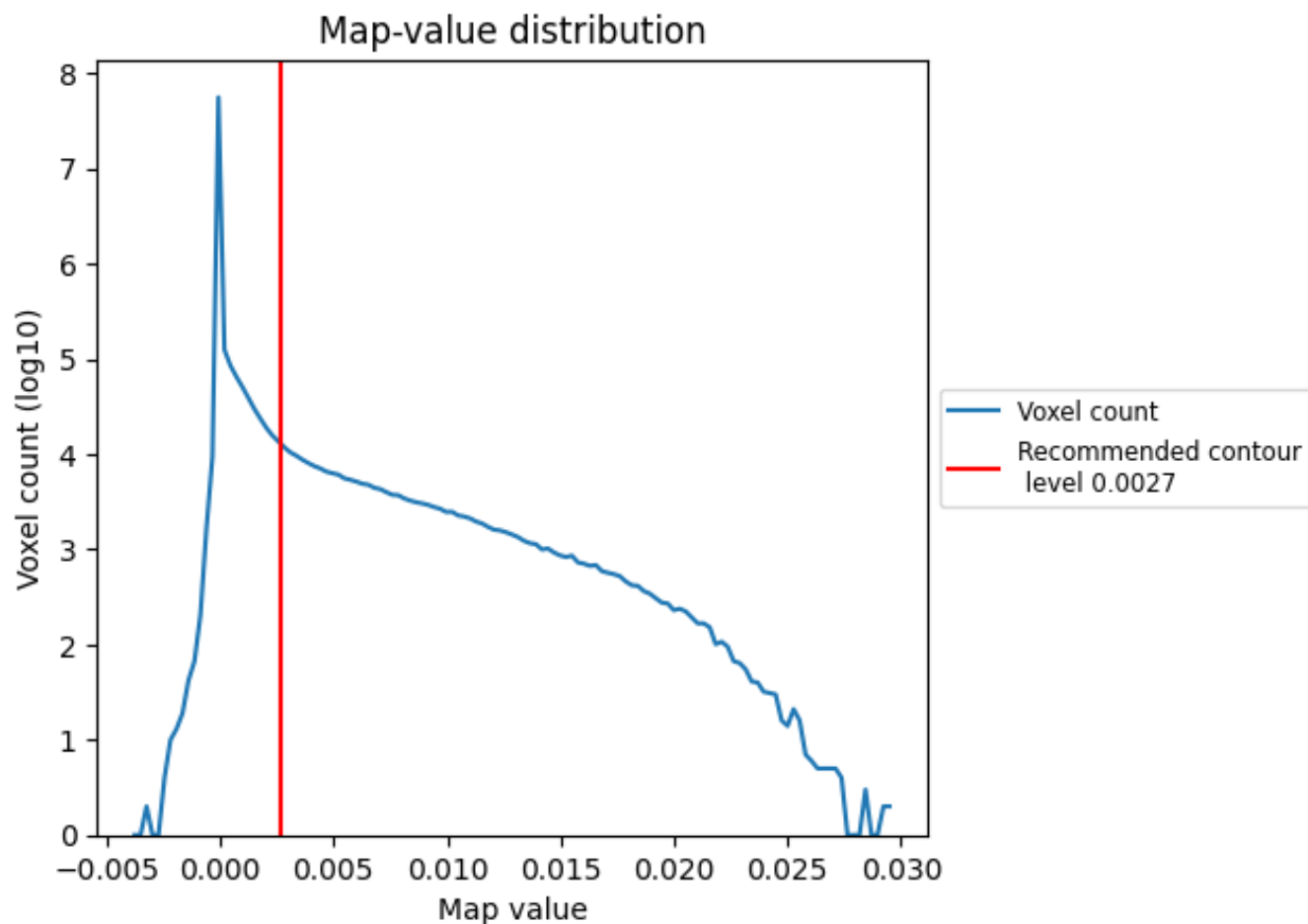
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

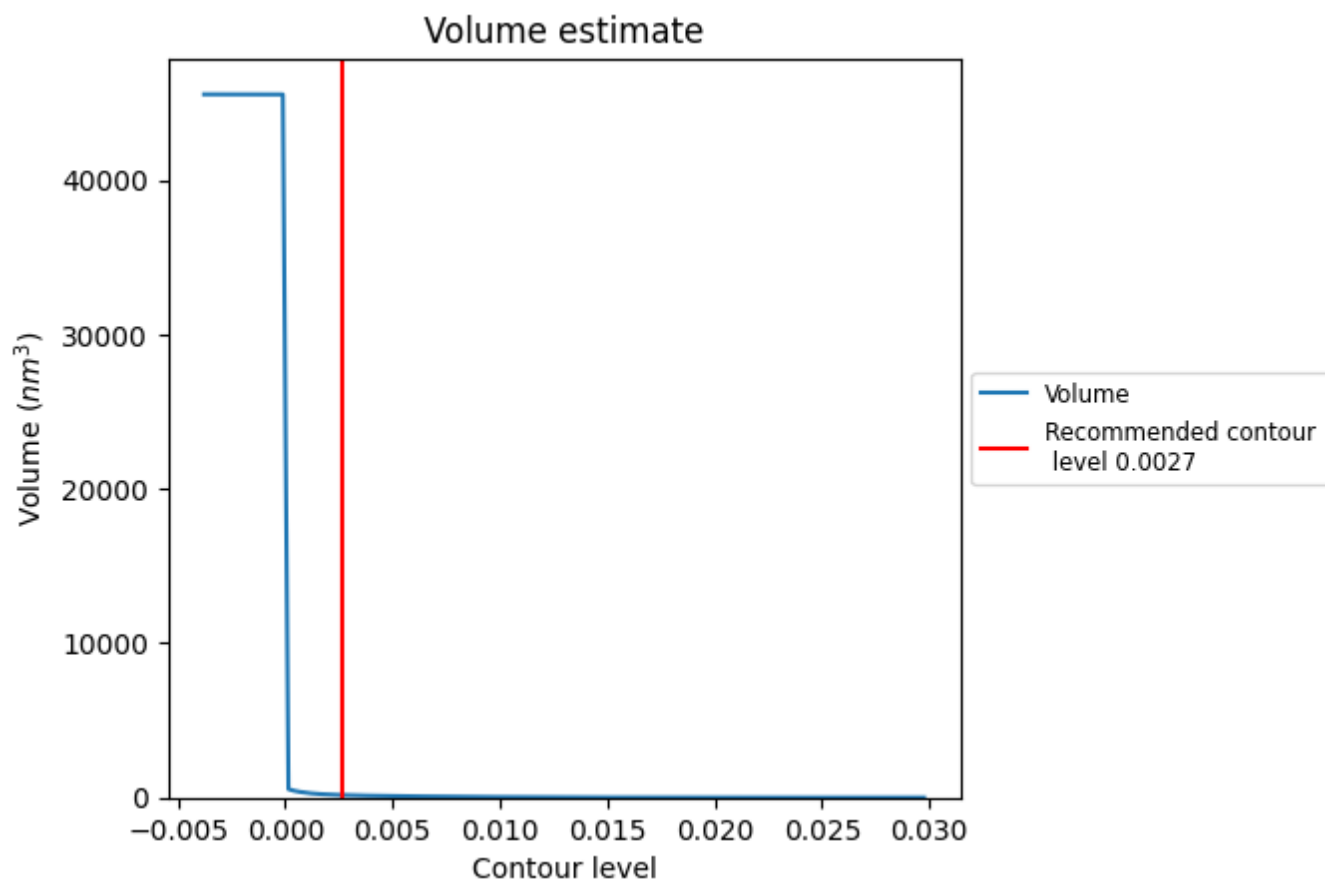
This section contains the results of statistical analysis of the map.

### 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](#)

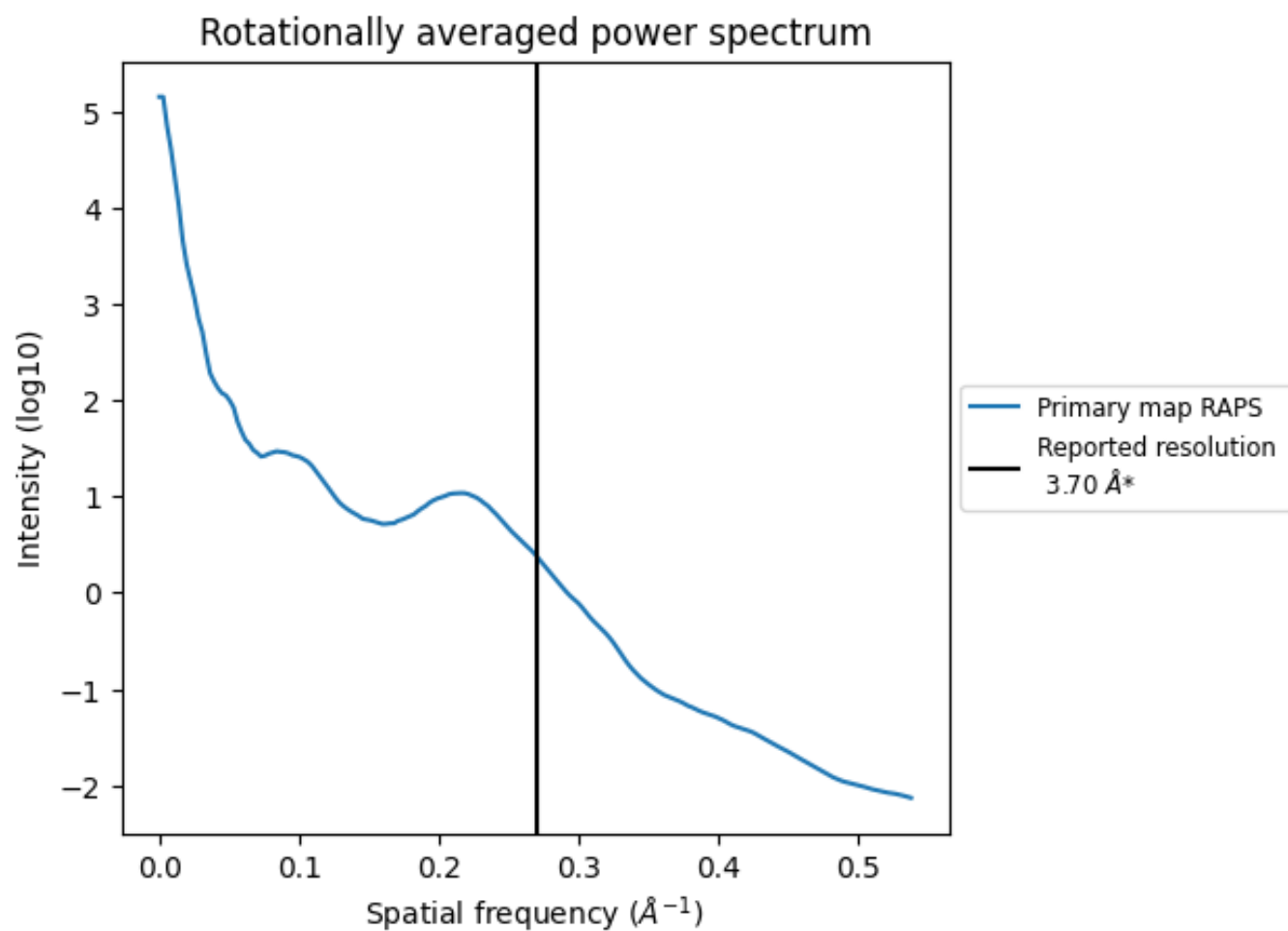


The volume at the recommended contour level is 161 nm<sup>3</sup>; this corresponds to an approximate mass of 145 kDa.

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 0.270 Å<sup>-1</sup>

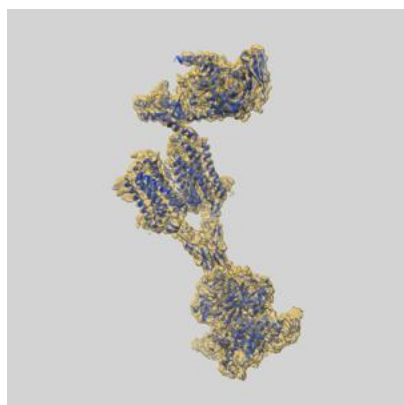
## 8 Fourier-Shell correlation

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

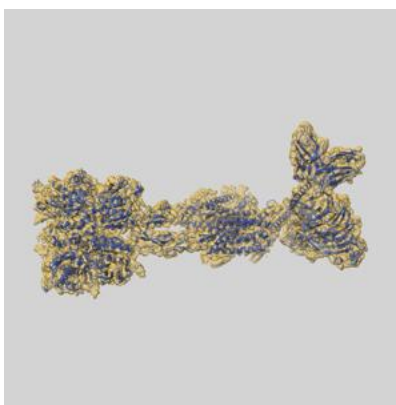
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-66174 and PDB model 9WQK. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

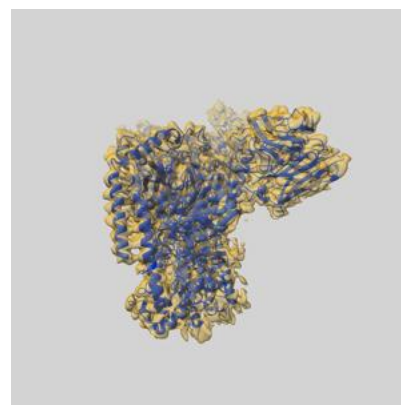
### 9.1 Map-model overlay [i](#)



X



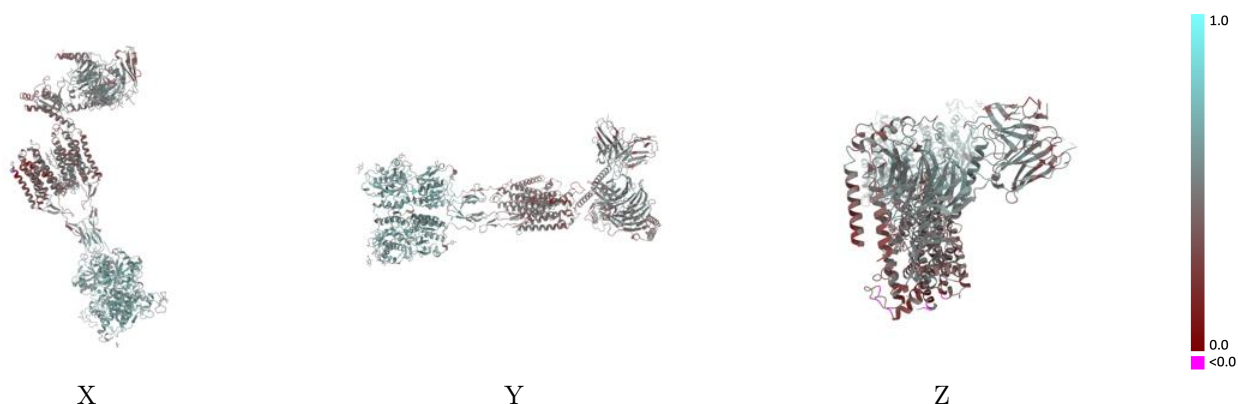
Y



Z

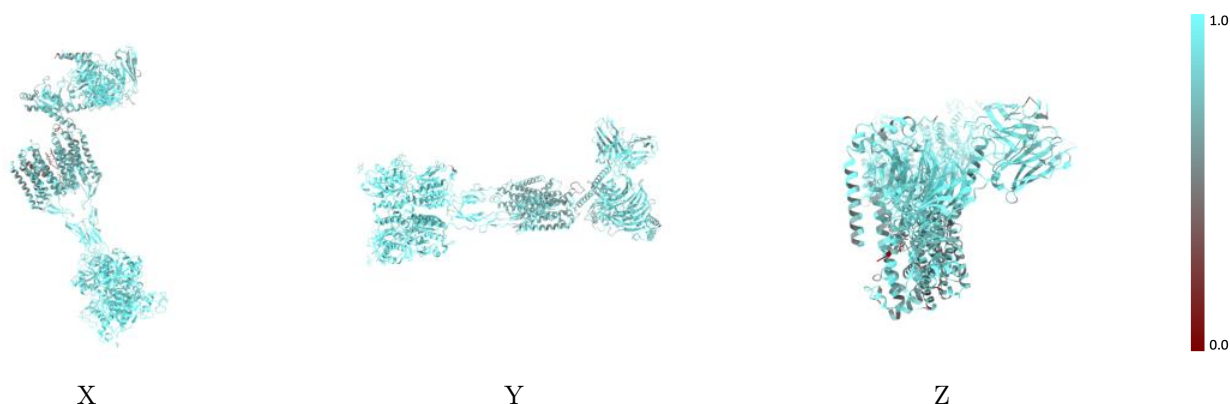
The images above show the 3D surface view of the map at the recommended contour level 0.0027 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



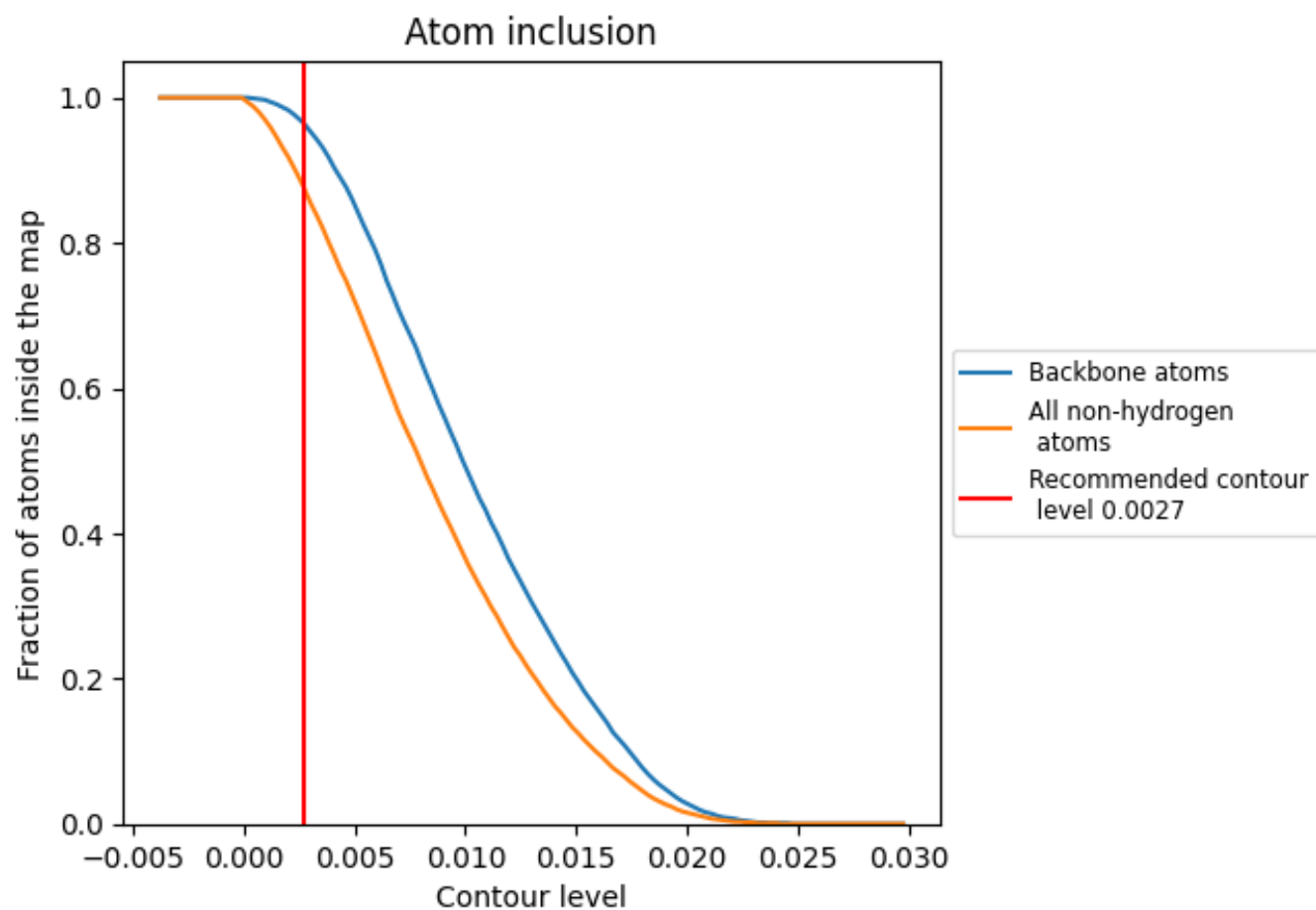
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0027).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 88% 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 (0.0027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8770	<div><div></div></div> 0.4970
A	<div><div></div></div> 0.7940	<div><div></div></div> 0.4160
B	<div><div></div></div> 0.8940	<div><div></div></div> 0.4920
F	<div><div></div></div> 0.8570	<div><div></div></div> 0.4710
G	<div><div></div></div> 0.7860	<div><div></div></div> 0.4180
X	<div><div></div></div> 0.8900	<div><div></div></div> 0.5180
Y	<div><div></div></div> 0.8910	<div><div></div></div> 0.5150

1.0

0.0

<0.0