



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:58 AM UTC

PDB ID : 7LDD / pdb_00007ldd
EMDB ID : EMD-23283
Title : native AMPA receptor
Authors : Yu, J.; Rao, P.; Gouaux, E.
Deposited on : 2021-01-13
Resolution : 3.40 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

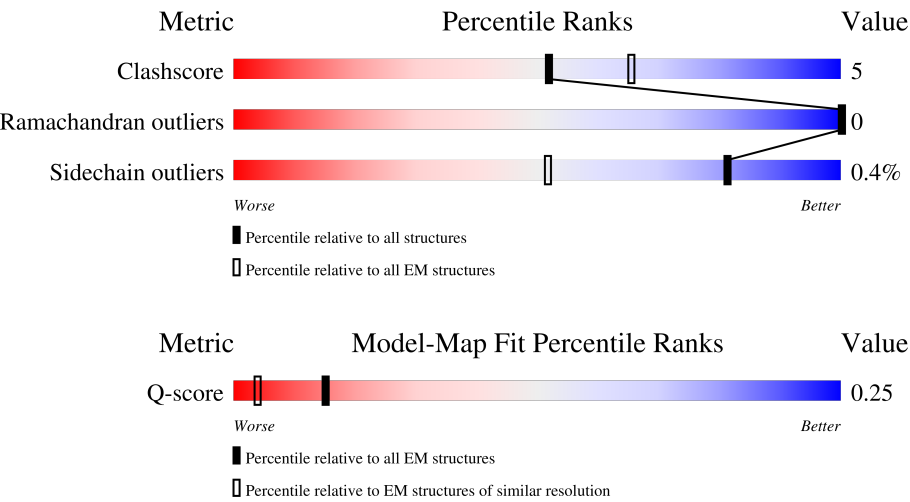
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	907	23% 70% 15% 14%
1	C	907	23% 70% 16% 14%
2	B	883	24% 78% 10% 12%
2	D	883	23% 77% 11% 12%

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Mol	Chain	Length	Quality of chain
3	E	160	 69% 72% 5% 22%
3	F	160	 66% 74% 22%
4	G	423	 31% 34% 5% 62%
4	H	423	 31% 34% 5% 62%
5	I	257	 16% 82% 7% 11%
5	L	257	 16% 83% 6% 11%
6	J	225	 18% 91% 6%
6	M	225	 18% 91% 6%
7	K	262	 15% 79% 18%
7	N	262	 15% 78% 18%
8	O	2	 100%
8	P	2	 50% 50%
8	Q	2	 50% 50%
8	R	2	 100%
8	S	2	 50% 50%
8	T	2	 50% 50%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 34528 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 Glutamate receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	776	Total	C	N	O	S	1	0
			5868	3792	977	1069	30		
1	C	776	Total	C	N	O	S	1	0
			5868	3792	977	1069	30		

- Molecule 2 is a protein called Glutamate receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	778	Total	C	N	O	S	0	0
			5687	3664	925	1070	28		
2	D	778	Total	C	N	O	S	0	0
			5687	3664	925	1070	28		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	586	ARG	GLN	variant	UNP G5E8H1
D	586	ARG	GLN	variant	UNP G5E8H1

- Molecule 3 is a protein called Protein cornichon homolog 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	124	Total	C	N	O	S	0	0
			974	671	142	150	11		
3	F	124	Total	C	N	O	S	0	0
			978	673	142	152	11		

- Molecule 4 is a protein called Voltage-dependent calcium channel gamma-8 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	162	Total	C	N	O	S	0	0
			1134	751	182	196	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	162	Total	C	N	O	S	0	0
			1134	751	182	196	5		

- Molecule 5 is a protein called 11B8 scFv.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	229	Total	C	N	O		0	0
			1124	666	229	229			
5	L	229	Total	C	N	O		0	0
			1124	666	229	229			

- Molecule 6 is a protein called 15F1 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	211	Total	C	N	O		0	0
			1042	620	211	211			
6	M	211	Total	C	N	O		0	0
			1042	620	211	211			

- Molecule 7 is a protein called 15F1 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	215	Total	C	N	O		0	0
			1059	629	215	215			
7	N	215	Total	C	N	O		0	0
			1059	629	215	215			

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



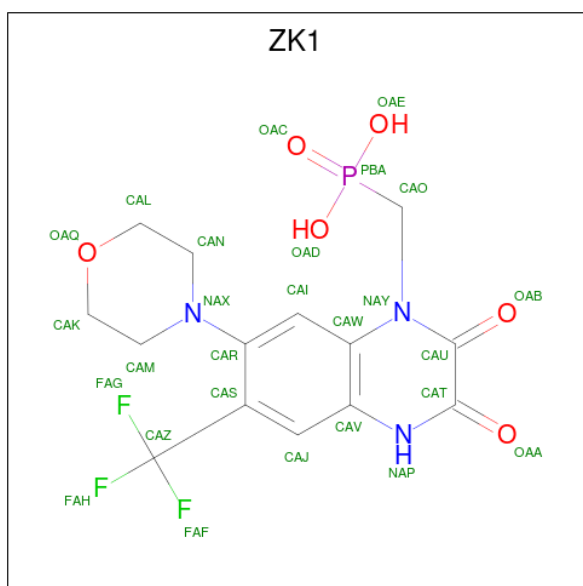
Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	2	Total	C	N	O		0	0
			28	16	2	10			
8	P	2	Total	C	N	O		0	0
			28	16	2	10			
8	Q	2	Total	C	N	O		0	0
			28	16	2	10			

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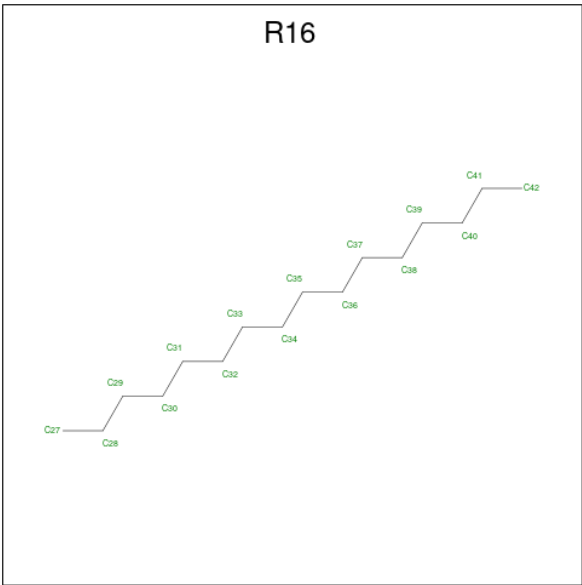
Mol	Chain	Residues	Atoms				AltConf	Trace
8	R	2	Total	C	N	O	0	0
			28	16	2	10		
8	S	2	Total	C	N	O	0	0
			28	16	2	10		
8	T	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (CCD ID: ZK1) (formula: C₁₄H₁₅F₃N₃O₆P).



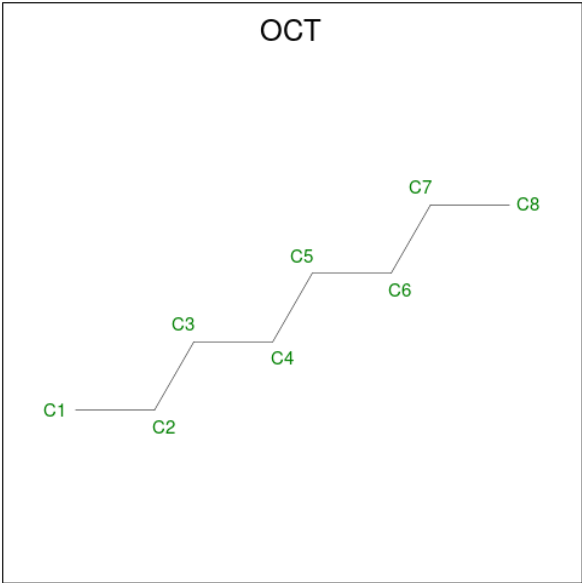
Mol	Chain	Residues	Atoms						AltConf
9	A	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
9	B	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
9	C	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
9	D	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	

- Molecule 10 is HEXADECANE (CCD ID: R16) (formula: C₁₆H₃₄).



Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	C	0
			13	13	
10	C	1	Total	C	0
			13	13	

- Molecule 11 is N-OCTANE (CCD ID: OCT) (formula: C₈H₁₈).



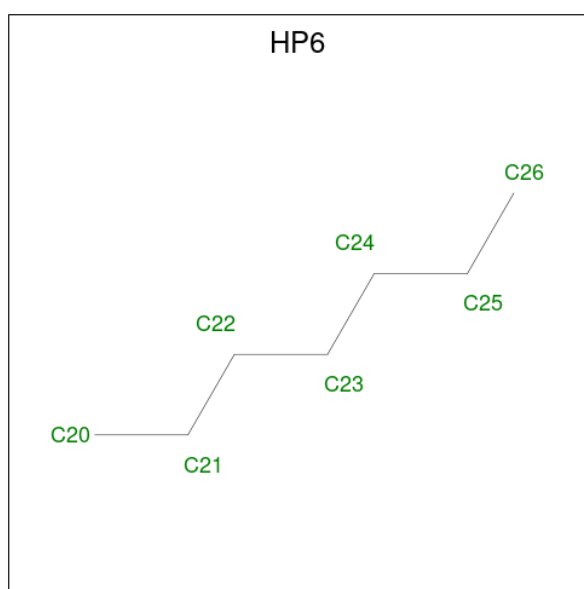
Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	C	0
			8	8	
11	B	1	Total	C	0
			8	8	

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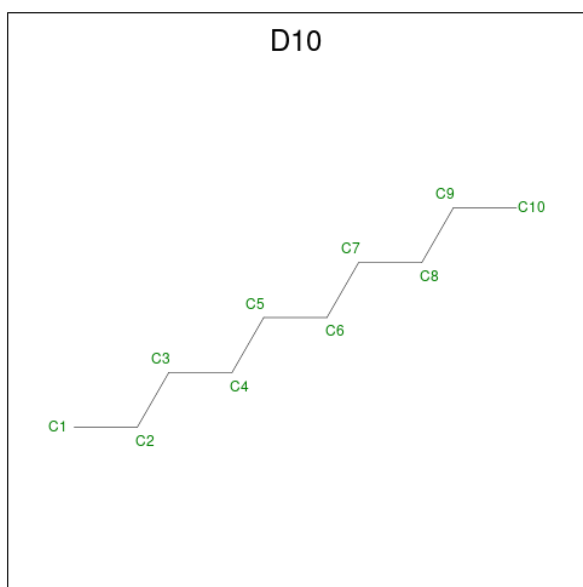
Mol	Chain	Residues	Atoms	AltConf
11	C	1	Total C 8 8	0
11	D	1	Total C 8 8	0
11	G	1	Total C 8 8	0
11	H	1	Total C 8 8	0

- Molecule 12 is HEPTANE (CCD ID: HP6) (formula: C_7H_{16}).



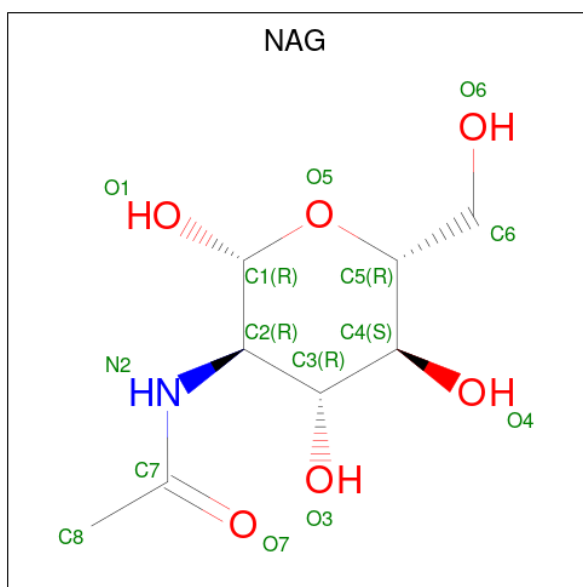
Mol	Chain	Residues	Atoms	AltConf
12	A	1	Total C 7 7	0
12	A	1	Total C 7 7	0
12	C	1	Total C 7 7	0
12	C	1	Total C 7 7	0

- Molecule 13 is DECANE (CCD ID: D10) (formula: $C_{10}H_{22}$).



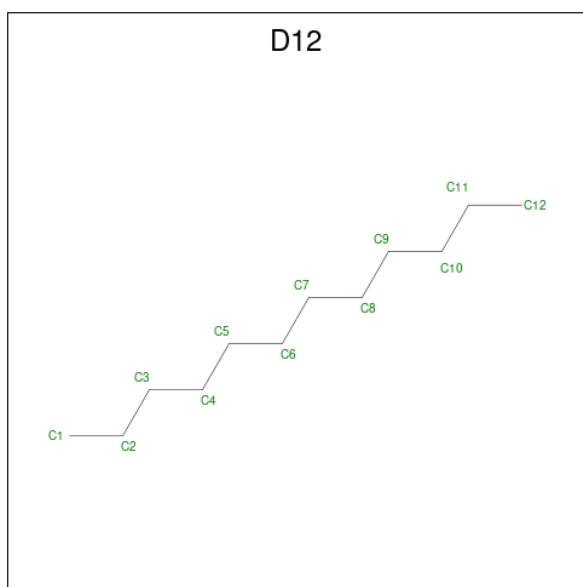
Mol	Chain	Residues	Atoms	AltConf
13	A	1	Total C 10 10	0
13	C	1	Total C 10 10	0
13	E	1	Total C 7 7	0
13	F	1	Total C 7 7	0
13	G	1	Total C 10 10	0
13	H	1	Total C 10 10	0

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



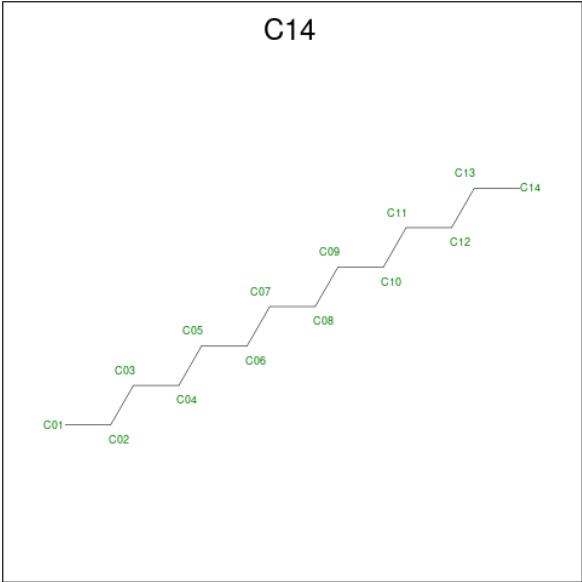
Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	C	N	O	0
			14	8	1	5	
14	A	1	Total	C	N	O	0
			14	8	1	5	
14	B	1	Total	C	N	O	0
			14	8	1	5	
14	C	1	Total	C	N	O	0
			14	8	1	5	
14	C	1	Total	C	N	O	0
			14	8	1	5	
14	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 15 is DODECANE (CCD ID: D12) (formula: C₁₂H₂₆).



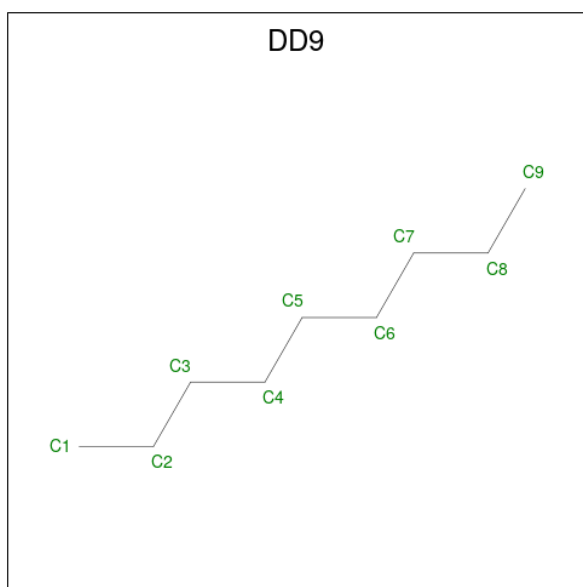
Mol	Chain	Residues	Atoms		AltConf
15	B	1	Total	C	0
			12	12	
15	D	1	Total	C	0
			12	12	
15	G	1	Total	C	0
			12	12	
15	G	1	Total	C	0
			12	12	
15	H	1	Total	C	0
			12	12	
15	H	1	Total	C	0
			12	12	

- Molecule 16 is TETRADECANE (CCD ID: C14) (formula: C₁₄H₃₀).



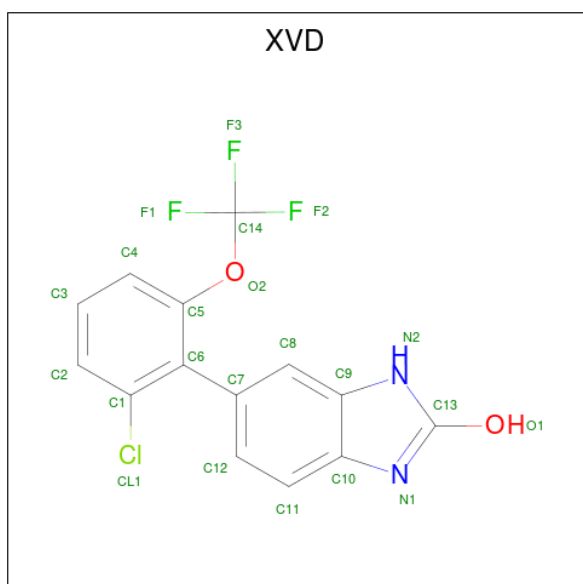
Mol	Chain	Residues	Atoms		AltConf
16	B	1	Total	C	0
			14	14	
16	D	1	Total	C	0
			14	14	
16	E	1	Total	C	0
			14	14	
16	F	1	Total	C	0
			14	14	
16	G	1	Total	C	0
			13	13	
16	H	1	Total	C	0
			13	13	

- Molecule 17 is nonane (CCD ID: DD9) (formula: C₉H₂₀).



Mol	Chain	Residues	Atoms	AltConf
17	B	1	Total C 8 8	0
17	B	1	Total C 9 9	0
17	D	1	Total C 8 8	0
17	D	1	Total C 9 9	0

- Molecule 18 is 6-[2-chloro-6-(trifluoromethoxy)phenyl]-1H-benzimidazol-2-ol (CCD ID: XVD) (formula: $C_{14}H_8ClF_3N_2O_2$) (labeled as "Ligand of Interest" by depositor).

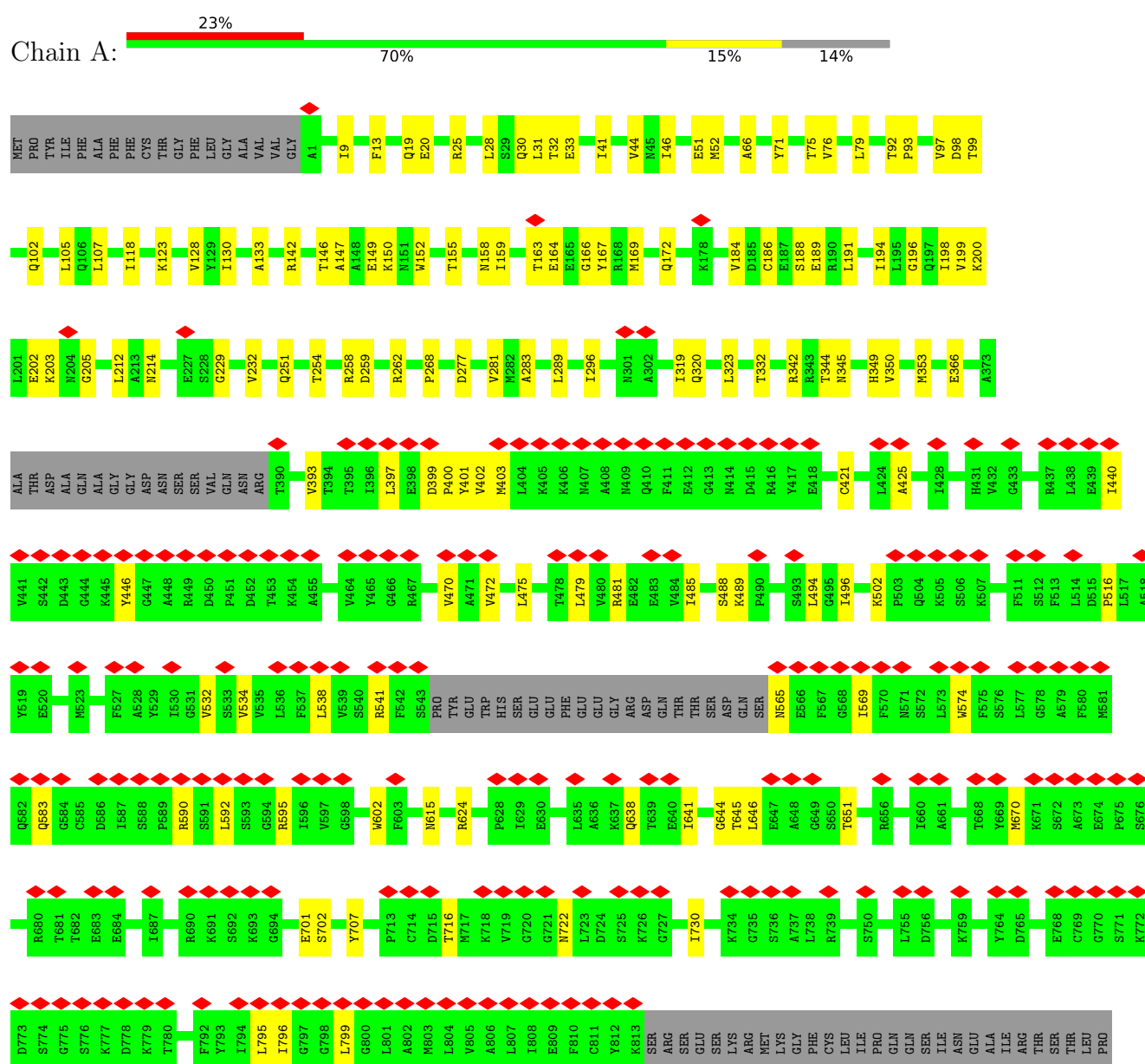


Mol	Chain	Residues	Atoms						AltConf
18	G	1	Total 22	C 14	Cl 1	F 3	N 2	O 2	0
18	H	1	Total 22	C 14	Cl 1	F 3	N 2	O 2	0

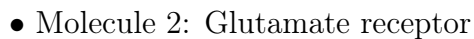
3 Residue-property plots

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

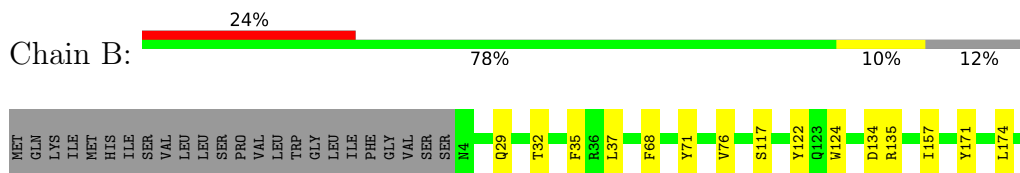
• Molecule 1: Glutamate receptor 1

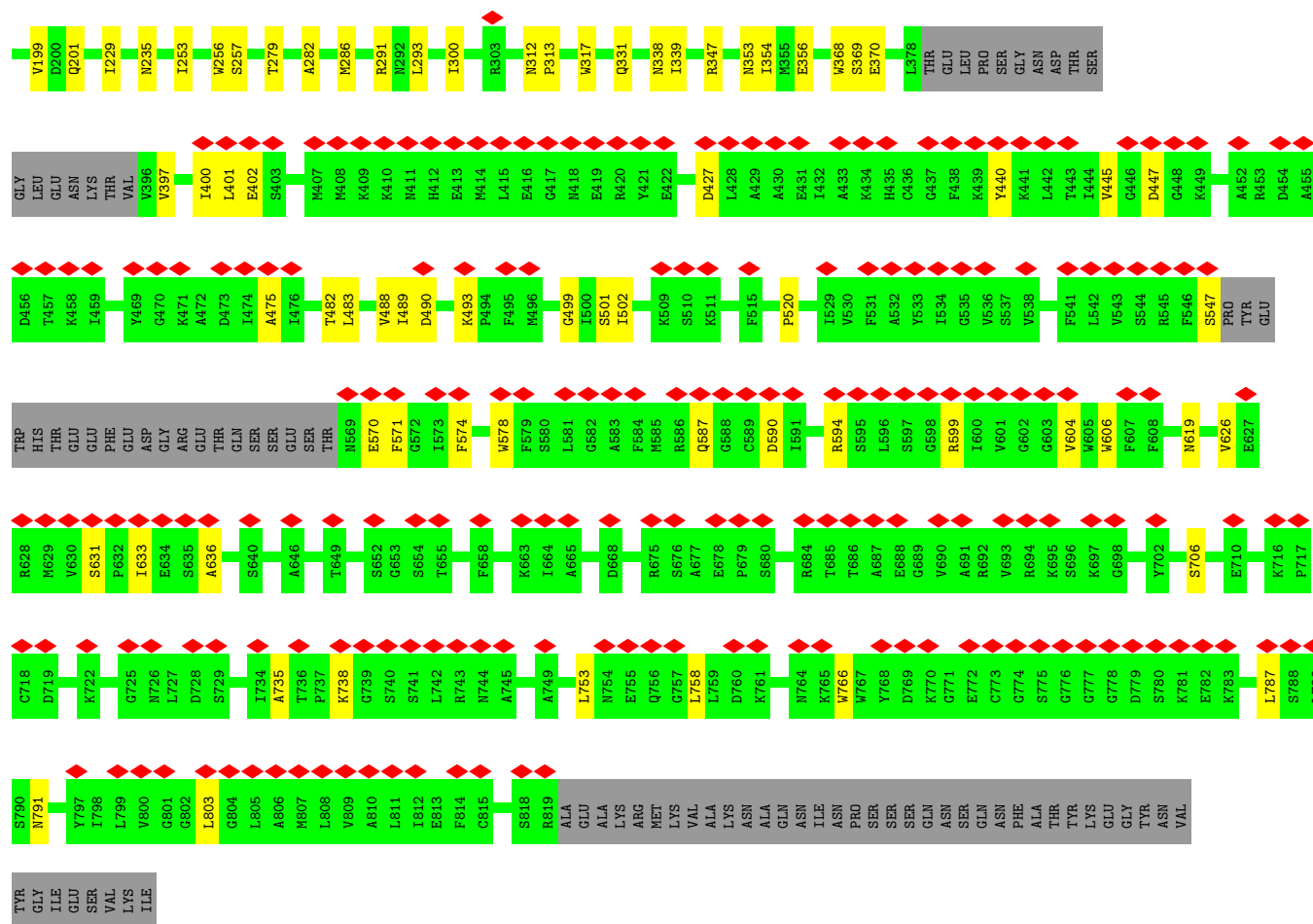


Chain C:

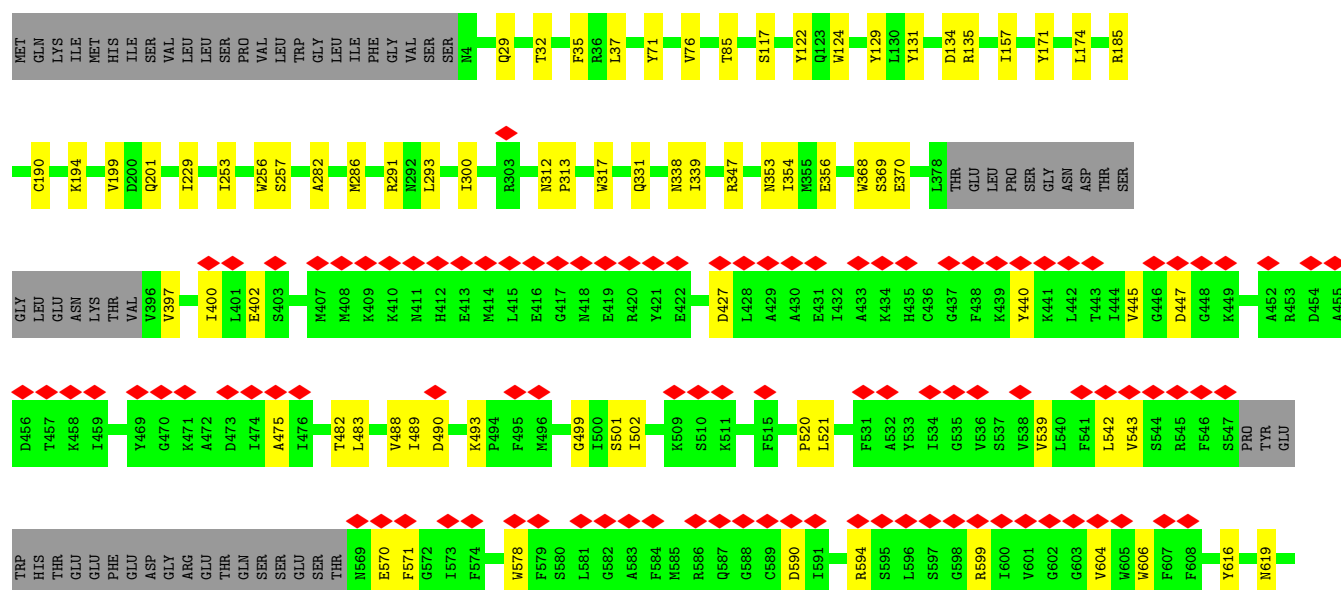
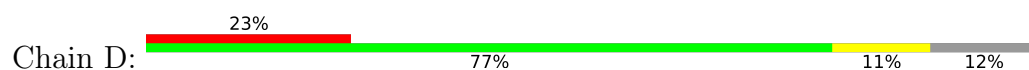


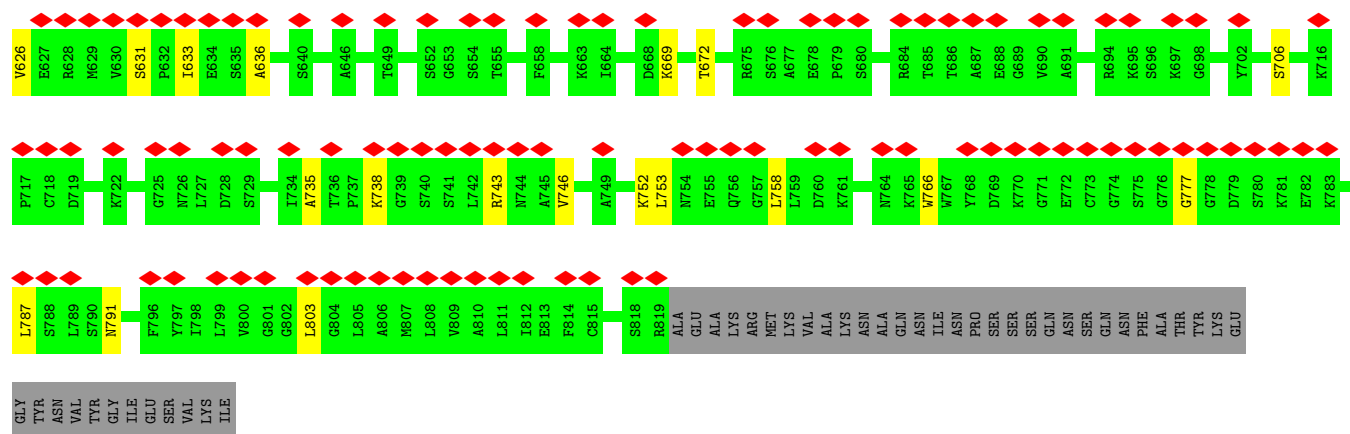
Chain B:



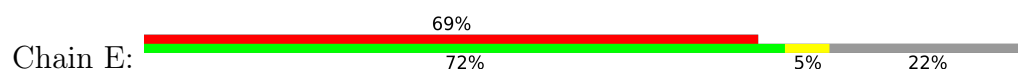


• Molecule 2: Glutamate receptor

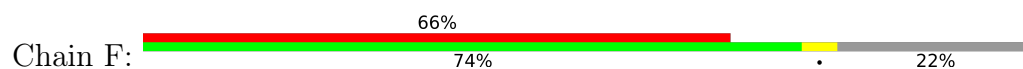




• Molecule 3: Protein cornichon homolog 2

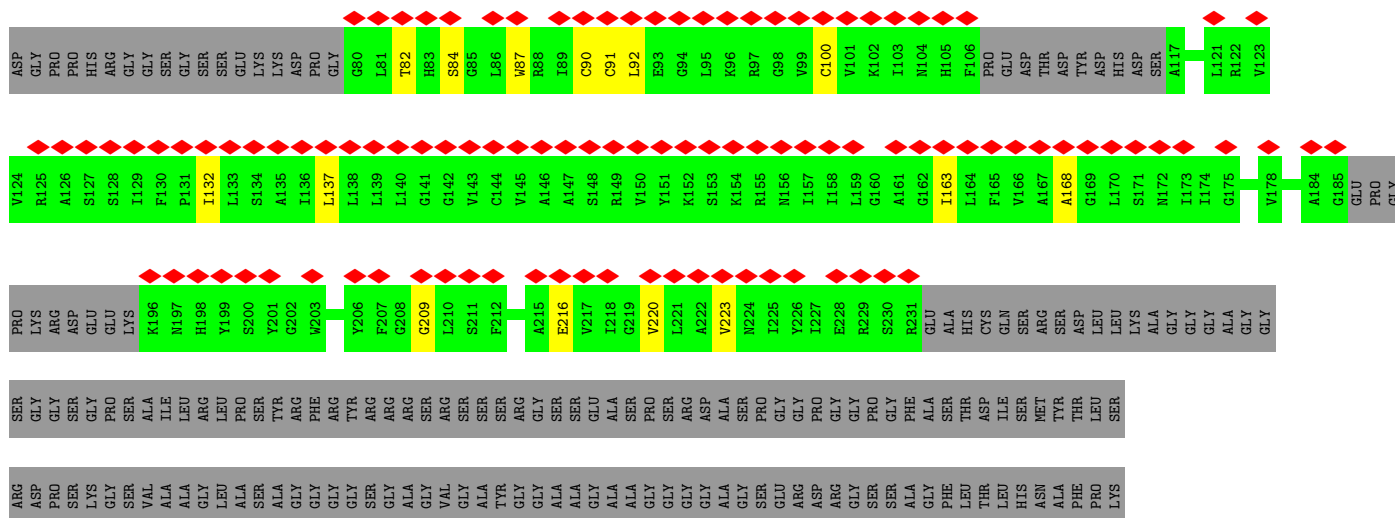


• Molecule 3: Protein cornichon homolog 2

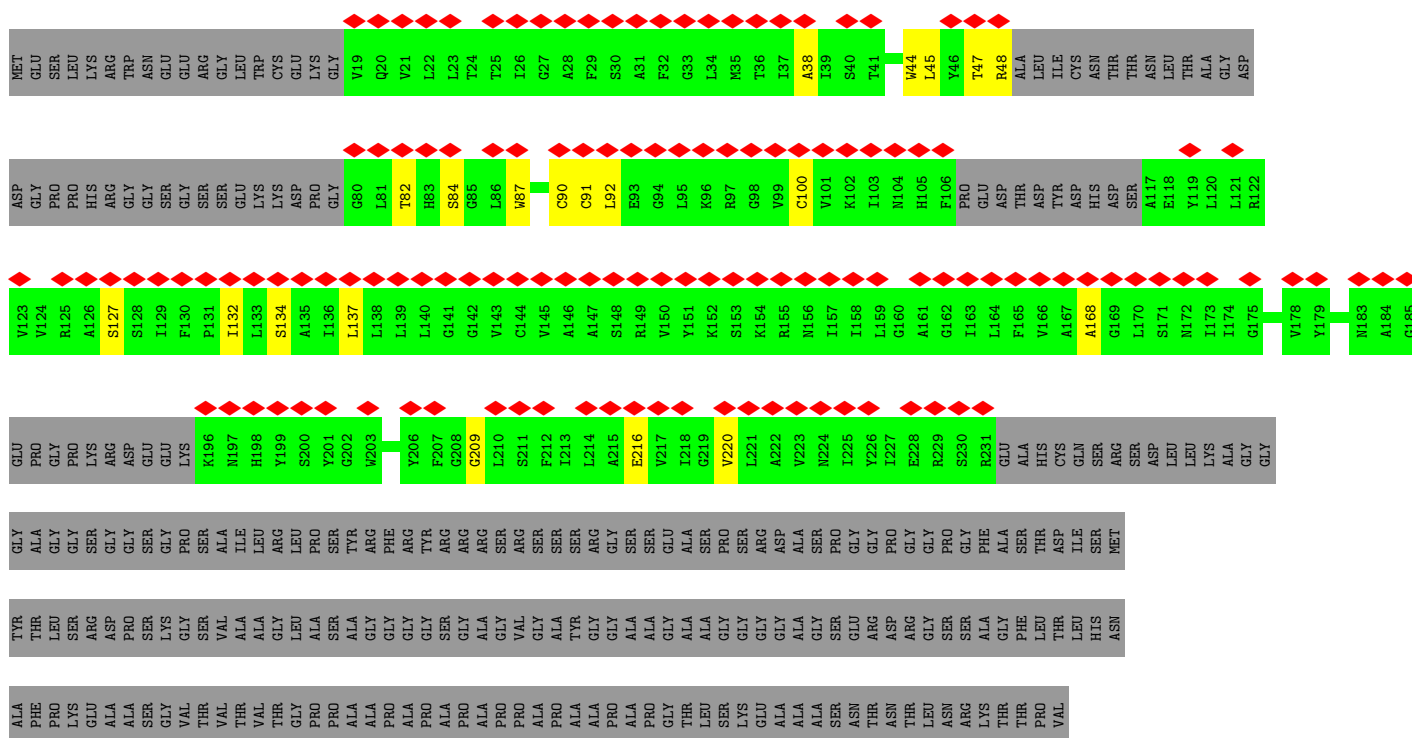


• Molecule 4: Voltage-dependent calcium channel gamma-8 subunit

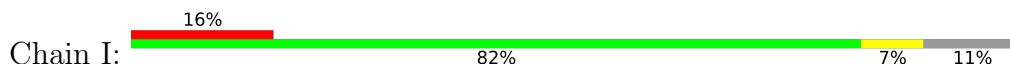




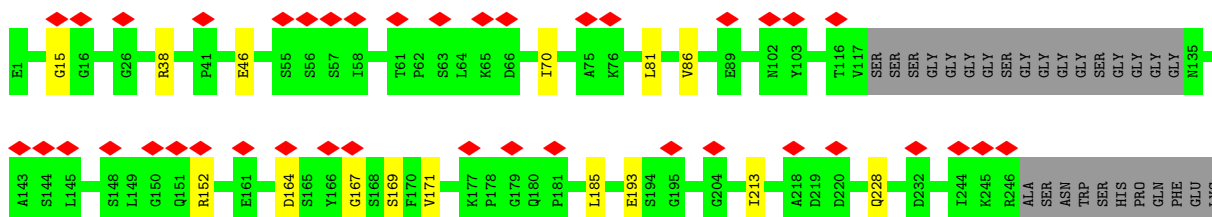
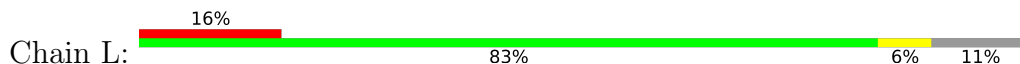
- Molecule 4: Voltage-dependent calcium channel gamma-8 subunit



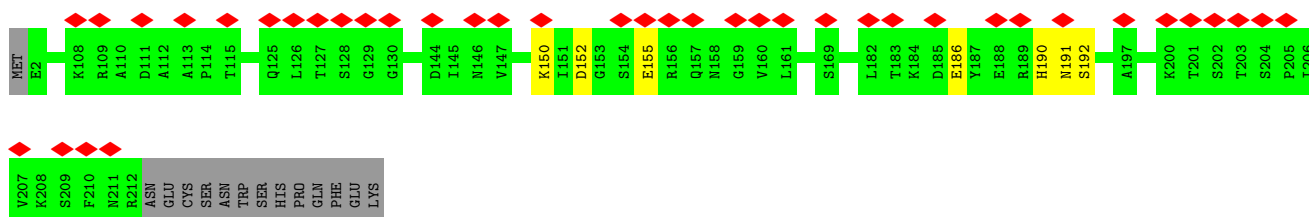
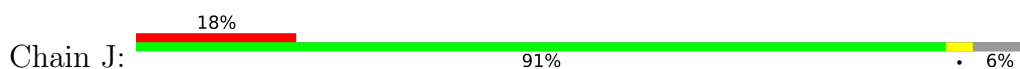
- Molecule 5: 11B8 scFv



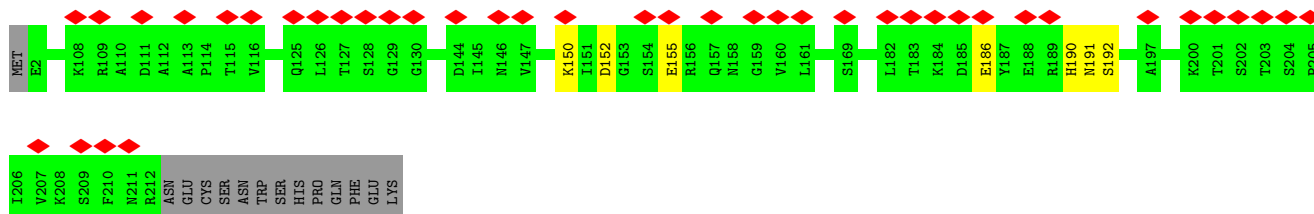
- Molecule 5: 11B8 scFv



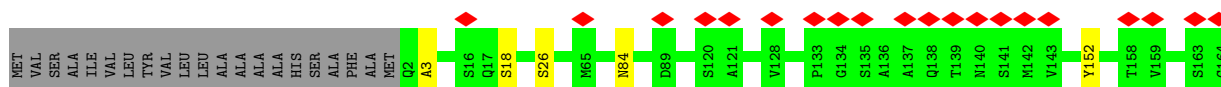
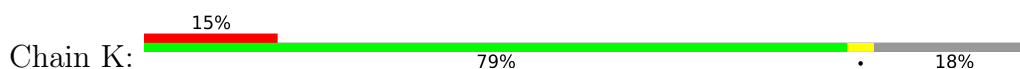
- Molecule 6: 15F1 Fab light chain

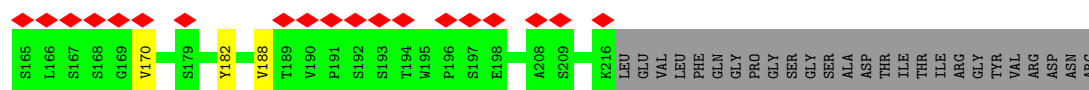


- Molecule 6: 15F1 Fab light chain

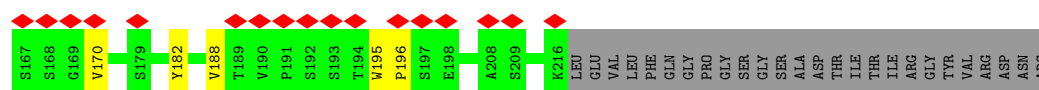
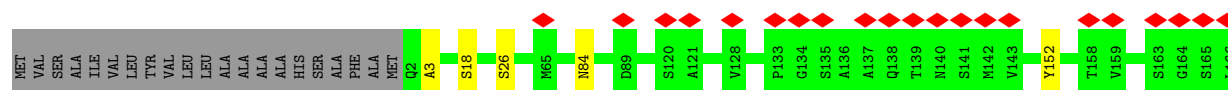
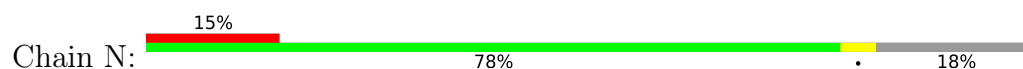


- Molecule 7: 15F1 Fab heavy chain





- Molecule 7: 15F1 Fab heavy chain



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  50% 50%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  50% 50%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	829000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.621	Depositor
Minimum map value	-0.962	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	515.51746, 515.51746, 515.51746	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.00687, 1.00687, 1.00687	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: OCT, HP6, XVD, R16, NAG, DD9, ZK1, D10, C14, D12

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	0.11	0/6007	0.26	0/8170
1	C	0.11	0/6007	0.26	0/8170
2	B	0.10	0/5811	0.24	0/7931
2	D	0.10	0/5811	0.24	0/7931
3	E	0.08	0/1005	0.25	0/1371
3	F	0.08	0/1009	0.25	0/1376
4	G	0.09	0/1154	0.26	0/1574
4	H	0.09	0/1154	0.26	0/1574
5	I	0.09	0/1122	0.25	0/1555
5	L	0.09	0/1122	0.25	0/1555
6	J	0.07	0/1041	0.23	0/1448
6	M	0.07	0/1041	0.23	0/1448
7	K	0.07	0/1058	0.24	0/1470
7	N	0.08	0/1058	0.24	0/1470
All	All	0.10	0/34400	0.25	0/47043

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5868	0	5591	92	0
1	C	5868	0	5591	93	0
2	B	5687	0	5261	53	0
2	D	5687	0	5261	57	0
3	E	974	0	923	5	0
3	F	978	0	927	3	0
4	G	1134	0	1096	14	0
4	H	1134	0	1096	15	0
5	I	1124	0	513	10	0
5	L	1124	0	513	8	0
6	J	1042	0	453	4	0
6	M	1042	0	453	4	0
7	K	1059	0	470	4	0
7	N	1059	0	470	5	0
8	O	28	0	25	0	0
8	P	28	0	25	1	0
8	Q	28	0	25	3	0
8	R	28	0	25	0	0
8	S	28	0	25	1	0
8	T	28	0	25	3	0
9	A	27	0	13	0	0
9	B	27	0	13	1	0
9	C	27	0	13	0	0
9	D	27	0	13	1	0
10	A	13	0	25	0	0
10	C	13	0	25	0	0
11	A	8	0	18	1	0
11	B	8	0	18	0	0
11	C	8	0	18	0	0
11	D	8	0	18	0	0
11	G	8	0	16	1	0
11	H	8	0	16	1	0
12	A	14	0	30	0	0
12	C	14	0	30	0	0
13	A	10	0	22	0	0
13	C	10	0	22	0	0
13	E	7	0	13	0	0
13	F	7	0	13	0	0
13	G	10	0	22	0	0
13	H	10	0	22	0	0
14	A	28	0	26	1	0
14	B	14	0	13	0	0
14	C	28	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	D	14	0	13	0	0
15	B	12	0	26	0	0
15	D	12	0	26	1	0
15	G	24	0	52	0	0
15	H	24	0	52	0	0
16	B	14	0	30	0	0
16	D	14	0	30	0	0
16	E	14	0	30	0	0
16	F	14	0	30	0	0
16	G	13	0	25	0	0
16	H	13	0	25	0	0
17	B	17	0	35	0	0
17	D	17	0	35	0	0
18	G	22	0	0	1	0
18	H	22	0	0	1	0
All	All	34528	0	29622	345	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 5.

All (345) 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:I:152:ARG:HA	5:I:213:ILE:O	1.82	0.80
5:L:152:ARG:HA	5:L:213:ILE:O	1.82	0.79
5:L:15:GLY:HA2	5:L:86:VAL:H	1.55	0.72
5:I:15:GLY:HA2	5:I:86:VAL:H	1.55	0.71
1:A:258:ARG:NH1	1:A:259:ASP:OD2	2.27	0.67
2:D:185:ARG:HH21	8:T:2:NAG:H81	1.59	0.67
2:B:185:ARG:HH21	8:Q:2:NAG:H81	1.59	0.66
1:C:258:ARG:NH1	1:C:259:ASP:OD2	2.27	0.66
1:C:199:VAL:HA	1:C:202:GLU:HG2	1.78	0.65
2:D:475:ALA:HB3	2:D:735:ALA:HB3	1.79	0.65
1:A:199:VAL:HA	1:A:202:GLU:HG2	1.78	0.65
2:B:475:ALA:HB3	2:B:735:ALA:HB3	1.78	0.64
1:A:196:GLY:O	1:A:200:LYS:NZ	2.31	0.63
1:C:196:GLY:O	1:C:200:LYS:NZ	2.31	0.63
2:B:338:ASN:O	2:B:347:ARG:NH2	2.33	0.62
2:D:400:ILE:HG23	2:D:402:GLU:H	1.65	0.62
2:B:400:ILE:HG23	2:B:402:GLU:H	1.65	0.62
2:D:338:ASN:O	2:D:347:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:520:PRO:O	2:B:619:ASN:ND2	2.33	0.61
1:C:133:ALA:HB2	1:C:158:ASN:HD21	1.65	0.61
1:A:133:ALA:HB2	1:A:158:ASN:HD21	1.65	0.61
8:S:1:NAG:O4	8:S:1:NAG:O7	2.19	0.61
1:C:502:LYS:H	1:C:716:THR:HA	1.66	0.60
1:A:142:ARG:NH1	1:A:146:THR:OG1	2.35	0.60
8:P:1:NAG:O4	8:P:1:NAG:O7	2.19	0.60
1:C:186:CYS:O	1:C:214:ASN:ND2	2.35	0.60
2:D:520:PRO:O	2:D:619:ASN:ND2	2.33	0.60
4:G:90:CYS:HA	4:G:100:CYS:HA	1.84	0.60
1:A:186:CYS:O	1:A:214:ASN:ND2	2.35	0.59
1:C:142:ARG:NH1	1:C:146:THR:OG1	2.35	0.59
4:H:90:CYS:HA	4:H:100:CYS:HA	1.84	0.59
2:B:122:TYR:OH	2:B:356:GLU:OE2	2.20	0.59
1:A:502:LYS:H	1:A:716:THR:HA	1.67	0.59
4:G:45:LEU:HB3	4:G:84:SER:HB3	1.84	0.58
1:A:289:LEU:HD11	1:A:319:ILE:HA	1.86	0.58
1:A:163:THR:HG23	1:A:166:GLY:H	1.69	0.58
2:B:199:VAL:HG13	2:B:229:ILE:HD11	1.86	0.58
1:A:130:ILE:HB	1:A:184:VAL:HG12	1.86	0.58
1:A:574:TRP:CG	2:D:599:ARG:HE	2.22	0.58
1:C:130:ILE:HB	1:C:184:VAL:HG12	1.86	0.57
1:C:163:THR:HG23	1:C:166:GLY:H	1.69	0.57
1:C:289:LEU:HD11	1:C:319:ILE:HA	1.85	0.57
4:H:45:LEU:HB3	4:H:84:SER:HB3	1.84	0.57
2:D:199:VAL:HG13	2:D:229:ILE:HD11	1.86	0.57
1:A:401:TYR:HB3	1:A:421:CYS:HB2	1.87	0.57
8:T:2:NAG:H83	8:T:2:NAG:H3	1.87	0.57
8:Q:2:NAG:H83	8:Q:2:NAG:H3	1.87	0.57
1:A:102:GLN:O	1:A:320:GLN:NE2	2.38	0.57
6:J:150:LYS:HA	6:J:155:GLU:HA	1.87	0.56
1:A:397:LEU:HB2	1:A:440:ILE:HD13	1.87	0.56
1:C:534:VAL:HG21	4:H:216:GLU:HB3	1.85	0.56
2:B:594:ARG:O	2:B:599:ARG:NH1	2.39	0.56
1:C:397:LEU:HB2	1:C:440:ILE:HD13	1.87	0.56
1:A:128:VAL:HG23	1:A:155:THR:HG23	1.88	0.56
2:B:570:GLU:HG2	2:B:571:PHE:H	1.71	0.56
2:D:787:LEU:HD11	2:D:791:ASN:HD21	1.69	0.56
3:E:35:ARG:HD3	3:E:128:LEU:HD21	1.86	0.56
1:C:128:VAL:HG23	1:C:155:THR:HG23	1.88	0.56
2:D:594:ARG:O	2:D:599:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:132:GLN:HE21	3:E:136:TRP:HE1	1.53	0.56
2:D:570:GLU:HG2	2:D:571:PHE:H	1.70	0.56
7:N:18:SER:HA	7:N:84:ASN:HA	1.88	0.56
1:C:102:GLN:O	1:C:320:GLN:NE2	2.38	0.55
1:C:702:SER:HB2	1:C:722:ASN:HD21	1.71	0.55
2:B:599:ARG:HE	1:C:574:TRP:CG	2.23	0.55
6:M:150:LYS:HA	6:M:155:GLU:HA	1.87	0.55
1:C:401:TYR:HB3	1:C:421:CYS:HB2	1.89	0.55
1:A:538:LEU:HD21	4:G:163:ILE:HD13	1.88	0.54
1:C:188:SER:OG	1:C:189:GLU:OE1	2.26	0.54
3:F:35:ARG:HD3	3:F:128:LEU:HD21	1.88	0.54
7:K:18:SER:HA	7:K:84:ASN:HA	1.88	0.54
4:G:220:VAL:HG11	11:G:505:OCT:H42	1.89	0.54
1:A:393:VAL:HG22	1:A:470:VAL:HB	1.89	0.54
1:A:538:LEU:HD13	4:G:223:VAL:HG21	1.90	0.54
2:B:499:GLY:O	2:B:706:SER:N	2.41	0.54
2:D:122:TYR:OH	2:D:356:GLU:OE2	2.20	0.54
1:A:20:GLU:OE1	1:A:20:GLU:N	2.39	0.54
1:C:644:GLY:HA2	1:C:670:MET:HE3	1.90	0.54
1:C:664:GLU:O	1:C:668:THR:HG23	2.08	0.54
4:H:220:VAL:HG11	11:H:505:OCT:H42	1.90	0.53
1:A:534:VAL:HG21	4:G:216:GLU:HB3	1.89	0.53
2:B:445:VAL:HG22	2:B:447:ASP:H	1.74	0.53
1:A:188:SER:OG	1:A:189:GLU:OE1	2.26	0.53
5:I:38:ARG:O	5:I:46:GLU:N	2.39	0.53
1:A:46:ILE:O	1:A:75:THR:OG1	2.25	0.53
1:A:702:SER:HB2	1:A:722:ASN:HD21	1.73	0.53
2:D:190:CYS:HB3	2:D:194:LYS:HB3	1.92	0.52
1:C:98:ASP:O	1:C:342:ARG:NH2	2.40	0.52
1:C:289:LEU:HD13	1:C:296:ILE:HD11	1.92	0.52
1:A:44:VAL:HG23	1:A:51:GLU:HG3	1.91	0.52
2:D:157:ILE:HD13	2:D:174:LEU:HD11	1.91	0.52
1:A:644:GLY:HA2	1:A:670:MET:HE3	1.91	0.52
1:C:516:PRO:O	1:C:615:ASN:ND2	2.41	0.52
1:C:20:GLU:OE1	1:C:20:GLU:N	2.39	0.52
1:C:399:ASP:OD2	1:C:446:TYR:OH	2.27	0.52
2:D:499:GLY:O	2:D:706:SER:N	2.43	0.52
3:F:132:GLN:HE21	3:F:136:TRP:HE1	1.56	0.52
4:G:82:THR:HB	4:G:91:CYS:HA	1.92	0.52
1:A:399:ASP:OD2	1:A:446:TYR:OH	2.28	0.51
1:A:345:ASN:N	1:A:366:GLU:OE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:LEU:HD22	2:D:539:VAL:HG11	1.90	0.51
2:B:157:ILE:HD13	2:B:174:LEU:HD11	1.91	0.51
2:B:190:CYS:HB3	2:B:194:LYS:HB3	1.91	0.51
4:H:82:THR:HB	4:H:91:CYS:HA	1.92	0.51
1:A:289:LEU:HD13	1:A:296:ILE:HD11	1.92	0.51
1:C:44:VAL:HG23	1:C:51:GLU:HG3	1.91	0.51
8:Q:1:NAG:O4	8:Q:1:NAG:O7	2.29	0.51
8:T:1:NAG:O4	8:T:1:NAG:O7	2.29	0.51
1:C:345:ASN:N	1:C:366:GLU:OE2	2.43	0.51
1:C:393:VAL:HG22	1:C:470:VAL:HB	1.92	0.51
5:L:38:ARG:O	5:L:46:GLU:N	2.39	0.51
1:C:169:MET:SD	1:C:172:GLN:NE2	2.84	0.50
1:C:595:ARG:HE	2:D:578:TRP:CG	2.30	0.50
1:C:759:LYS:O	1:C:763:TRP:HB2	2.11	0.50
1:A:98:ASP:O	1:A:342:ARG:NH2	2.40	0.50
1:A:205:GLY:HA3	1:A:229:GLY:H	1.76	0.50
4:H:209:GLY:HA3	18:H:504:XVD:CL1	2.49	0.50
7:K:3:ALA:HA	7:K:26:SER:O	2.12	0.50
1:C:205:GLY:HA3	1:C:229:GLY:H	1.76	0.50
1:A:169:MET:SD	1:A:172:GLN:NE2	2.84	0.50
7:K:170:VAL:HA	7:K:188:VAL:HA	1.94	0.49
1:C:9:ILE:HD12	1:C:66:ALA:HB3	1.94	0.49
1:C:402:VAL:HG23	1:C:421:CYS:HB3	1.95	0.49
1:A:402:VAL:HG23	1:A:421:CYS:HB3	1.93	0.49
4:G:209:GLY:HA3	18:G:504:XVD:CL1	2.49	0.49
7:N:3:ALA:HA	7:N:26:SER:O	2.12	0.49
1:A:9:ILE:HD12	1:A:66:ALA:HB3	1.94	0.49
1:A:595:ARG:HE	2:B:578:TRP:CG	2.31	0.49
1:C:32:THR:N	1:C:33:GLU:OE1	2.46	0.49
1:C:638:GLN:HE22	1:C:641:ILE:HG13	1.79	0.48
7:N:170:VAL:HA	7:N:188:VAL:HA	1.94	0.48
1:A:19:GLN:HE22	1:A:268:PRO:HA	1.78	0.48
1:C:400:PRO:HA	1:C:403:MET:HE3	1.95	0.48
1:A:488:SER:O	2:D:493:LYS:NZ	2.47	0.48
1:A:541:ARG:NH1	1:A:565:ASN:O	2.46	0.48
1:C:254:THR:O	1:C:258:ARG:HG2	2.14	0.48
1:C:639:THR:H	2:D:777:GLY:HA3	1.78	0.48
1:A:32:THR:N	1:A:33:GLU:OE1	2.46	0.48
1:A:638:GLN:HE22	1:A:641:ILE:HG13	1.79	0.48
1:A:105:LEU:HD11	1:A:323:LEU:HB3	1.96	0.47
1:A:496:ILE:HD13	1:A:651:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:LEU:HD21	1:C:481:ARG:HD3	1.96	0.47
2:D:539:VAL:O	2:D:543:VAL:HG23	2.14	0.47
2:B:493:LYS:NZ	1:C:488:SER:O	2.47	0.47
4:H:87:TRP:HZ2	4:H:132:ILE:HD11	1.79	0.47
2:B:604:VAL:HG12	1:C:795:LEU:HD12	1.95	0.47
1:A:400:PRO:HA	1:A:403:MET:HE3	1.95	0.47
2:D:312:ASN:HD22	2:D:313:PRO:HA	1.80	0.47
1:A:254:THR:O	1:A:258:ARG:HG2	2.14	0.47
1:C:262:ARG:HG3	5:I:167:GLY:HA3	1.97	0.47
1:C:496:ILE:HD13	1:C:651:THR:HG23	1.96	0.47
2:B:631:SER:OG	2:B:633:ILE:O	2.31	0.47
1:C:19:GLN:HE22	1:C:268:PRO:HA	1.78	0.47
2:B:312:ASN:HD22	2:B:313:PRO:HA	1.80	0.47
1:C:71:TYR:HB3	1:C:79:LEU:HD12	1.97	0.47
4:H:91:CYS:SG	4:H:92:LEU:N	2.88	0.47
1:C:481:ARG:O	1:C:485:ILE:HG22	2.15	0.47
1:C:488:SER:OG	1:C:489:LYS:N	2.48	0.47
1:A:163:THR:O	1:A:167:TYR:N	2.41	0.47
1:C:425:ALA:HB2	1:C:472:VAL:HG11	1.97	0.47
2:B:369:SER:OG	2:B:370:GLU:N	2.48	0.47
1:C:105:LEU:HD11	1:C:323:LEU:HB3	1.96	0.47
2:D:29:GLN:NE2	2:D:29:GLN:O	2.47	0.47
4:H:134:SER:OG	4:H:168:ALA:O	2.32	0.47
1:A:488:SER:OG	1:A:489:LYS:N	2.48	0.46
1:C:541:ARG:NH1	1:C:565:ASN:O	2.48	0.46
1:A:349:HIS:CE1	14:A:907:NAG:H82	2.51	0.46
1:C:349:HIS:CE1	14:C:907:NAG:H82	2.51	0.46
3:F:16:LEU:O	3:F:19:SER:OG	2.33	0.46
1:A:592:LEU:HA	2:B:574:PHE:HZ	1.79	0.46
1:C:199:VAL:HG22	1:C:203:LYS:HD3	1.97	0.46
5:I:164:ASP:HA	5:I:169:SER:HA	1.98	0.46
1:A:71:TYR:HB3	1:A:79:LEU:HD12	1.97	0.46
1:A:481:ARG:O	1:A:485:ILE:HG22	2.16	0.46
2:B:29:GLN:O	2:B:29:GLN:NE2	2.47	0.46
2:B:235:ASN:OD1	2:B:235:ASN:N	2.46	0.46
1:C:25:ARG:HD3	1:C:262:ARG:HH12	1.80	0.46
1:C:46:ILE:O	1:C:75:THR:OG1	2.25	0.46
2:D:134:ASP:OD1	2:D:135:ARG:N	2.49	0.46
2:D:354:ILE:HD11	2:D:368:TRP:HB2	1.98	0.46
2:D:427:ASP:OD2	2:D:766:TRP:NE1	2.43	0.46
4:G:87:TRP:HZ2	4:G:132:ILE:HD11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:185:LEU:O	5:L:193:GLU:N	2.49	0.46
1:A:25:ARG:HD3	1:A:262:ARG:HH12	1.80	0.46
1:A:475:LEU:HD21	1:A:481:ARG:HD3	1.97	0.46
1:C:158:ASN:OD1	1:C:159:ILE:N	2.49	0.46
1:C:537:PHE:CE2	4:H:220:VAL:HG23	2.51	0.46
2:D:369:SER:OG	2:D:370:GLU:N	2.48	0.46
1:C:30:GLN:NE2	1:C:251:GLN:OE1	2.50	0.45
2:B:32:THR:HG21	2:B:291:ARG:HD2	1.98	0.45
1:C:97:VAL:HG22	1:C:99:THR:H	1.81	0.45
1:C:645:THR:OG1	1:C:646:LEU:N	2.49	0.45
2:D:590:ASP:OD1	2:D:590:ASP:N	2.48	0.45
1:A:30:GLN:NE2	1:A:251:GLN:OE1	2.50	0.45
1:A:199:VAL:HG22	1:A:203:LYS:HD3	1.98	0.45
1:A:583:GLN:HG3	2:D:606:TRP:CG	2.51	0.45
2:B:501:SER:OG	2:B:502:ILE:N	2.50	0.45
1:C:163:THR:O	1:C:167:TYR:N	2.41	0.45
4:G:91:CYS:SG	4:G:92:LEU:N	2.88	0.45
1:A:31:LEU:HD22	1:A:283:ALA:HB2	1.99	0.45
1:A:532:VAL:HA	2:B:803:LEU:HD21	1.99	0.45
1:A:624:ARG:NH2	2:D:626:VAL:O	2.50	0.45
5:I:185:LEU:O	5:I:193:GLU:N	2.49	0.45
5:L:70:ILE:HA	5:L:81:LEU:HA	1.98	0.45
1:A:796:ILE:HG21	3:E:11:MET:HG2	1.99	0.45
5:L:164:ASP:HA	5:L:169:SER:HA	1.97	0.45
1:A:277:ASP:OD2	1:A:332:THR:OG1	2.22	0.45
1:A:472:VAL:HA	1:A:730:ILE:HG22	1.99	0.45
2:B:293:LEU:HD13	2:B:300:ILE:HD13	1.99	0.45
6:M:186:GLU:O	6:M:190:HIS:N	2.49	0.45
2:B:354:ILE:HD11	2:B:368:TRP:HB2	1.98	0.45
1:C:590:ARG:O	1:C:595:ARG:NH1	2.50	0.45
6:J:186:GLU:O	6:J:190:HIS:N	2.49	0.45
2:B:124:TRP:CD2	2:B:185:ARG:HD3	2.52	0.44
1:A:158:ASN:OD1	1:A:159:ILE:N	2.49	0.44
1:A:191:LEU:HD21	1:A:212:LEU:HD22	1.99	0.44
1:A:516:PRO:O	1:A:615:ASN:ND2	2.50	0.44
1:C:421:CYS:SG	1:C:472:VAL:HG22	2.58	0.44
2:D:32:THR:HG21	2:D:291:ARG:HD2	1.98	0.44
1:A:590:ARG:O	1:A:595:ARG:NH1	2.51	0.44
1:A:645:THR:OG1	1:A:646:LEU:N	2.50	0.44
7:N:152:TYR:O	7:N:182:TYR:N	2.49	0.44
1:C:169:MET:O	1:C:172:GLN:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:743:ARG:HA	2:D:746:VAL:HG22	1.98	0.44
1:A:97:VAL:HG22	1:A:99:THR:H	1.81	0.44
1:A:569:ILE:HG12	4:G:220:VAL:HG21	1.99	0.44
2:D:124:TRP:CD2	2:D:185:ARG:HD3	2.52	0.44
2:D:445:VAL:HG22	2:D:447:ASP:H	1.82	0.44
2:D:502:ILE:HD11	2:D:636:ALA:HB2	1.99	0.44
1:C:31:LEU:HD22	1:C:283:ALA:HB2	1.99	0.44
1:C:52:MET:HE3	1:C:52:MET:HB3	1.90	0.44
1:C:118:ILE:HD11	1:C:350:VAL:HG21	2.00	0.44
2:D:35:PHE:HE2	2:D:37:LEU:HG	1.83	0.44
2:D:501:SER:OG	2:D:502:ILE:N	2.49	0.44
1:C:532:VAL:HG22	2:D:803:LEU:HD11	1.99	0.44
2:D:293:LEU:HD13	2:D:300:ILE:HD13	1.99	0.44
2:B:134:ASP:OD1	2:B:135:ARG:N	2.49	0.44
2:B:502:ILE:HD11	2:B:636:ALA:HB2	1.99	0.44
5:I:70:ILE:HA	5:I:81:LEU:HA	1.98	0.43
4:G:137:LEU:HB2	4:G:168:ALA:HB2	2.00	0.43
1:A:28:LEU:HD23	1:A:28:LEU:HA	1.86	0.43
1:C:191:LEU:HD21	1:C:212:LEU:HD22	1.98	0.43
1:C:569:ILE:HG12	4:H:220:VAL:HG21	2.00	0.43
2:B:35:PHE:HE2	2:B:37:LEU:HG	1.83	0.43
2:B:606:TRP:CG	1:C:583:GLN:HG3	2.53	0.43
2:B:787:LEU:HD11	2:B:791:ASN:HD21	1.83	0.43
7:N:195:TRP:HA	7:N:196:PRO:HA	1.73	0.43
1:A:52:MET:HE3	1:A:52:MET:HB3	1.90	0.43
1:A:425:ALA:HB2	1:A:472:VAL:HG11	2.00	0.43
1:A:118:ILE:HD11	1:A:350:VAL:HG21	2.00	0.43
1:A:169:MET:O	1:A:172:GLN:HG2	2.18	0.43
2:B:427:ASP:OD2	2:B:766:TRP:NE1	2.42	0.43
2:B:633:ILE:HD12	2:B:633:ILE:HA	1.93	0.43
1:A:13:PHE:HD2	1:A:41:ILE:HG23	1.84	0.43
1:A:421:CYS:SG	1:A:472:VAL:HG22	2.59	0.43
1:C:13:PHE:HD2	1:C:41:ILE:HG23	1.84	0.43
1:C:472:VAL:HA	1:C:730:ILE:HG22	2.01	0.43
4:H:137:LEU:HB2	4:H:168:ALA:HB2	2.00	0.43
2:D:317:TRP:CD1	2:D:317:TRP:H	2.37	0.43
2:D:397:VAL:HG23	2:D:440:TYR:HB2	2.01	0.43
1:C:194:ILE:O	1:C:198:ILE:HG12	2.19	0.42
1:A:71:TYR:HE1	1:A:92:THR:HG21	1.83	0.42
1:A:258:ARG:HG3	1:A:259:ASP:H	1.84	0.42
1:C:71:TYR:HE1	1:C:92:THR:HG21	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:753:LEU:HD22	2:D:758:LEU:HD23	2.01	0.42
2:B:317:TRP:CD1	2:B:317:TRP:H	2.37	0.42
1:A:147:ALA:HB1	1:A:152:TRP:HB2	2.02	0.42
1:C:147:ALA:HB1	1:C:152:TRP:HB2	2.02	0.42
5:I:232:ASP:HA	5:I:233:PRO:HA	1.80	0.42
1:A:194:ILE:O	1:A:198:ILE:HG12	2.19	0.42
1:C:149:GLU:OE1	1:C:150:LYS:HG3	2.19	0.42
1:C:258:ARG:HG3	1:C:259:ASP:H	1.84	0.42
2:D:488:VAL:HG13	2:D:489:ILE:HG13	2.01	0.42
6:M:152:ASP:HA	6:M:192:SER:H	1.85	0.42
1:A:93:PRO:HA	1:A:107:LEU:HB2	2.01	0.42
2:B:171:TYR:CD2	2:B:201:GLN:HG3	2.55	0.42
2:B:753:LEU:HD22	2:B:758:LEU:HD23	2.02	0.42
7:K:152:TYR:O	7:K:182:TYR:N	2.49	0.42
2:B:490:ASP:OD2	2:B:738:LYS:NZ	2.51	0.42
1:A:79:LEU:HD23	1:A:79:LEU:HA	1.88	0.42
1:A:123:LYS:HD2	1:A:123:LYS:HA	1.98	0.42
1:A:149:GLU:OE1	1:A:150:LYS:HG3	2.19	0.42
2:B:547:SER:O	2:B:547:SER:OG	2.33	0.42
2:B:590:ASP:OD1	2:B:590:ASP:N	2.48	0.42
1:C:400:PRO:HB3	1:C:707:TYR:CZ	2.55	0.42
4:H:47:THR:OG1	4:H:48:ARG:N	2.53	0.42
5:I:171:VAL:HA	5:I:228:GLN:HA	2.02	0.42
1:A:795:LEU:HD12	2:D:604:VAL:HG12	2.01	0.42
2:B:282:ALA:O	2:B:286:MET:HG3	2.20	0.42
2:D:490:ASP:OD2	2:D:738:LYS:NZ	2.53	0.42
2:D:631:SER:OG	2:D:633:ILE:O	2.33	0.42
9:D:906:ZK1:HAOA	9:D:906:ZK1:HAI	1.82	0.42
11:A:903:OCT:H62	15:D:901:D12:H12	2.00	0.41
2:D:171:TYR:CD2	2:D:201:GLN:HG3	2.55	0.41
2:D:282:ALA:O	2:D:286:MET:HG3	2.20	0.41
2:B:253:ILE:HA	2:B:256:TRP:HB3	2.03	0.41
2:B:482:THR:OG1	2:B:483:LEU:N	2.54	0.41
2:B:488:VAL:HG13	2:B:489:ILE:HG13	2.02	0.41
1:C:93:PRO:HA	1:C:107:LEU:HB2	2.01	0.41
1:A:163:THR:OG1	1:A:164:GLU:N	2.54	0.41
1:C:489:LYS:HD3	1:C:489:LYS:HA	1.87	0.41
2:D:71:TYR:CD2	2:D:76:VAL:HG22	2.55	0.41
1:A:479:LEU:HD22	2:D:752:LYS:HD3	2.03	0.41
2:B:397:VAL:HG23	2:B:440:TYR:HB2	2.00	0.41
1:C:683:GLU:O	1:C:687:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:47:THR:OG1	4:G:48:ARG:N	2.53	0.41
6:J:152:ASP:HA	6:J:192:SER:H	1.85	0.41
1:A:262:ARG:HG3	5:L:167:GLY:HA3	2.02	0.41
4:H:38:ALA:O	4:H:44:TRP:NE1	2.53	0.41
2:B:71:TYR:CD2	2:B:76:VAL:HG22	2.55	0.41
2:B:331:GLN:HA	2:B:339:ILE:O	2.21	0.41
1:C:52:MET:HG3	1:C:75:THR:HG21	2.02	0.41
1:C:55:ARG:HD3	1:C:55:ARG:HA	1.91	0.41
1:C:502:LYS:N	1:C:716:THR:HA	2.34	0.41
1:C:660:ILE:HG22	1:C:662:VAL:H	1.86	0.41
4:H:127:SER:O	4:H:127:SER:OG	2.36	0.41
5:L:171:VAL:HA	5:L:228:GLN:HA	2.02	0.41
6:M:152:ASP:HA	6:M:191:ASN:H	1.86	0.41
1:C:123:LYS:HD2	1:C:123:LYS:HA	1.98	0.41
6:J:152:ASP:HA	6:J:191:ASN:H	1.86	0.41
2:D:253:ILE:HA	2:D:256:TRP:HB3	2.03	0.40
2:D:331:GLN:HA	2:D:339:ILE:O	2.21	0.40
1:A:400:PRO:HB3	1:A:707:TYR:CZ	2.56	0.40
1:A:489:LYS:HA	1:A:489:LYS:HD3	1.88	0.40
1:C:163:THR:OG1	1:C:164:GLU:N	2.54	0.40
1:C:587:ILE:HD12	1:C:587:ILE:HA	1.98	0.40
1:C:590:ARG:HH11	1:C:595:ARG:HH12	1.68	0.40
2:D:129:TYR:CE2	2:D:131:TYR:HB3	2.56	0.40
5:I:6:GLU:HA	5:I:21:SER:O	2.21	0.40
1:A:602:TRP:CE2	2:B:587:GLN:HG3	2.56	0.40
2:B:68:PHE:CZ	2:B:279:THR:HG23	2.56	0.40
2:B:400:ILE:HG13	2:B:401:LEU:H	1.86	0.40
9:B:901:ZK1:HAI	9:B:901:ZK1:HAOA	1.82	0.40
1:C:50:PHE:CD2	2:D:85:THR:HG21	2.57	0.40
2:D:482:THR:OG1	2:D:483:LEU:N	2.54	0.40
2:D:521:LEU:HD13	2:D:616:TYR:HD2	1.85	0.40
3:E:154:VAL:O	3:E:158:VAL:HG12	2.21	0.40
1:A:494:LEU:HD12	1:A:701:GLU:HB3	2.04	0.40
2:B:626:VAL:O	1:C:624:ARG:NH2	2.54	0.40
2:D:400:ILE:HD12	2:D:400:ILE:HA	1.99	0.40
2:D:542:LEU:HD21	3:E:74:ILE:HD11	2.03	0.40
4:G:38:ALA:O	4:G:44:TRP:NE1	2.53	0.40
1:A:232:VAL:HG22	1:A:353:MET:HB3	2.03	0.40
1:C:137:LEU:HD23	1:C:137:LEU:HA	1.96	0.40
2:D:669:LYS:HA	2:D:672:THR:HG22	2.02	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	771/907 (85%)	749 (97%)	22 (3%)	0	100	100
1	C	771/907 (85%)	750 (97%)	21 (3%)	0	100	100
2	B	772/883 (87%)	753 (98%)	19 (2%)	0	100	100
2	D	772/883 (87%)	754 (98%)	18 (2%)	0	100	100
3	E	118/160 (74%)	117 (99%)	1 (1%)	0	100	100
3	F	118/160 (74%)	117 (99%)	1 (1%)	0	100	100
4	G	154/423 (36%)	151 (98%)	3 (2%)	0	100	100
4	H	154/423 (36%)	151 (98%)	3 (2%)	0	100	100
5	I	225/257 (88%)	213 (95%)	12 (5%)	0	100	100
5	L	225/257 (88%)	213 (95%)	12 (5%)	0	100	100
6	J	209/225 (93%)	197 (94%)	12 (6%)	0	100	100
6	M	209/225 (93%)	196 (94%)	13 (6%)	0	100	100
7	K	213/262 (81%)	207 (97%)	6 (3%)	0	100	100
7	N	213/262 (81%)	207 (97%)	6 (3%)	0	100	100
All	All	4924/6234 (79%)	4775 (97%)	149 (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	A	583/770 (76%)	580 (100%)	3 (0%)	81	81
1	C	583/770 (76%)	580 (100%)	3 (0%)	81	81
2	B	551/755 (73%)	548 (100%)	3 (0%)	81	81
2	D	551/755 (73%)	548 (100%)	3 (0%)	81	81
3	E	95/143 (66%)	95 (100%)	0	100	100
3	F	96/143 (67%)	96 (100%)	0	100	100
4	G	105/310 (34%)	105 (100%)	0	100	100
4	H	105/310 (34%)	105 (100%)	0	100	100
All	All	2669/3956 (68%)	2657 (100%)	12 (0%)	81	83

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	VAL
1	A	281	VAL
1	A	344	THR
2	B	117	SER
2	B	257	SER
2	B	353	ASN
1	C	76	VAL
1	C	281	VAL
1	C	344	THR
2	D	117	SER
2	D	257	SER
2	D	353	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	349	HIS
1	A	431	HIS
1	A	571	ASN
1	A	722	ASN
2	B	161	ASN
2	B	312	ASN
2	B	418	ASN
2	B	714	GLN
2	B	756	GLN

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Mol	Chain	Res	Type
1	C	19	GLN
1	C	349	HIS
1	C	431	HIS
1	C	722	ASN
2	D	161	ASN
2	D	312	ASN
2	D	418	ASN
2	D	756	GLN
2	D	791	ASN
3	E	75	HIS
3	E	94	ASN
3	E	132	GLN
3	F	75	HIS
3	F	94	ASN
3	F	132	GLN
4	G	172	ASN
4	H	172	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

12 monosaccharides 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	$\# Z > 2$
8	NAG	O	1	8,1	14,14,15	0.18	0	17,19,21	0.43	0
8	NAG	O	2	8	14,14,15	0.22	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	P	1	8,1	14,14,15	0.61	1 (7%)	17,19,21	0.77	0
8	NAG	P	2	8	14,14,15	0.48	0	17,19,21	0.35	0
8	NAG	Q	1	2,8	14,14,15	0.56	0	17,19,21	0.76	0
8	NAG	Q	2	8	14,14,15	0.46	0	17,19,21	1.32	2 (11%)
8	NAG	R	1	8,1	14,14,15	0.20	0	17,19,21	0.44	0
8	NAG	R	2	8	14,14,15	0.22	0	17,19,21	0.42	0
8	NAG	S	1	8,1	14,14,15	0.60	1 (7%)	17,19,21	0.78	0
8	NAG	S	2	8	14,14,15	0.48	0	17,19,21	0.36	0
8	NAG	T	1	2,8	14,14,15	0.58	0	17,19,21	0.77	0
8	NAG	T	2	8	14,14,15	0.47	0	17,19,21	1.33	2 (11%)

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	O	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	O	2	8	-	2/6/23/26	0/1/1/1
8	NAG	P	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	P	2	8	-	0/6/23/26	0/1/1/1
8	NAG	Q	1	2,8	-	4/6/23/26	0/1/1/1
8	NAG	Q	2	8	-	6/6/23/26	0/1/1/1
8	NAG	R	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	R	2	8	-	2/6/23/26	0/1/1/1
8	NAG	S	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	S	2	8	-	0/6/23/26	0/1/1/1
8	NAG	T	1	2,8	-	4/6/23/26	0/1/1/1
8	NAG	T	2	8	-	6/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	1	NAG	O5-C1	-2.11	1.40	1.43
8	S	1	NAG	O5-C1	-2.06	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	T	2	NAG	C2-N2-C7	4.55	129.00	122.90
8	Q	2	NAG	C2-N2-C7	4.52	128.96	122.90
8	T	2	NAG	C1-C2-N2	2.12	113.77	110.43
8	Q	2	NAG	C1-C2-N2	2.12	113.77	110.43

There are no chirality outliers.

All (32) torsion outliers are listed below:

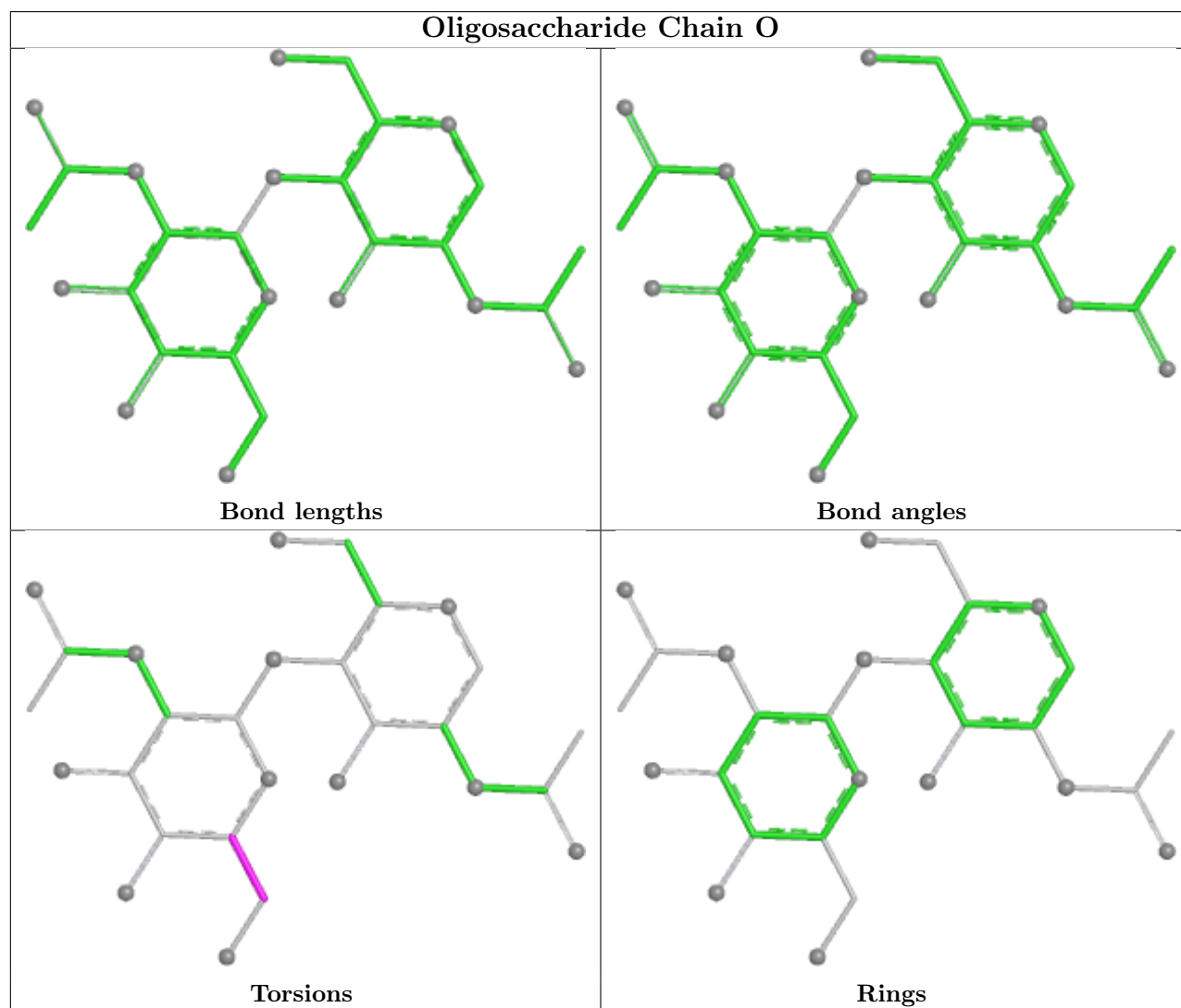
Mol	Chain	Res	Type	Atoms
8	P	1	NAG	O5-C5-C6-O6
8	S	1	NAG	O5-C5-C6-O6
8	O	2	NAG	O5-C5-C6-O6
8	R	2	NAG	O5-C5-C6-O6
8	Q	1	NAG	O5-C5-C6-O6
8	T	1	NAG	O5-C5-C6-O6
8	Q	1	NAG	C4-C5-C6-O6
8	T	1	NAG	C4-C5-C6-O6
8	P	1	NAG	C4-C5-C6-O6
8	S	1	NAG	C4-C5-C6-O6
8	Q	2	NAG	C8-C7-N2-C2
8	Q	2	NAG	O7-C7-N2-C2
8	T	2	NAG	C8-C7-N2-C2
8	T	2	NAG	O7-C7-N2-C2
8	Q	2	NAG	O5-C5-C6-O6
8	T	2	NAG	O5-C5-C6-O6
8	O	2	NAG	C4-C5-C6-O6
8	R	2	NAG	C4-C5-C6-O6
8	T	2	NAG	C4-C5-C6-O6
8	Q	2	NAG	C4-C5-C6-O6
8	P	1	NAG	C1-C2-N2-C7
8	Q	1	NAG	C1-C2-N2-C7
8	S	1	NAG	C1-C2-N2-C7
8	T	1	NAG	C1-C2-N2-C7
8	P	1	NAG	C3-C2-N2-C7
8	S	1	NAG	C3-C2-N2-C7
8	Q	2	NAG	C1-C2-N2-C7
8	T	2	NAG	C1-C2-N2-C7
8	Q	1	NAG	C3-C2-N2-C7
8	Q	2	NAG	C3-C2-N2-C7
8	T	1	NAG	C3-C2-N2-C7
8	T	2	NAG	C3-C2-N2-C7

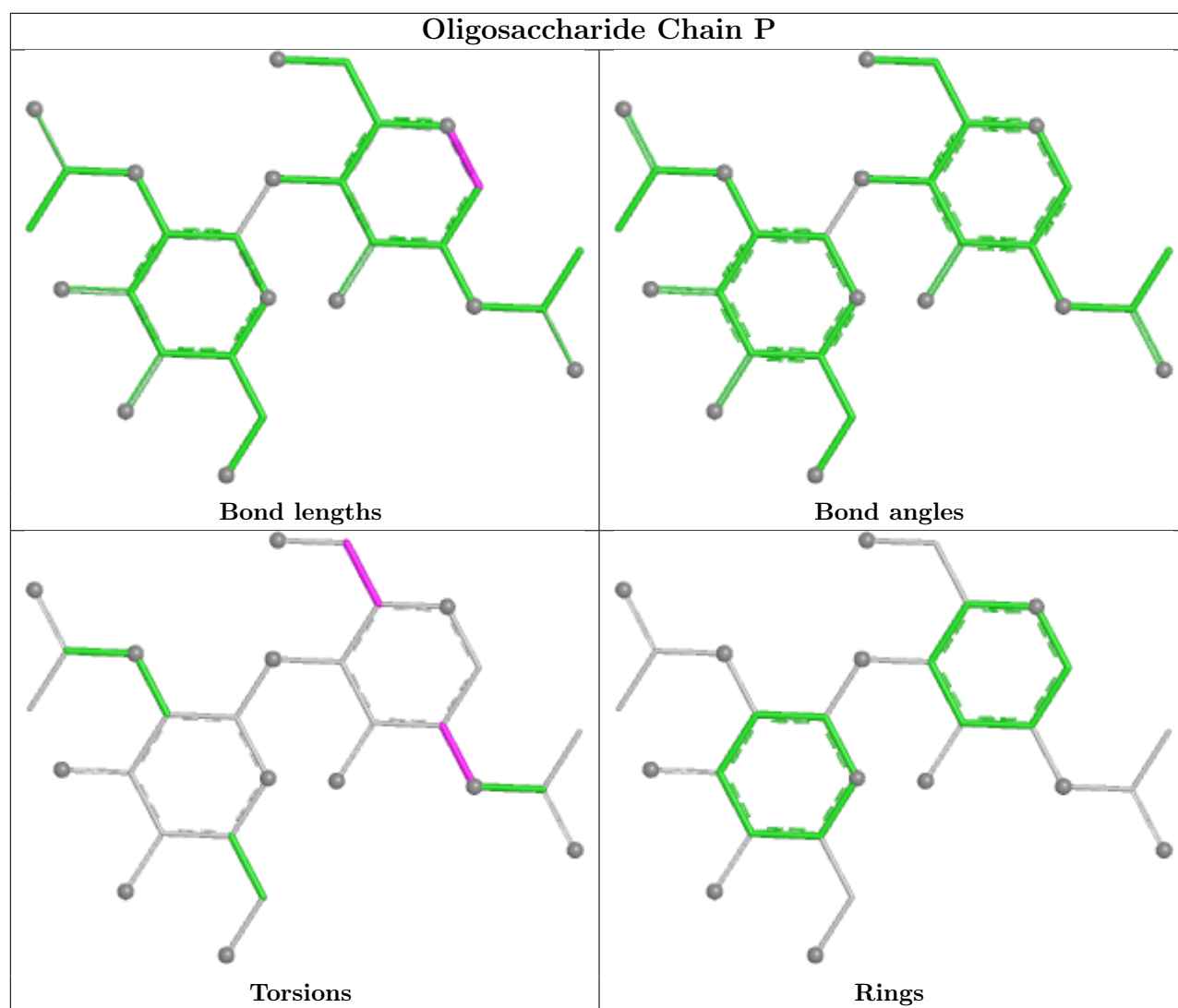
There are no ring outliers.

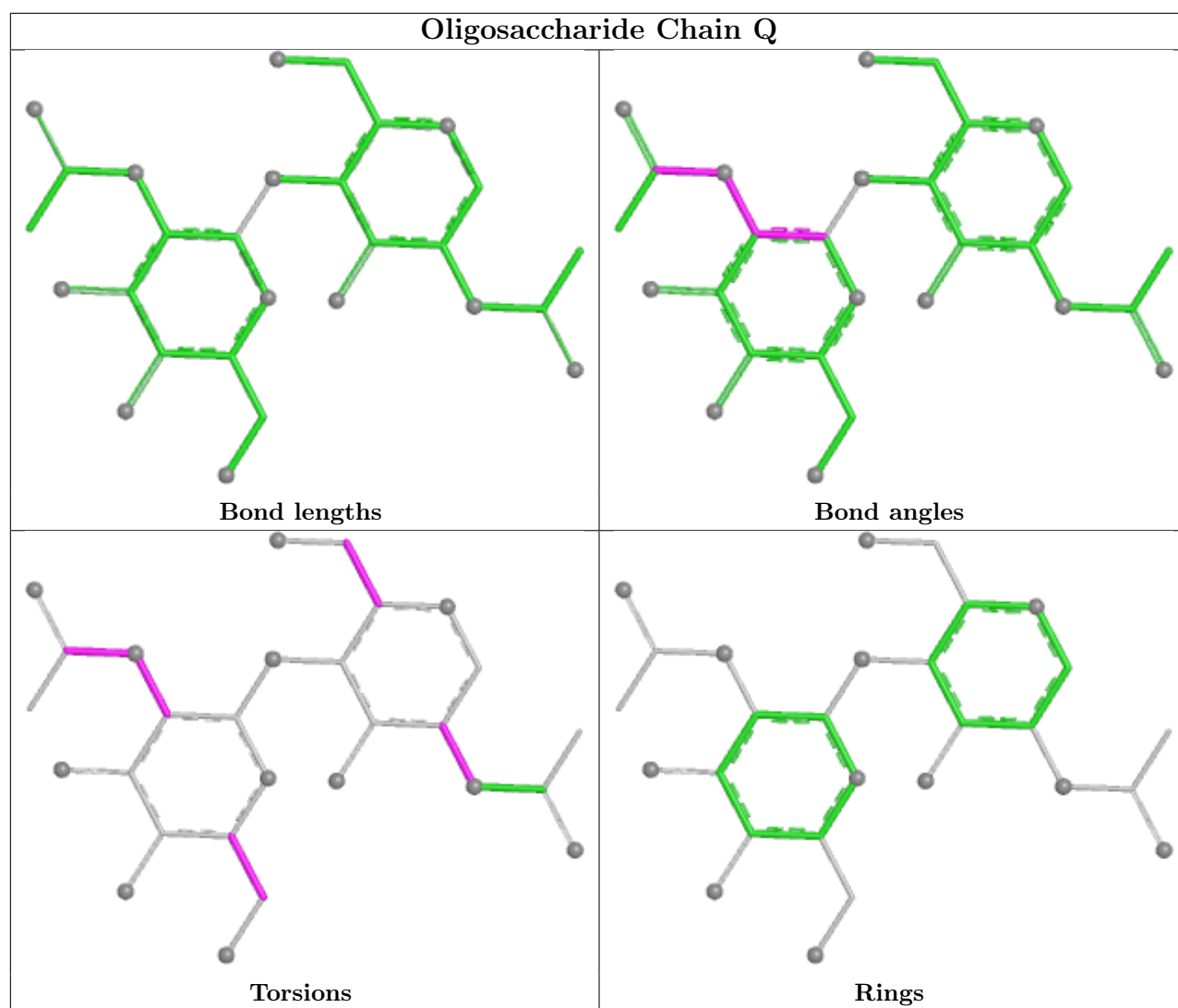
6 monomers are involved in 8 short contacts:

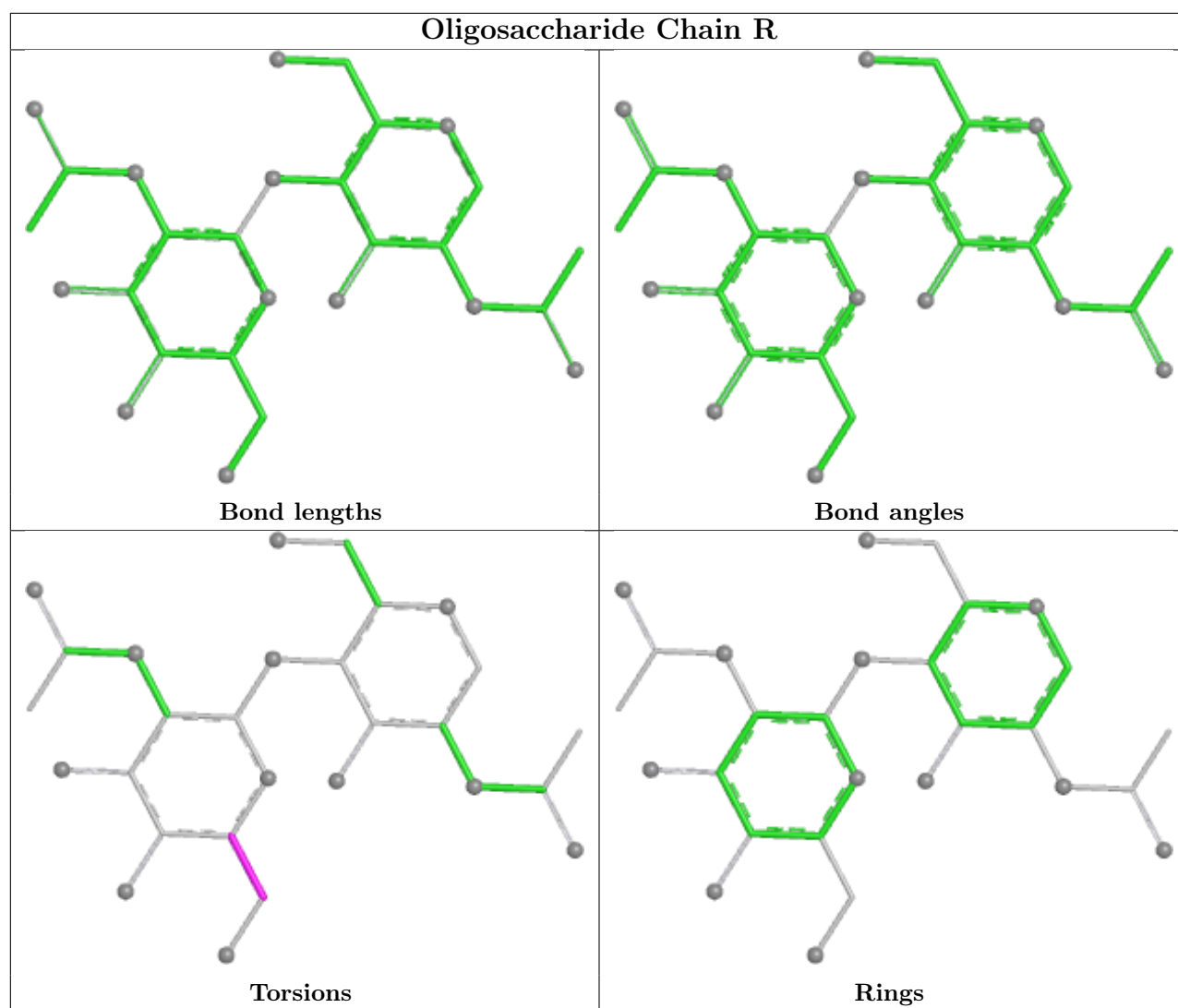
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	Q	2	NAG	2	0
8	Q	1	NAG	1	0
8	P	1	NAG	1	0
8	T	2	NAG	2	0
8	S	1	NAG	1	0
8	T	1	NAG	1	0

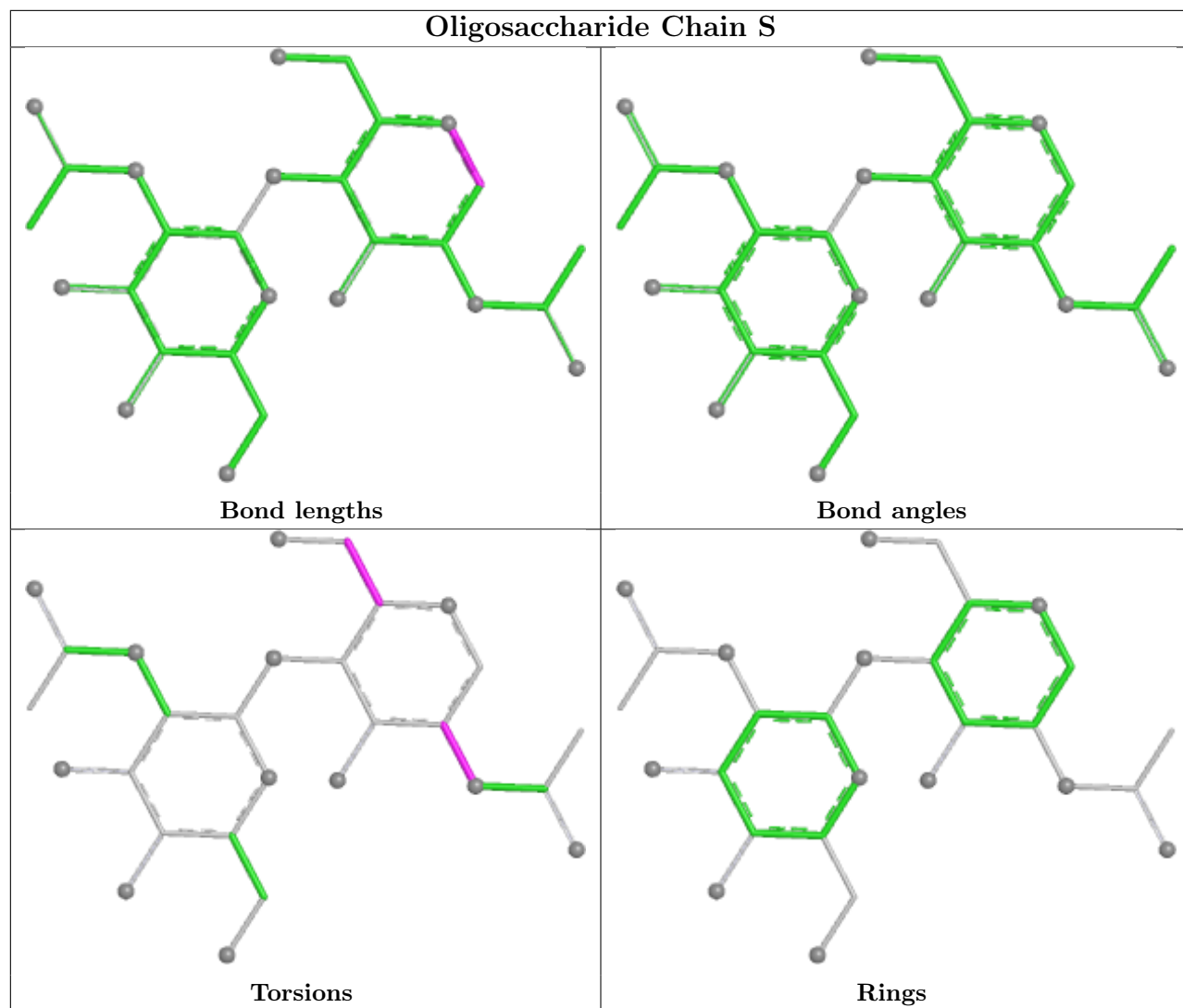
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

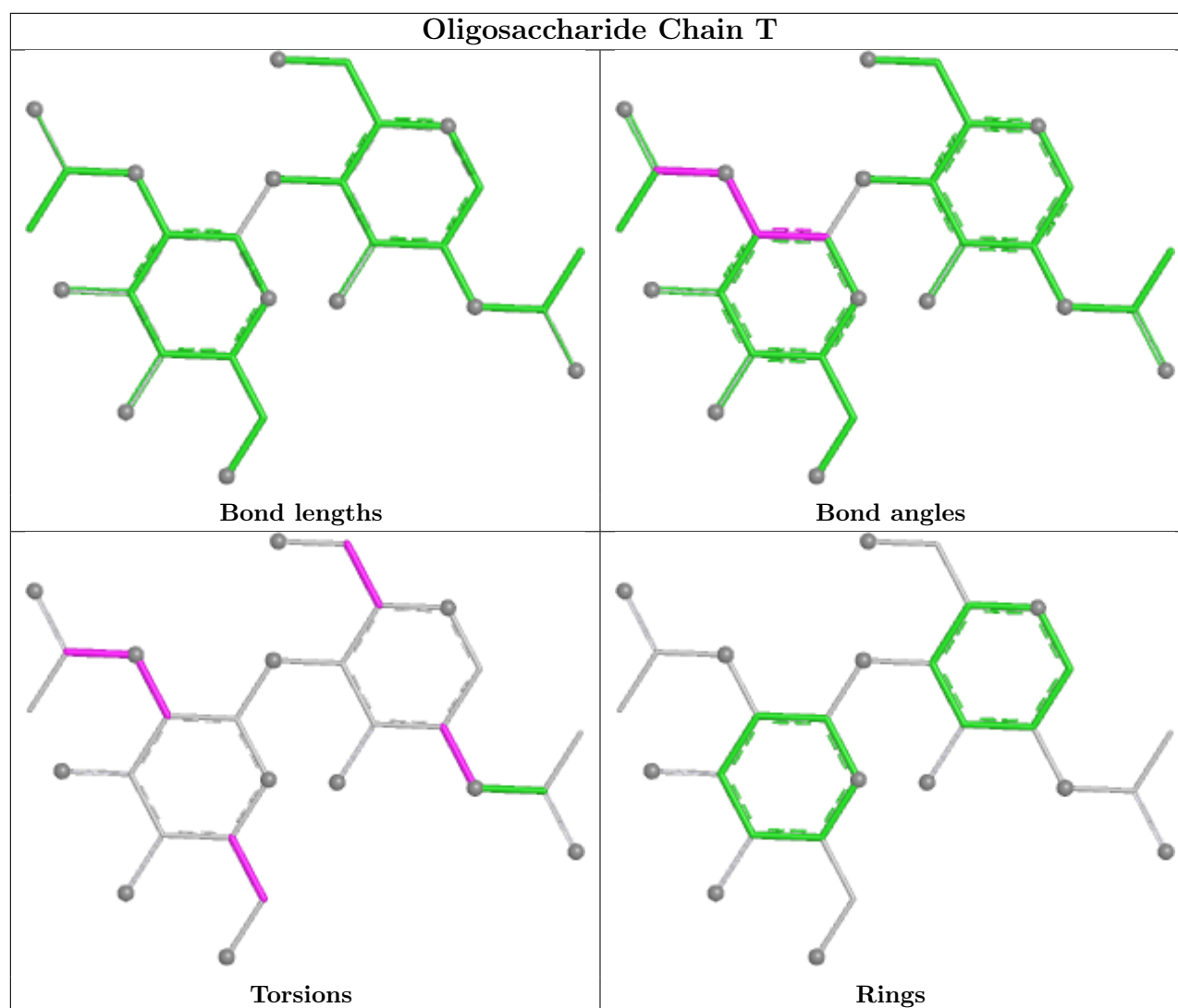












5.6 Ligand geometry [i](#)

46 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	$\# Z > 2$
10	R16	C	902	-	12,12,15	0.30	0	11,11,14	0.38	0
11	OCT	B	906	-	7,7,7	0.31	0	6,6,6	0.32	0
14	NAG	C	906	1	14,14,15	0.20	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	D10	A	905	-	9,9,9	0.30	0	8,8,8	0.35	0
12	HP6	C	908	-	6,6,6	0.31	0	5,5,5	0.30	0
16	C14	G	506	-	12,12,13	0.29	0	11,11,12	0.36	0
11	OCT	A	903	-	7,7,7	0.31	0	6,6,6	0.32	0
13	D10	F	201	-	6,6,9	0.31	0	5,5,8	0.31	0
11	OCT	C	903	-	7,7,7	0.31	0	6,6,6	0.32	0
12	HP6	A	904	-	6,6,6	0.31	0	5,5,5	0.30	0
14	NAG	D	907	2	14,14,15	0.22	0	17,19,21	0.43	0
11	OCT	G	505	-	7,7,7	0.31	0	6,6,6	0.32	0
18	XVD	H	504	-	22,24,24	2.00	7 (31%)	32,36,36	1.00	3 (9%)
15	D12	D	901	-	11,11,11	0.30	0	10,10,10	0.35	0
15	D12	B	903	-	11,11,11	0.30	0	10,10,10	0.36	0
9	ZK1	B	901	-	29,29,29	3.34	12 (41%)	45,45,45	1.45	6 (13%)
15	D12	G	502	-	11,11,11	0.30	0	10,10,10	0.37	0
17	DD9	B	905	-	7,7,8	0.31	0	6,6,7	0.32	0
12	HP6	C	904	-	6,6,6	0.31	0	5,5,5	0.30	0
14	NAG	A	906	1	14,14,15	0.19	0	17,19,21	0.44	0
14	NAG	A	907	1	14,14,15	0.23	0	17,19,21	0.46	0
16	C14	F	202	-	13,13,13	0.29	0	12,12,12	0.37	0
15	D12	H	501	-	11,11,11	0.30	0	10,10,10	0.36	0
17	DD9	B	907	-	8,8,8	0.30	0	7,7,7	0.33	0
17	DD9	D	903	-	7,7,8	0.31	0	6,6,7	0.32	0
17	DD9	D	905	-	8,8,8	0.31	0	7,7,7	0.34	0
9	ZK1	C	901	-	29,29,29	3.34	12 (41%)	45,45,45	1.46	6 (13%)
10	R16	A	902	-	12,12,15	0.29	0	11,11,14	0.37	0
13	D10	G	501	-	9,9,9	0.30	0	8,8,8	0.34	0
11	OCT	D	904	-	7,7,7	0.31	0	6,6,6	0.32	0
16	C14	B	904	-	13,13,13	0.29	0	12,12,12	0.37	0
13	D10	H	503	-	9,9,9	0.30	0	8,8,8	0.34	0
11	OCT	H	505	-	7,7,7	0.31	0	6,6,6	0.33	0
13	D10	E	201	-	6,6,9	0.32	0	5,5,8	0.30	0
9	ZK1	D	906	-	29,29,29	3.34	12 (41%)	45,45,45	1.45	6 (13%)
13	D10	C	905	-	9,9,9	0.30	0	8,8,8	0.34	0
15	D12	H	502	-	11,11,11	0.30	0	10,10,10	0.36	0
16	C14	D	902	-	13,13,13	0.29	0	12,12,12	0.37	0
12	HP6	A	908	-	6,6,6	0.32	0	5,5,5	0.30	0
16	C14	E	202	-	13,13,13	0.29	0	12,12,12	0.37	0
15	D12	G	503	-	11,11,11	0.30	0	10,10,10	0.36	0
14	NAG	B	902	2	14,14,15	0.23	0	17,19,21	0.42	0
14	NAG	C	907	1	14,14,15	0.23	0	17,19,21	0.45	0
18	XVD	G	504	-	22,24,24	2.00	7 (31%)	32,36,36	1.01	2 (6%)
9	ZK1	A	901	-	29,29,29	3.33	12 (41%)	45,45,45	1.46	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	C14	H	506	-	12,12,13	0.29	0	11,11,12	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	R16	C	902	-	-	1/10/10/13	-
11	OCT	B	906	-	-	0/5/5/5	-
14	NAG	C	906	1	-	2/6/23/26	0/1/1/1
13	D10	A	905	-	-	0/7/7/7	-
12	HP6	C	908	-	-	0/4/4/4	-
16	C14	G	506	-	-	0/10/10/11	-
11	OCT	A	903	-	-	0/5/5/5	-
13	D10	F	201	-	-	0/4/4/7	-
11	OCT	C	903	-	-	0/5/5/5	-
12	HP6	A	904	-	-	0/4/4/4	-
14	NAG	D	907	2	-	2/6/23/26	0/1/1/1
11	OCT	G	505	-	-	0/5/5/5	-
18	XVD	H	504	-	-	0/9/9/9	0/3/3/3
15	D12	D	901	-	-	1/9/9/9	-
15	D12	B	903	-	-	1/9/9/9	-
9	ZK1	B	901	-	-	2/13/23/23	0/3/3/3
15	D12	G	502	-	-	0/9/9/9	-
17	DD9	B	905	-	-	0/5/5/6	-
12	HP6	C	904	-	-	0/4/4/4	-
14	NAG	A	906	1	-	2/6/23/26	0/1/1/1
14	NAG	A	907	1	-	2/6/23/26	0/1/1/1
16	C14	F	202	-	-	0/11/11/11	-
15	D12	H	501	-	-	0/9/9/9	-
17	DD9	B	907	-	-	0/6/6/6	-
17	DD9	D	903	-	-	0/5/5/6	-
17	DD9	D	905	-	-	0/6/6/6	-
9	ZK1	C	901	-	-	2/13/23/23	0/3/3/3
10	R16	A	902	-	-	1/10/10/13	-
13	D10	G	501	-	-	0/7/7/7	-
11	OCT	D	904	-	-	0/5/5/5	-
16	C14	B	904	-	-	0/11/11/11	-
13	D10	H	503	-	-	0/7/7/7	-
11	OCT	H	505	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	D10	E	201	-	-	0/4/4/7	-
9	ZK1	D	906	-	-	2/13/23/23	0/3/3/3
13	D10	C	905	-	-	0/7/7/7	-
15	D12	H	502	-	-	0/9/9/9	-
16	C14	D	902	-	-	0/11/11/11	-
12	HP6	A	908	-	-	0/4/4/4	-
16	C14	E	202	-	-	0/11/11/11	-
15	D12	G	503	-	-	0/9/9/9	-
14	NAG	B	902	2	-	2/6/23/26	0/1/1/1
14	NAG	C	907	1	-	2/6/23/26	0/1/1/1
18	XVD	G	504	-	-	0/9/9/9	0/3/3/3
9	ZK1	A	901	-	-	2/13/23/23	0/3/3/3
16	C14	H	506	-	-	0/10/10/11	-

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	901	ZK1	CAU-CAT	-9.88	1.39	1.53
9	B	901	ZK1	CAU-CAT	-9.87	1.39	1.53
9	D	906	ZK1	CAU-CAT	-9.84	1.39	1.53
9	A	901	ZK1	CAU-CAT	-9.81	1.39	1.53
9	C	901	ZK1	OAB-CAU	8.68	1.40	1.23
9	B	901	ZK1	OAB-CAU	8.68	1.40	1.23
9	A	901	ZK1	OAB-CAU	8.66	1.40	1.23
9	D	906	ZK1	OAB-CAU	8.64	1.40	1.23
9	C	901	ZK1	OAA-CAT	8.60	1.39	1.23
9	A	901	ZK1	OAA-CAT	8.59	1.39	1.23
9	B	901	ZK1	OAA-CAT	8.57	1.39	1.23
9	D	906	ZK1	OAA-CAT	8.54	1.39	1.23
18	G	504	XVD	C8-C9	3.99	1.45	1.39
18	H	504	XVD	C8-C9	3.97	1.45	1.39
18	H	504	XVD	C6-C7	3.81	1.56	1.50
18	G	504	XVD	C6-C7	3.77	1.56	1.50
9	C	901	ZK1	PBA-CAO	3.21	1.88	1.81
9	A	901	ZK1	PBA-CAO	3.17	1.88	1.81
9	B	901	ZK1	PBA-CAO	3.14	1.88	1.81
9	D	906	ZK1	PBA-CAO	3.13	1.88	1.81
18	G	504	XVD	C12-C11	3.11	1.43	1.38
18	G	504	XVD	C1-CL1	3.09	1.80	1.73
18	H	504	XVD	C1-CL1	3.07	1.80	1.73
18	H	504	XVD	C12-C11	3.04	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	906	ZK1	CAR-NAX	3.03	1.47	1.41
9	A	901	ZK1	CAR-NAX	3.02	1.47	1.41
9	B	901	ZK1	CAR-NAX	3.01	1.47	1.41
9	A	901	ZK1	CAU-NAY	-2.99	1.32	1.38
9	C	901	ZK1	CAR-NAX	2.99	1.47	1.41
9	B	901	ZK1	CAU-NAY	-2.98	1.32	1.38
9	D	906	ZK1	CAU-NAY	-2.97	1.32	1.38
9	C	901	ZK1	CAU-NAY	-2.95	1.33	1.38
9	A	901	ZK1	CAV-NAP	-2.88	1.35	1.39
9	D	906	ZK1	CAV-NAP	-2.86	1.35	1.39
9	C	901	ZK1	CAV-NAP	-2.81	1.35	1.39
9	B	901	ZK1	CAV-NAP	-2.79	1.35	1.39
9	D	906	ZK1	CAV-CAW	-2.61	1.37	1.40
9	B	901	ZK1	CAV-CAW	-2.60	1.37	1.40
9	C	901	ZK1	CAV-CAW	-2.52	1.37	1.40
18	H	504	XVD	O2-C14	2.49	1.44	1.31
18	G	504	XVD	O2-C14	2.48	1.44	1.31
9	A	901	ZK1	CAV-CAW	-2.48	1.37	1.40
9	D	906	ZK1	CAW-NAY	-2.35	1.37	1.41
9	B	901	ZK1	CAW-NAY	-2.35	1.37	1.41
9	C	901	ZK1	CAW-NAY	-2.31	1.37	1.41
18	H	504	XVD	C9-N2	-2.31	1.34	1.38
9	A	901	ZK1	CAW-NAY	-2.29	1.37	1.41
18	G	504	XVD	C9-N2	-2.26	1.34	1.38
9	C	901	ZK1	CAZ-CAS	2.23	1.55	1.50
9	A	901	ZK1	PBA-OAD	-2.19	1.50	1.55
9	C	901	ZK1	PBA-OAD	-2.17	1.50	1.55
9	A	901	ZK1	CAZ-CAS	2.17	1.55	1.50
18	H	504	XVD	C6-C1	2.16	1.42	1.39
9	D	906	ZK1	CAZ-CAS	2.15	1.55	1.50
9	B	901	ZK1	PBA-OAD	-2.15	1.50	1.55
9	B	901	ZK1	CAZ-CAS	2.14	1.55	1.50
9	D	906	ZK1	PBA-OAD	-2.11	1.50	1.55
18	G	504	XVD	C6-C1	2.11	1.42	1.39
9	A	901	ZK1	CAJ-CAV	2.08	1.42	1.39
9	B	901	ZK1	CAJ-CAV	2.08	1.42	1.39
9	D	906	ZK1	CAJ-CAV	2.05	1.42	1.39
9	C	901	ZK1	CAJ-CAV	2.04	1.42	1.39

All (29) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	901	ZK1	CAN-NAX-CAM	3.71	119.92	111.57
9	D	906	ZK1	CAN-NAX-CAM	3.70	119.89	111.57
9	A	901	ZK1	CAN-NAX-CAM	3.69	119.88	111.57
9	C	901	ZK1	CAN-NAX-CAM	3.66	119.81	111.57
9	C	901	ZK1	CAV-NAP-CAT	-3.45	119.98	124.82
9	B	901	ZK1	CAV-NAP-CAT	-3.39	120.07	124.82
9	D	906	ZK1	CAV-NAP-CAT	-3.39	120.07	124.82
9	A	901	ZK1	CAV-NAP-CAT	-3.39	120.07	124.82
9	A	901	ZK1	CAO-NAY-CAU	3.09	119.69	116.55
9	C	901	ZK1	CAO-NAY-CAU	3.03	119.64	116.55
9	B	901	ZK1	CAO-NAY-CAU	2.98	119.58	116.55
9	D	906	ZK1	CAO-NAY-CAU	2.97	119.57	116.55
9	B	901	ZK1	CAI-CAR-NAX	-2.84	118.45	122.59
9	C	901	ZK1	CAI-CAR-NAX	-2.82	118.49	122.59
9	A	901	ZK1	CAI-CAR-NAX	-2.81	118.50	122.59
9	D	906	ZK1	CAI-CAR-NAX	-2.79	118.53	122.59
9	C	901	ZK1	CAU-CAT-NAP	2.75	120.26	117.46
9	B	901	ZK1	CAU-CAT-NAP	2.74	120.26	117.46
9	A	901	ZK1	CAU-CAT-NAP	2.71	120.23	117.46
9	D	906	ZK1	CAU-CAT-NAP	2.69	120.20	117.46
18	H	504	XVD	C10-N1-C13	2.42	108.92	104.13
18	G	504	XVD	C10-N1-C13	2.42	108.92	104.13
18	G	504	XVD	C9-C10-N1	-2.06	106.60	109.42
9	B	901	ZK1	FAF-CAZ-CAS	-2.05	109.01	112.65
18	H	504	XVD	C9-C10-N1	-2.04	106.63	109.42
9	D	906	ZK1	FAF-CAZ-CAS	-2.03	109.04	112.65
9	A	901	ZK1	FAF-CAZ-CAS	-2.02	109.07	112.65
9	C	901	ZK1	FAF-CAZ-CAS	-2.01	109.08	112.65
18	H	504	XVD	C5-C6-C1	2.00	120.01	117.74

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	B	902	NAG	C4-C5-C6-O6
14	D	907	NAG	C4-C5-C6-O6
14	A	906	NAG	O5-C5-C6-O6
14	C	906	NAG	O5-C5-C6-O6
14	A	906	NAG	C4-C5-C6-O6
14	C	906	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
14	B	902	NAG	O5-C5-C6-O6
14	D	907	NAG	O5-C5-C6-O6
15	D	901	D12	C6-C7-C8-C9
15	B	903	D12	C6-C7-C8-C9
14	C	907	NAG	C4-C5-C6-O6
14	A	907	NAG	C4-C5-C6-O6
9	B	901	ZK1	CAI-CAR-NAX-CAM
9	D	906	ZK1	CAI-CAR-NAX-CAM
9	A	901	ZK1	CAI-CAR-NAX-CAM
9	C	901	ZK1	CAI-CAR-NAX-CAM
10	A	902	R16	C37-C38-C39-C40
10	C	902	R16	C37-C38-C39-C40
14	C	907	NAG	O5-C5-C6-O6
14	A	907	NAG	O5-C5-C6-O6
9	A	901	ZK1	CAI-CAR-NAX-CAN
9	C	901	ZK1	CAI-CAR-NAX-CAN
9	D	906	ZK1	CAI-CAR-NAX-CAN
9	B	901	ZK1	CAI-CAR-NAX-CAN

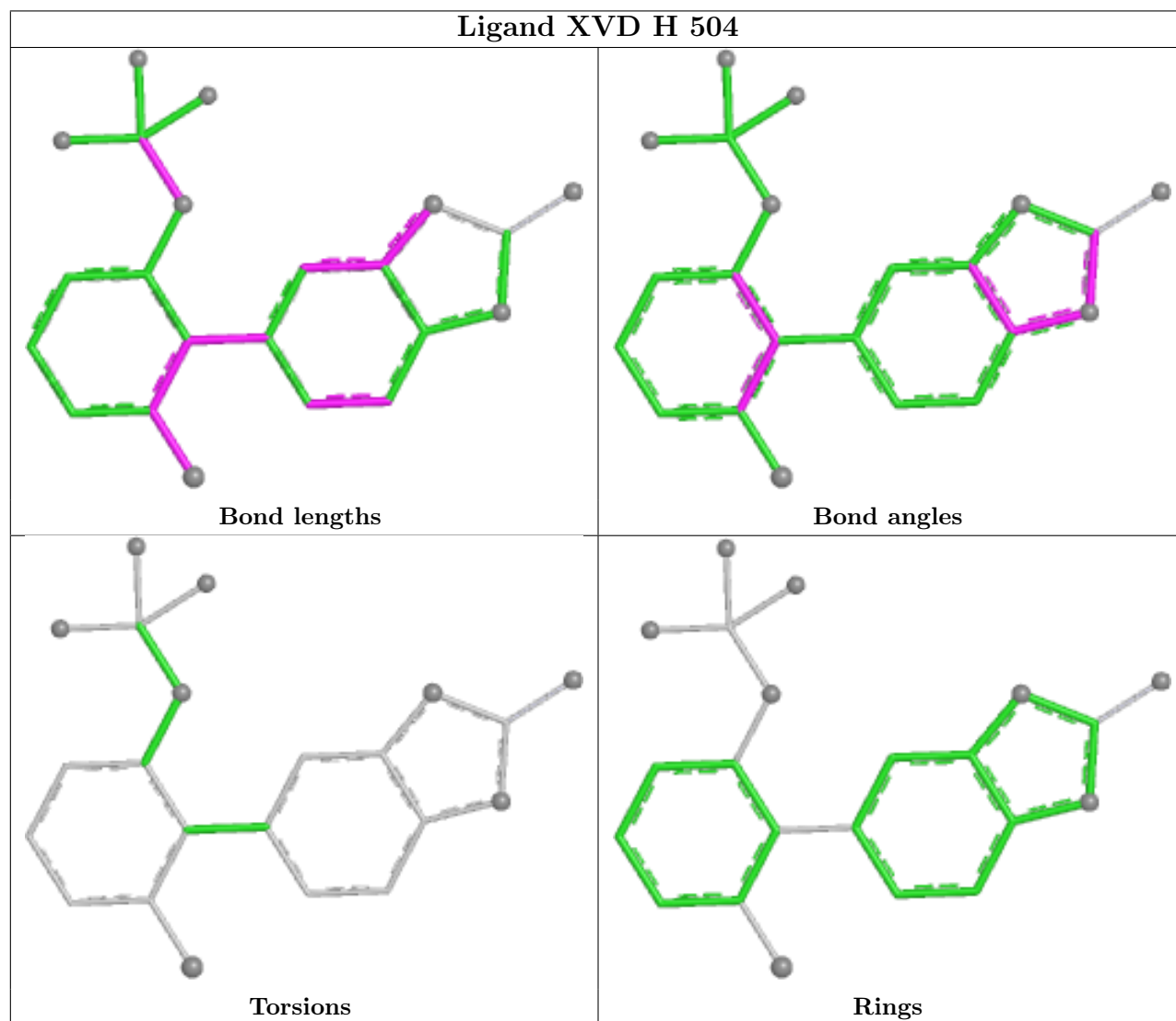
There are no ring outliers.

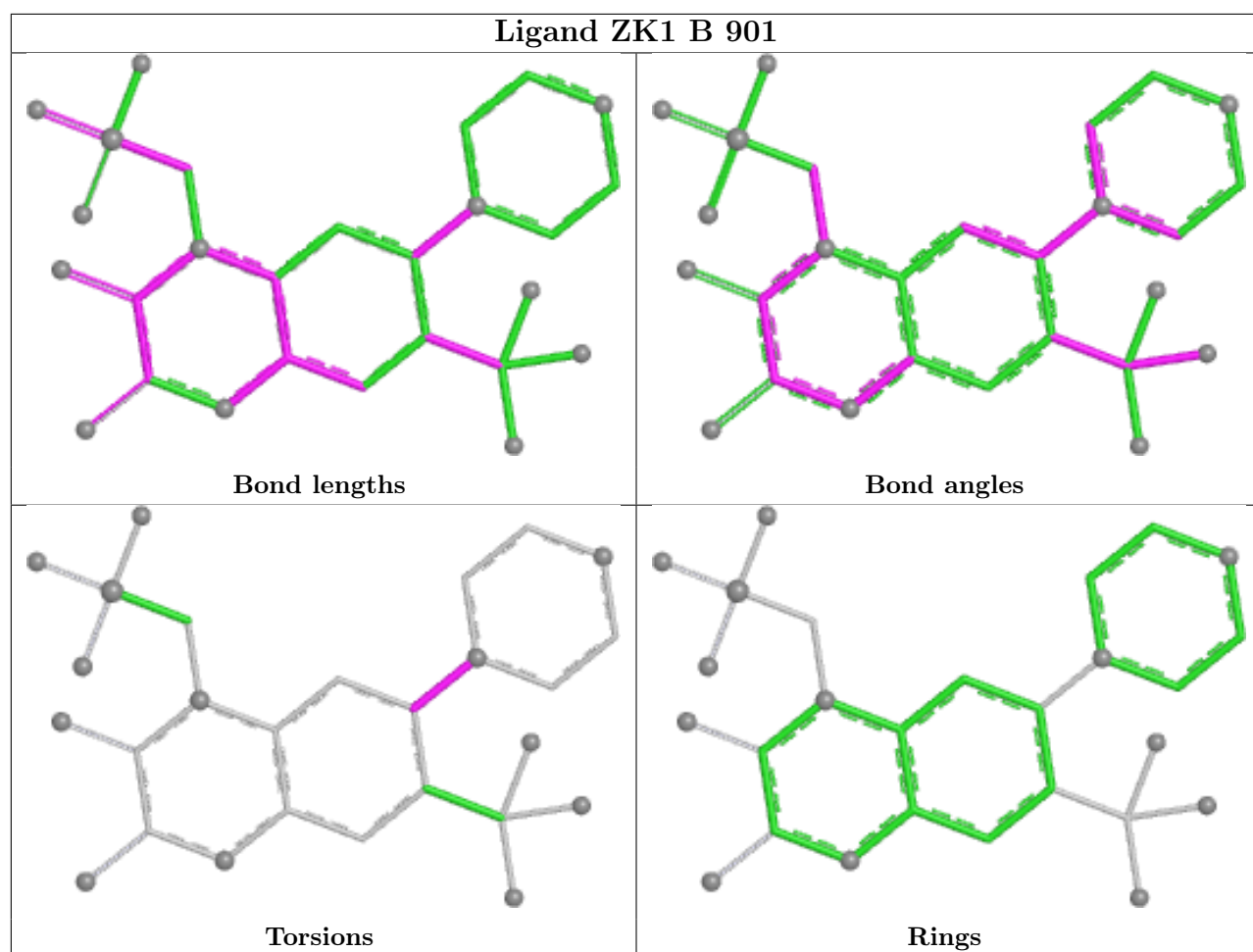
10 monomers are involved in 9 short contacts:

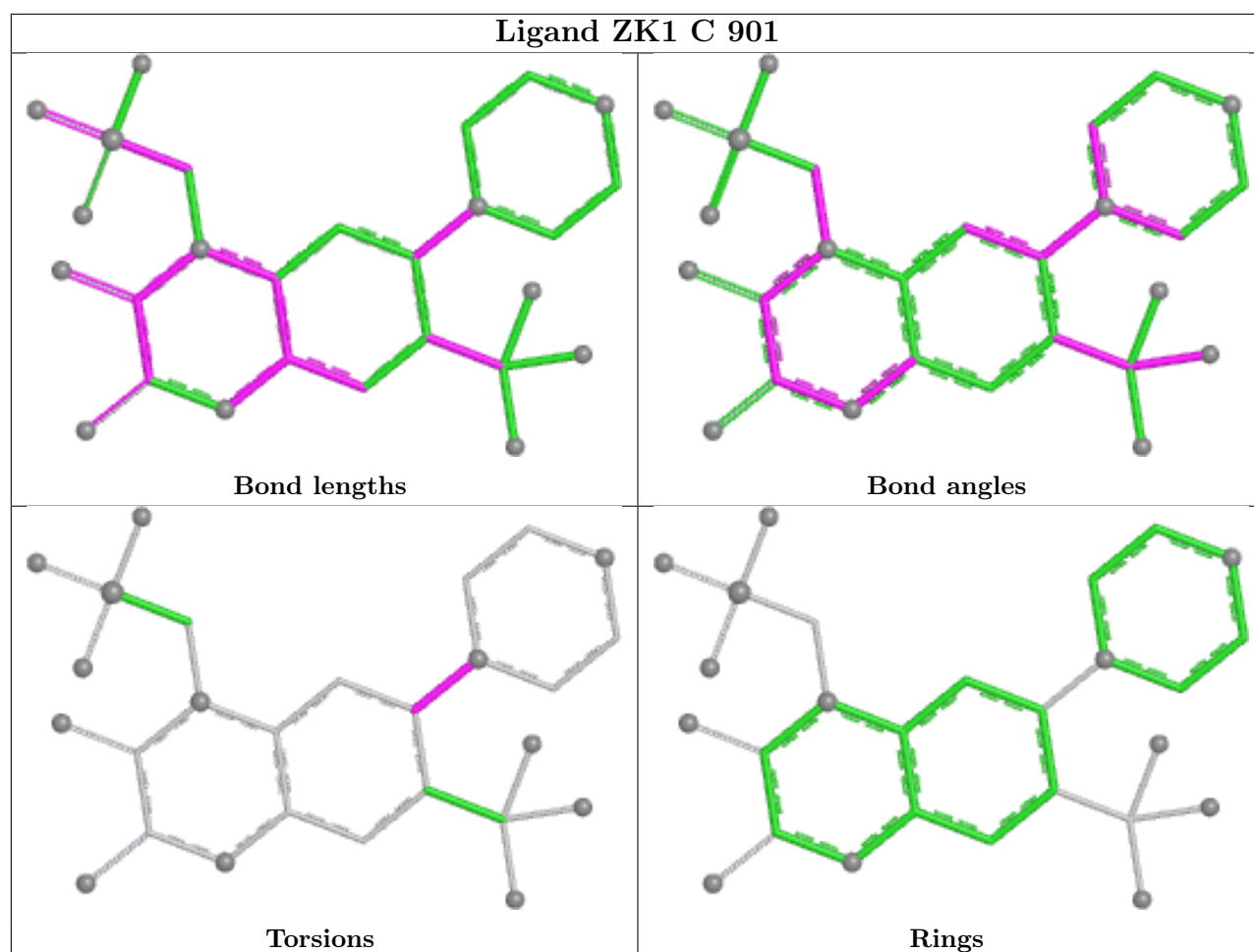
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	903	OCT	1	0
11	G	505	OCT	1	0
18	H	504	XVD	1	0
15	D	901	D12	1	0
9	B	901	ZK1	1	0
14	A	907	NAG	1	0
11	H	505	OCT	1	0
9	D	906	ZK1	1	0
14	C	907	NAG	1	0
18	G	504	XVD	1	0

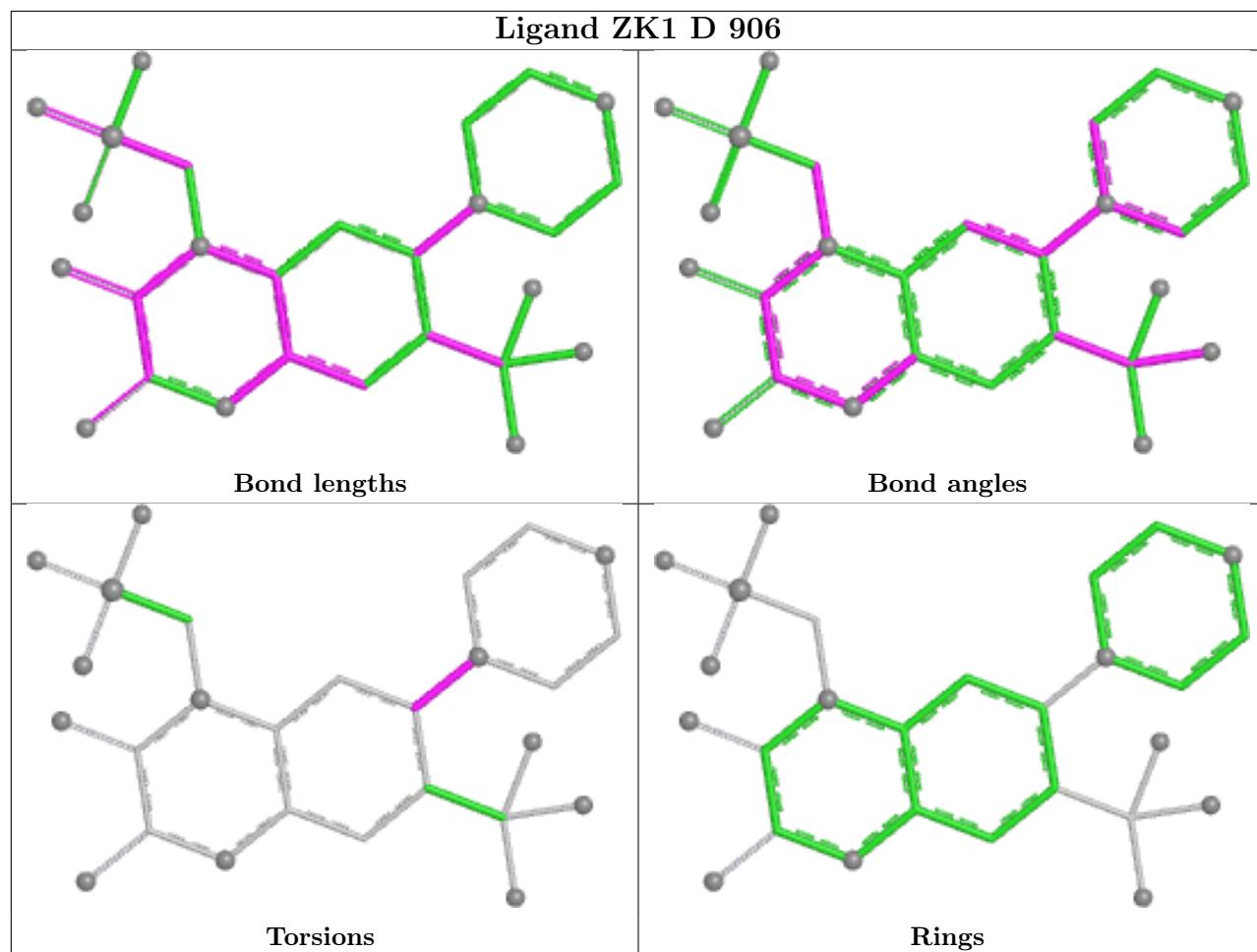
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

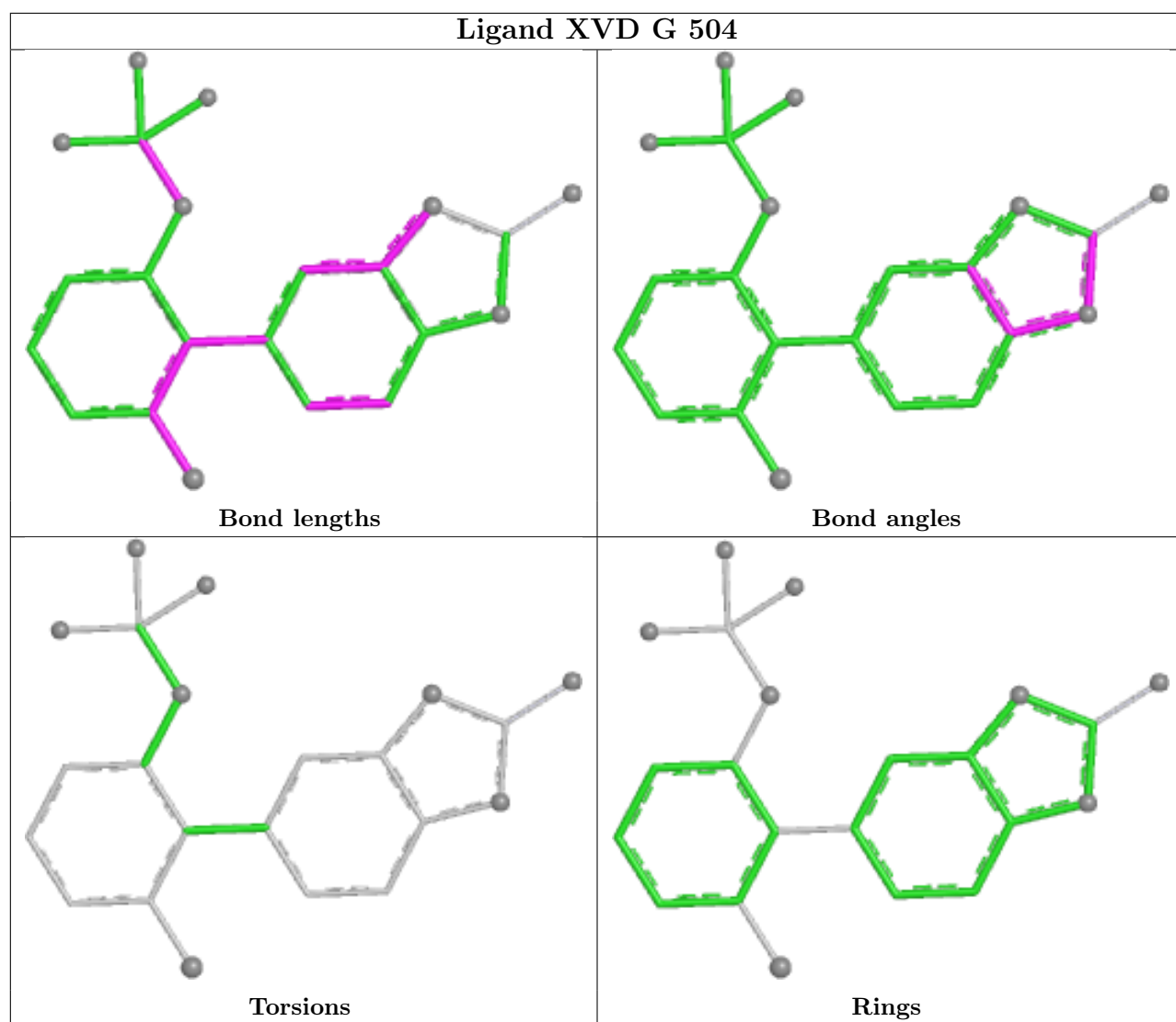
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

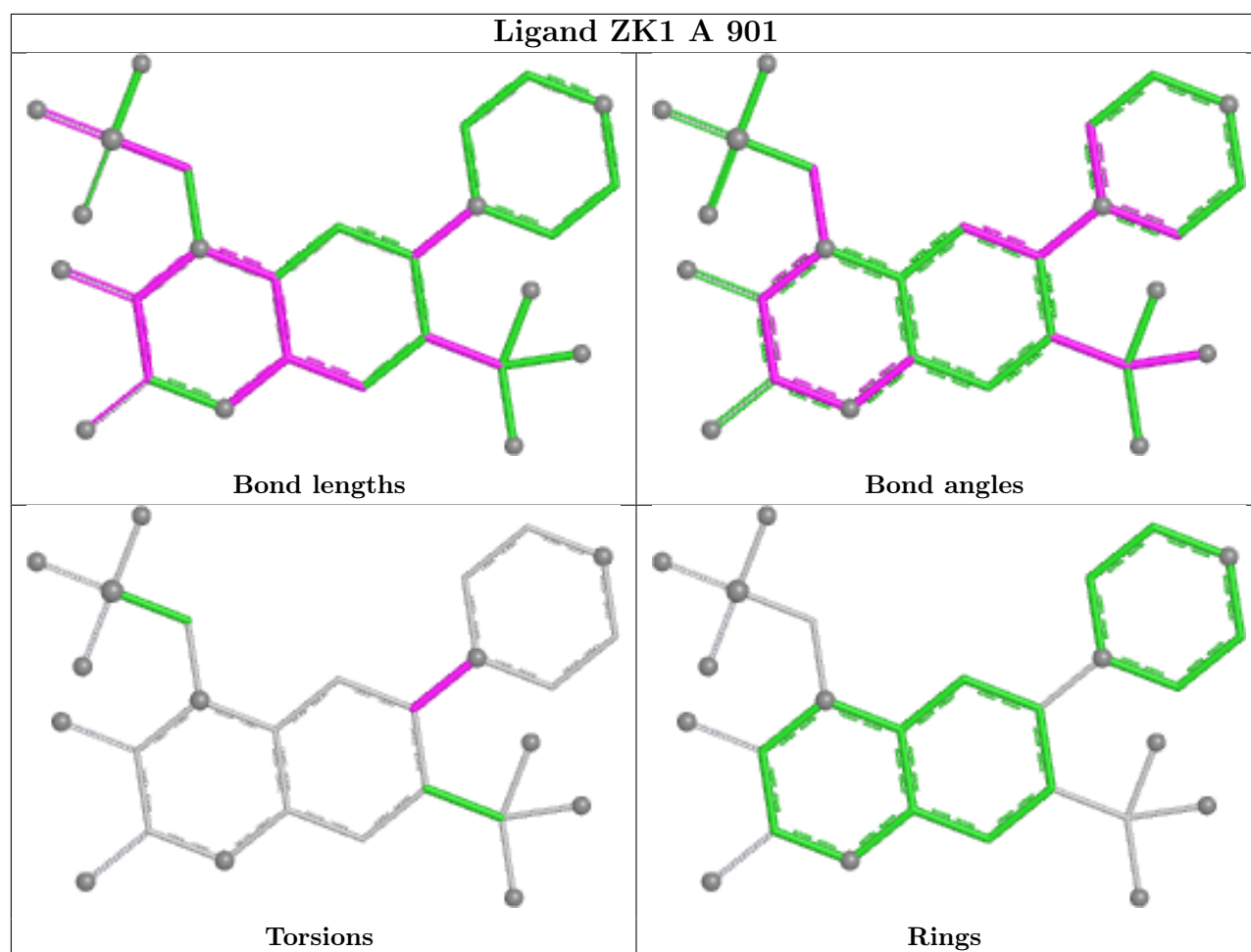












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

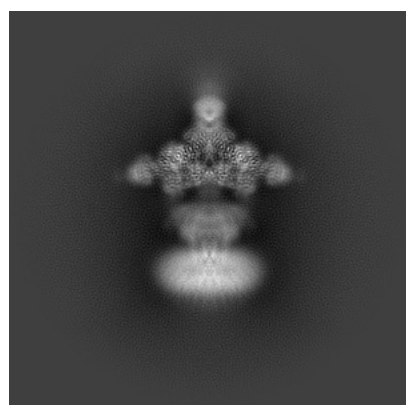
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23283. These allow visual inspection of the internal detail of the map and identification of artifacts.

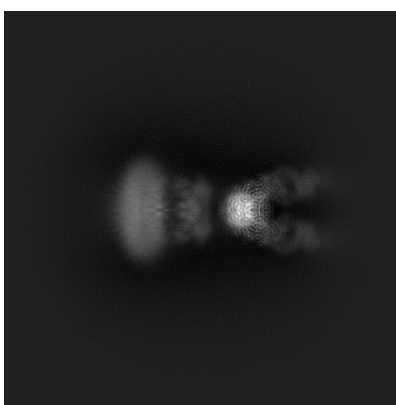
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

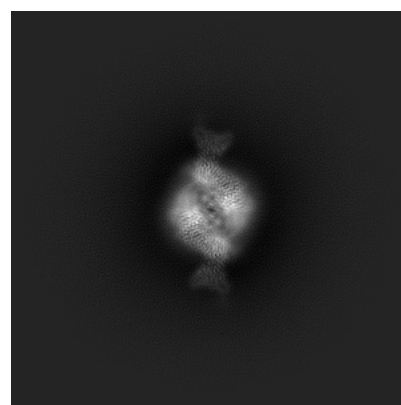
6.1.1 Primary map



X



Y

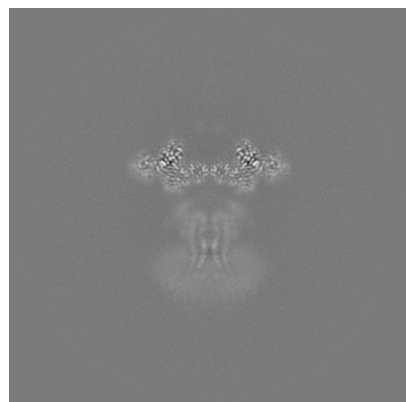


Z

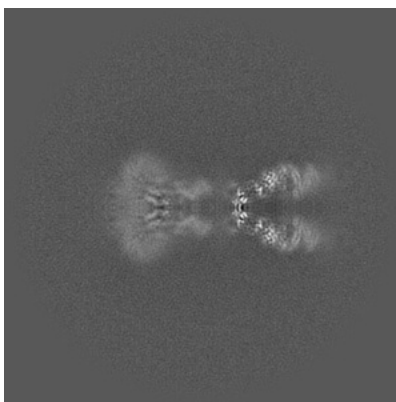
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

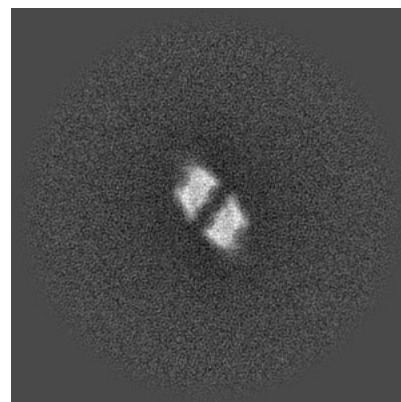
6.2.1 Primary map



X Index: 256



Y Index: 256

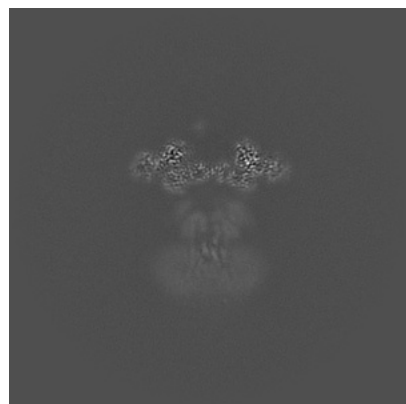


Z Index: 256

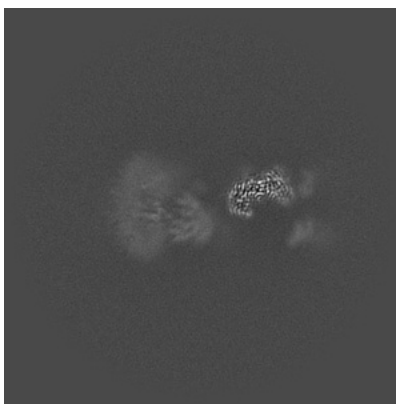
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

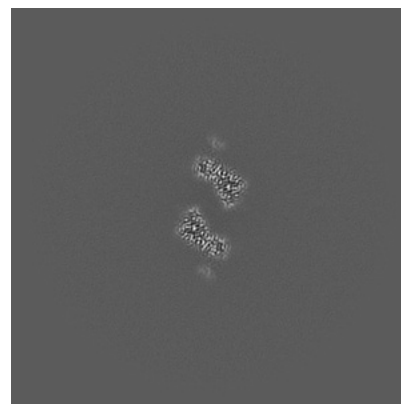
6.3.1 Primary map



X Index: 253



Y Index: 272



Z Index: 326

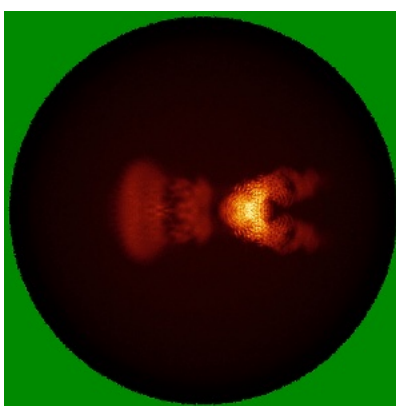
The images above show the largest variance slices of the map in three orthogonal directions.

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

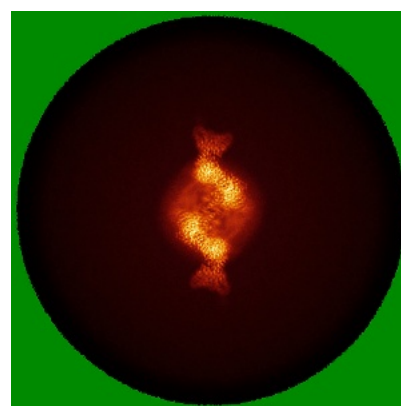
6.4.1 Primary map



X



Y

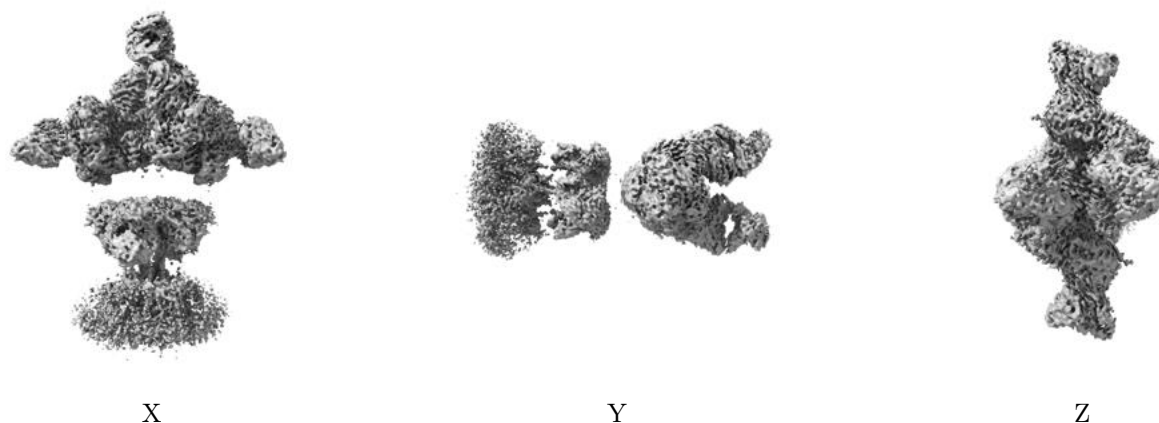


Z

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

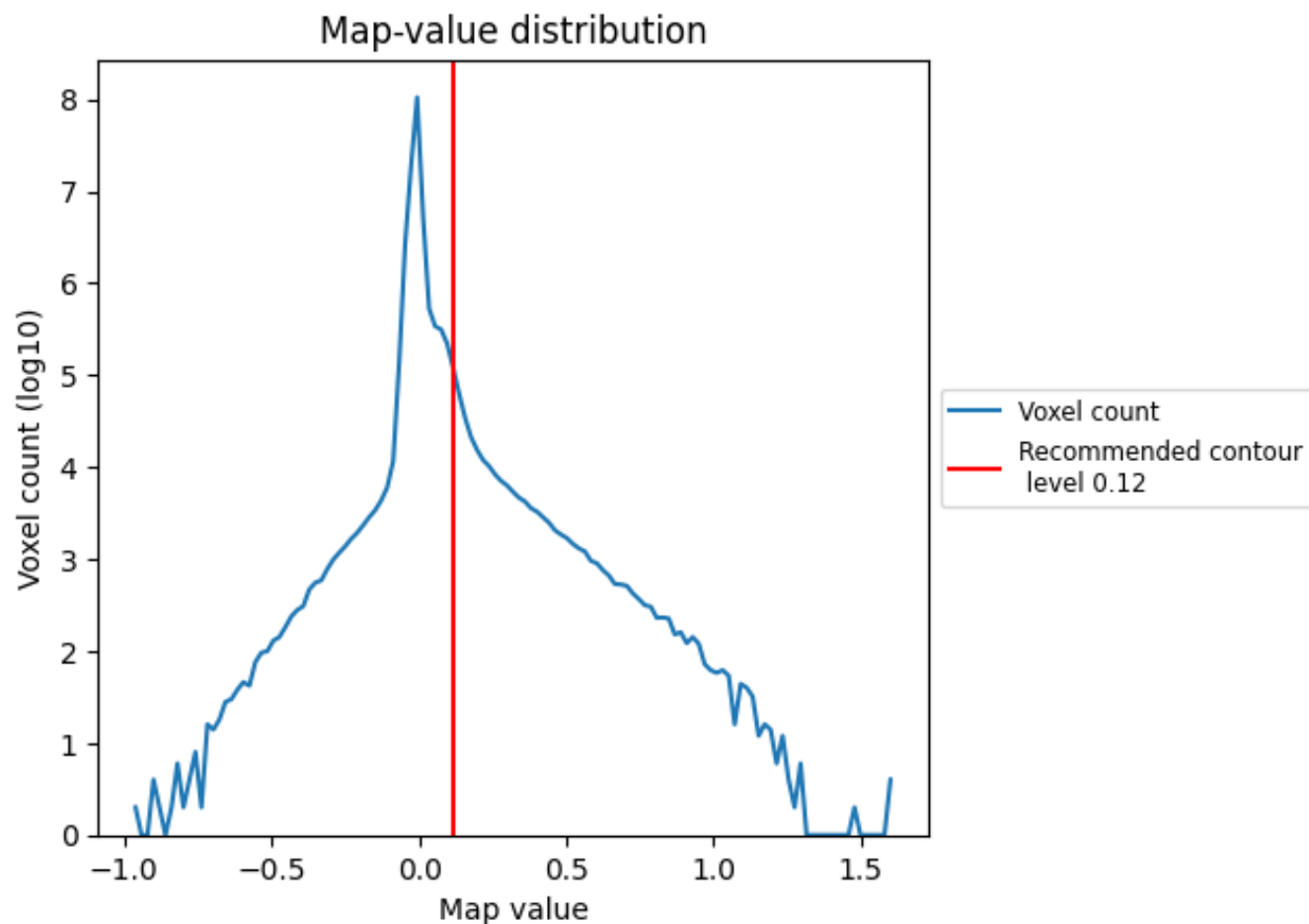
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

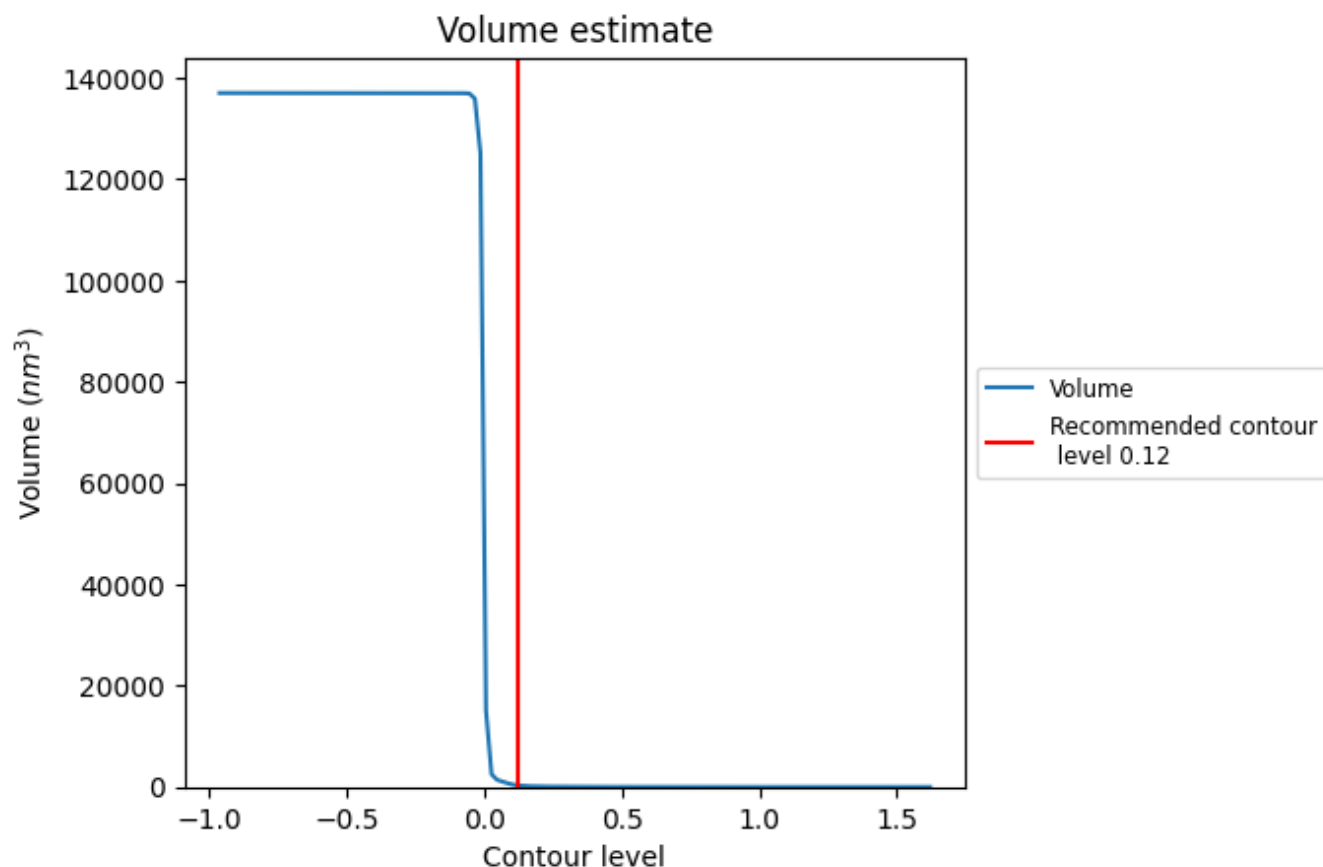
This section contains the results of statistical analysis of the map.

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.

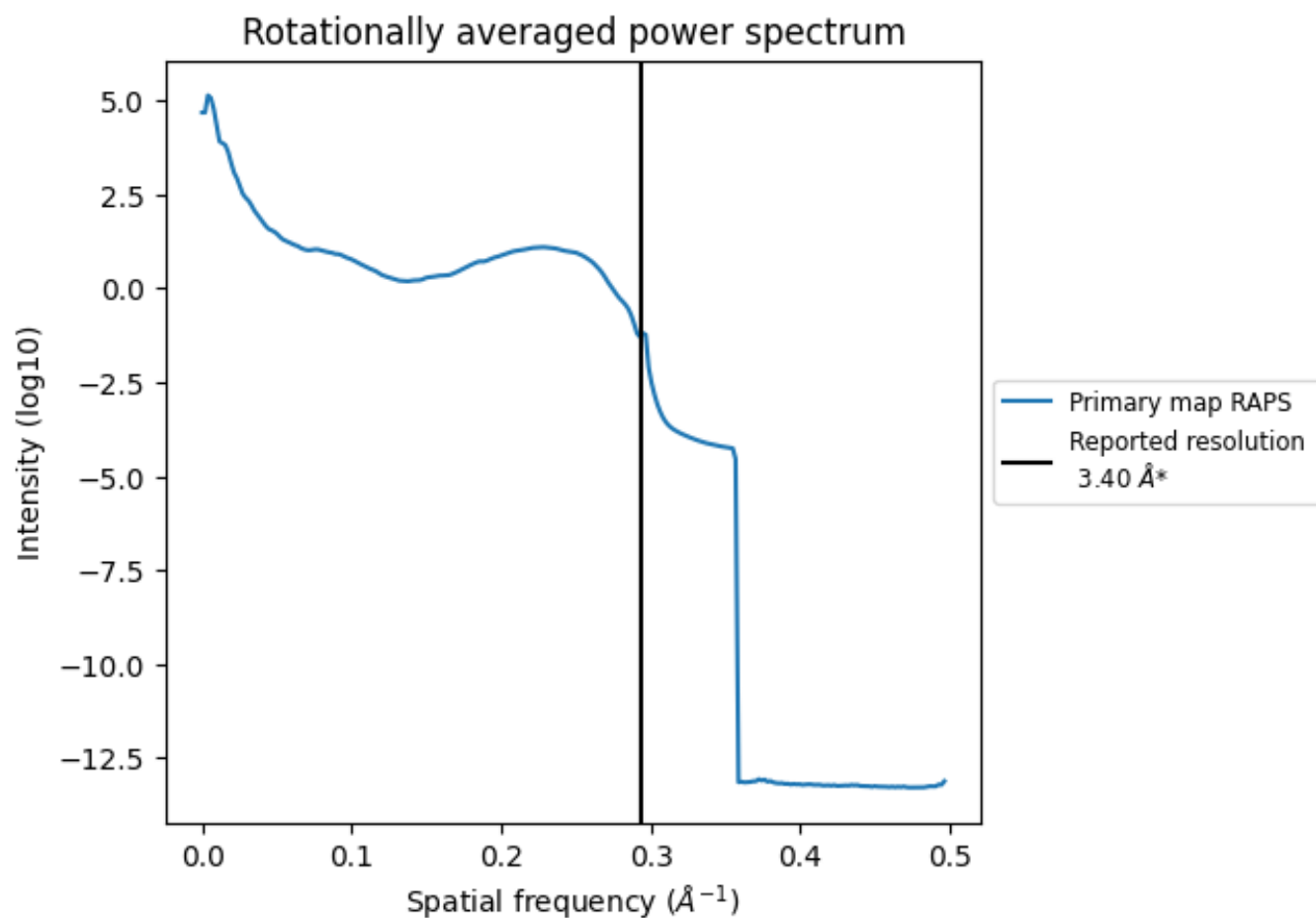
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 333 nm³; this corresponds to an approximate mass of 301 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 0.294 Å⁻¹

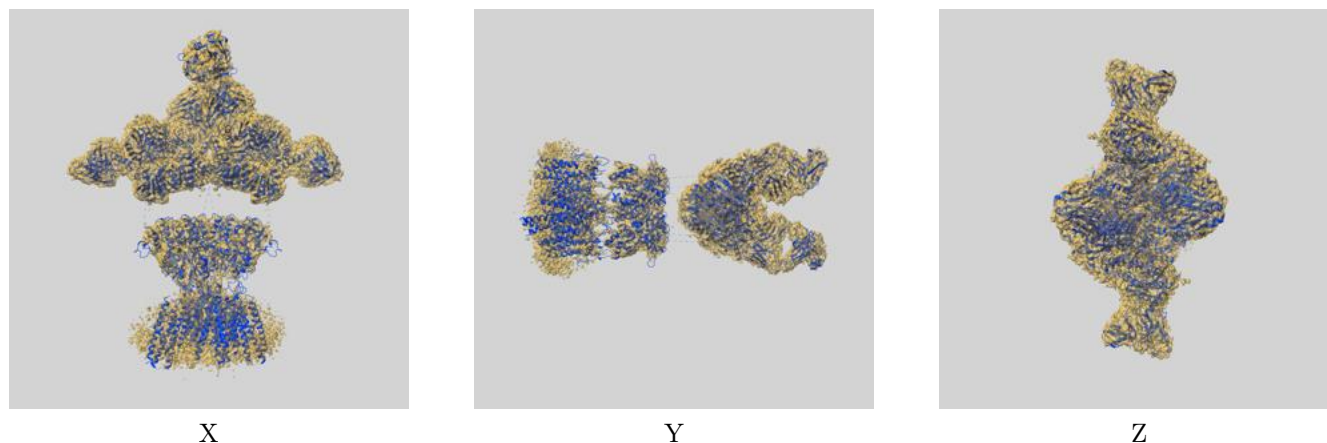
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

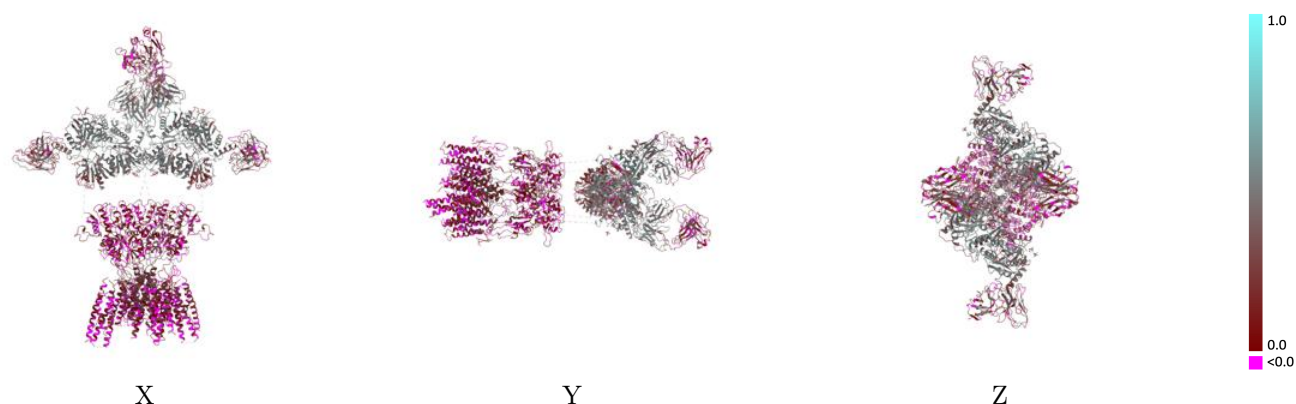
This section contains information regarding the fit between EMDB map EMD-23283 and PDB model 7LDD. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



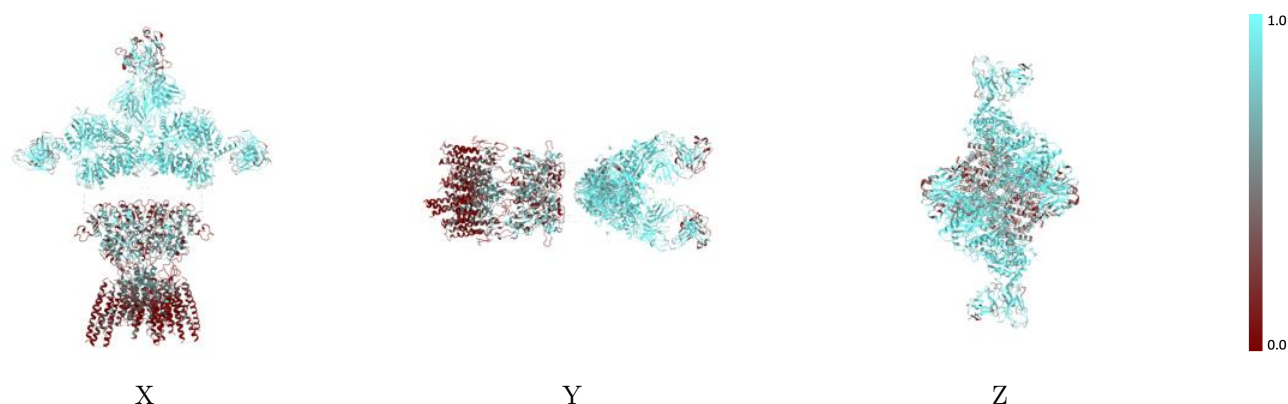
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



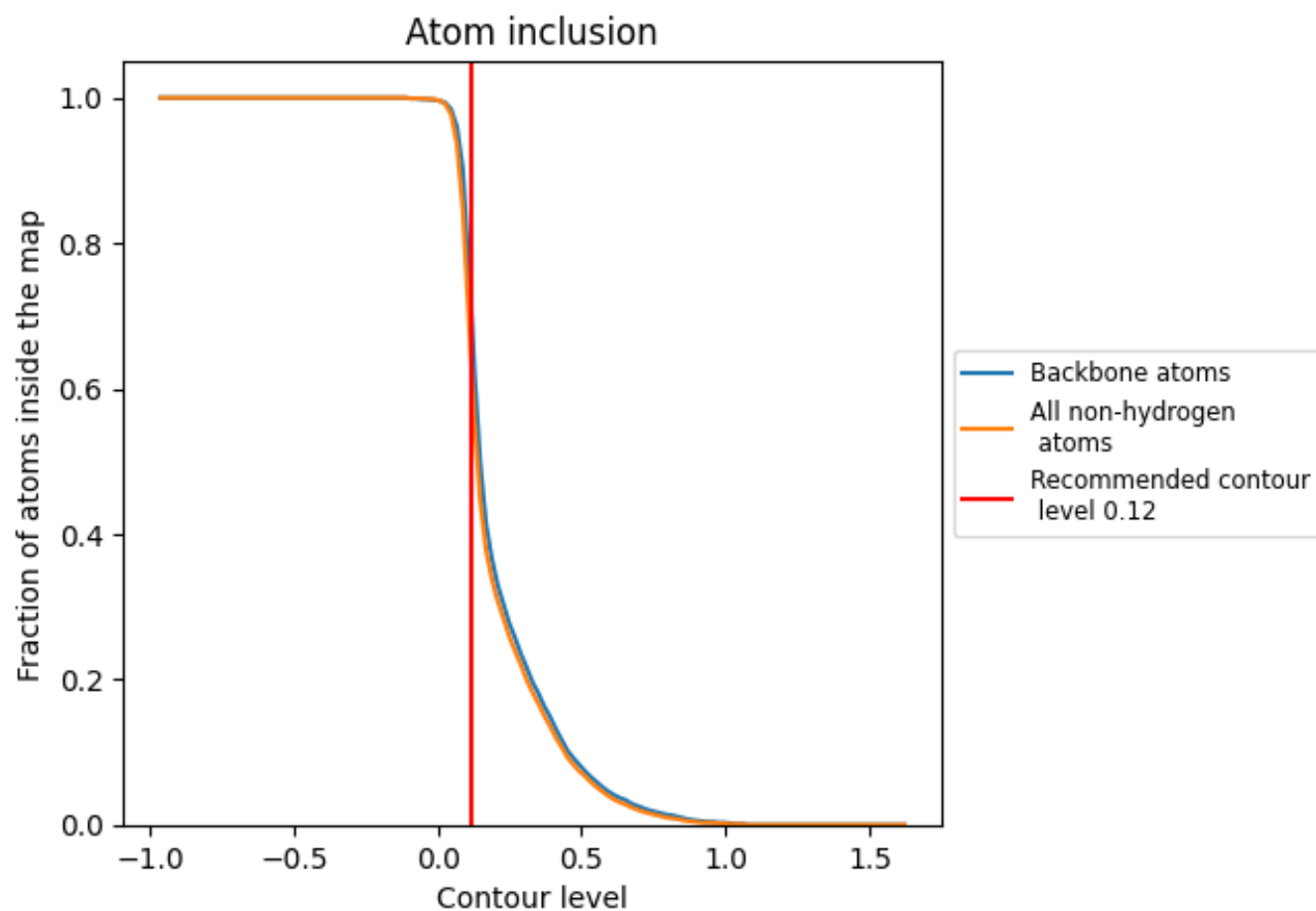
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 61% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6140	 0.2500
A	 0.6500	 0.2690
B	 0.6560	 0.2850
C	 0.6510	 0.2700
D	 0.6560	 0.2830
E	 0.1810	 0.0400
F	 0.1800	 0.0490
G	 0.1840	 0.0670
H	 0.1830	 0.0700
I	 0.7460	 0.2480
J	 0.7660	 0.2980
K	 0.7710	 0.3040
L	 0.7470	 0.2470
M	 0.7620	 0.2980
N	 0.7750	 0.3000
O	 0.8210	 0.3760
P	 0.8570	 0.3690
Q	 0.5360	 0.2210
R	 0.8210	 0.3650
S	 0.8570	 0.3600
T	 0.5360	 0.2320

