



wwPDB EM Validation Summary Report ⓘ

Apr 20, 2024 – 06:01 PM EDT

PDB ID : 9AXF
EMDB ID : EMD-43966
Title : Structure of human calcium-sensing receptor in complex with chimeric Gq (miniGisq) protein in detergent
Authors : Zuo, H.; Park, J.; Frangaj, A.; Ye, J.; Lu, G.; Manning, J.J.; Asher, W.B.; Lu, Z.; Hu, G.; Wang, L.; Mendez, J.; Eng, E.; Zhang, Z.; Lin, X.; Grasucci, R.; Hendrickson, W.A.; Clarke, O.B.; Javitch, J.A.; Conigrave, A.D.; Fan, Q.R.
Deposited on : 2024-03-06
Resolution : 3.50 Å(reported)
Based on initial models : 7SIL, 7RTB, 7P00

This is a wwPDB EM Validation Summary 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:

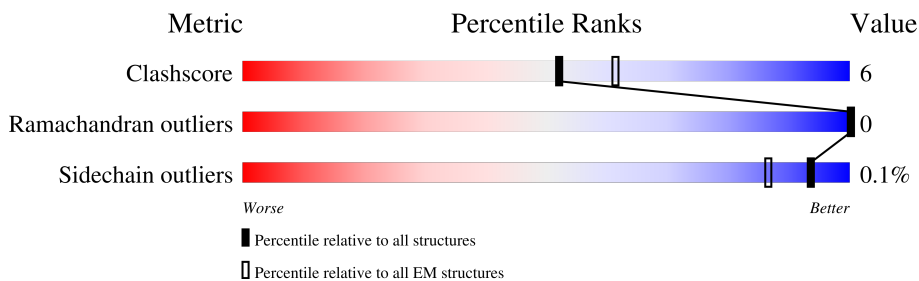
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 Å.

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




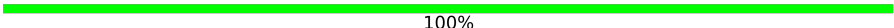
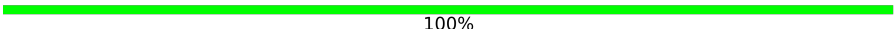

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	Q	911	
1	R	911	
2	A	246	
3	B	348	
4	G	71	
5	H	297	
6	N	160	

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Mol	Chain	Length	Quality of chain
7	C	2	 50% 50%
7	D	2	 100%
7	E	2	 100%
7	F	2	 50% 50%

2 Entry composition i

There are 15 unique types of molecules in this entry. The entry contains 21342 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 Extracellular calcium-sensing receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	R	832	Total	C	N	O	S	0	0
			6632	4307	1083	1204	38		
1	Q	791	Total	C	N	O	S	0	0
			6293	4088	1019	1149	37		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	904	ASP	-	expression tag	UNP P41180
R	905	TYR	-	expression tag	UNP P41180
R	906	LYS	-	expression tag	UNP P41180
R	907	ASP	-	expression tag	UNP P41180
R	908	ASP	-	expression tag	UNP P41180
R	909	ASP	-	expression tag	UNP P41180
R	910	ASP	-	expression tag	UNP P41180
R	911	LYS	-	expression tag	UNP P41180
Q	904	ASP	-	expression tag	UNP P41180
Q	905	TYR	-	expression tag	UNP P41180
Q	906	LYS	-	expression tag	UNP P41180
Q	907	ASP	-	expression tag	UNP P41180
Q	908	ASP	-	expression tag	UNP P41180
Q	909	ASP	-	expression tag	UNP P41180
Q	910	ASP	-	expression tag	UNP P41180
Q	911	LYS	-	expression tag	UNP P41180

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	228	Total	C	N	O	S	0	0
			1879	1188	332	351	8		

There are 53 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLU	ASP	engineered mutation	UNP P63096
A	21	LYS	ARG	engineered mutation	UNP P63096
A	22	GLN	ASN	engineered mutation	UNP P63096
A	24	GLN	ARG	engineered mutation	UNP P63096
A	25	LYS	GLU	engineered mutation	UNP P63096
A	27	LYS	GLY	engineered mutation	UNP P63096
A	28	GLN	GLU	engineered mutation	UNP P63096
A	29	VAL	LYS	engineered mutation	UNP P63096
A	30	TYR	ALA	engineered mutation	UNP P63096
A	31	ARG	ALA	engineered mutation	UNP P63096
A	32	ALA	ARG	engineered mutation	UNP P63096
A	33	THR	GLU	engineered mutation	UNP P63096
A	34	HIS	VAL	engineered mutation	UNP P63096
A	35	ARG	LYS	engineered mutation	UNP P63096
A	42	ASP	GLY	engineered mutation	UNP P63096
A	43	ASN	GLU	engineered mutation	UNP P63096
A	54	ARG	-	linker	UNP P63096
A	55	ILE	-	linker	UNP P63096
A	56	LEU	-	linker	UNP P63096
A	57	HIS	-	linker	UNP P63096
A	58	GLY	-	linker	UNP P63096
A	59	GLY	-	linker	UNP P63096
A	60	SER	-	linker	UNP P63096
A	61	GLY	-	linker	UNP P63096
A	62	GLY	-	linker	UNP P63096
A	63	SER	-	linker	UNP P63096
A	64	GLY	-	linker	UNP P63096
A	65	GLY	-	linker	UNP P63096
A	66	THR	-	linker	UNP P63096
A	67	SER	-	linker	UNP P63096
A	68	GLY	-	linker	UNP P63096
A	111	ASP	ALA	engineered mutation	UNP A0A590UJY2
A	114	ASP	SER	engineered mutation	UNP A0A590UJY2
A	?	-	ASN	deletion	UNP A0A590UJY2
A	?	-	MET	deletion	UNP A0A590UJY2
A	?	-	VAL	deletion	UNP A0A590UJY2
A	?	-	ILE	deletion	UNP A0A590UJY2
A	?	-	ARG	deletion	UNP A0A590UJY2
A	?	-	GLU	deletion	UNP A0A590UJY2
A	?	-	ASP	deletion	UNP A0A590UJY2
A	?	-	ASN	deletion	UNP A0A590UJY2
A	?	-	GLN	deletion	UNP A0A590UJY2
A	?	-	THR	deletion	UNP A0A590UJY2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	124	ASP	LEU	engineered mutation	UNP A0A590UJY2
A	224	ALA	ILE	engineered mutation	UNP A0A590UJY2
A	227	ILE	VAL	engineered mutation	UNP A0A590UJY2
A	232	LYS	ARG	engineered mutation	UNP A0A590UJY2
A	236	LEU	GLN	engineered mutation	UNP A0A590UJY2
A	237	GLN	ARG	engineered mutation	UNP A0A590UJY2
A	239	ASN	HIS	engineered mutation	UNP A0A590UJY2
A	242	GLU	GLN	engineered mutation	UNP A0A590UJY2
A	244	ASN	GLU	engineered mutation	UNP A0A590UJY2
A	246	VAL	LEU	engineered mutation	UNP A0A590UJY2

- 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
			Total	C	N	O	S		
3	B	338	2601	1604	467	509	21	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	initiating methionine	UNP P62873
B	-6	ASP	-	expression tag	UNP P62873
B	-5	TYR	-	expression tag	UNP P62873
B	-4	LYS	-	expression tag	UNP P62873
B	-3	ASP	-	expression tag	UNP P62873
B	-2	ASP	-	expression tag	UNP P62873
B	-1	ASP	-	expression tag	UNP P62873
B	0	ASP	-	expression tag	UNP P62873
B	1	LYS	-	expression tag	UNP P62873

- 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
			Total	C	N	O	S		
4	G	56	433	271	76	83	3	0	0

- Molecule 5 is a protein called Single-chain antibody fragment scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	234	1795	1137	297	351	10	0	0

- Molecule 6 is a protein called Nanobody Nb-35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	N	126	961	599	168	188	6	0	0

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



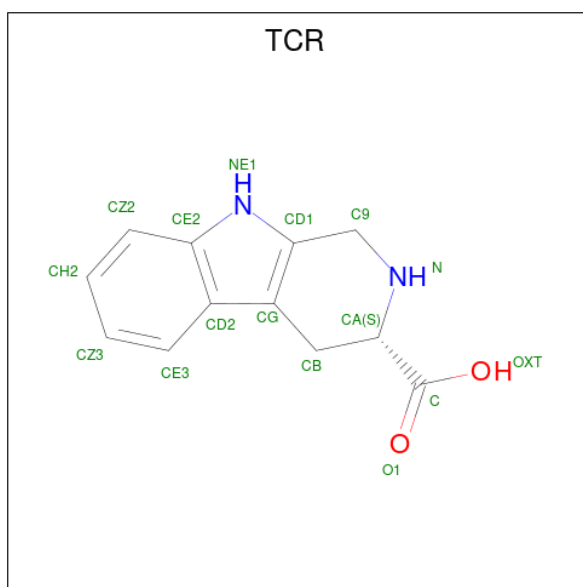
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	C	2	28	16	2	10	0	0
7	D	2	28	16	2	10	0	0
7	E	2	28	16	2	10	0	0
7	F	2	28	16	2	10	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



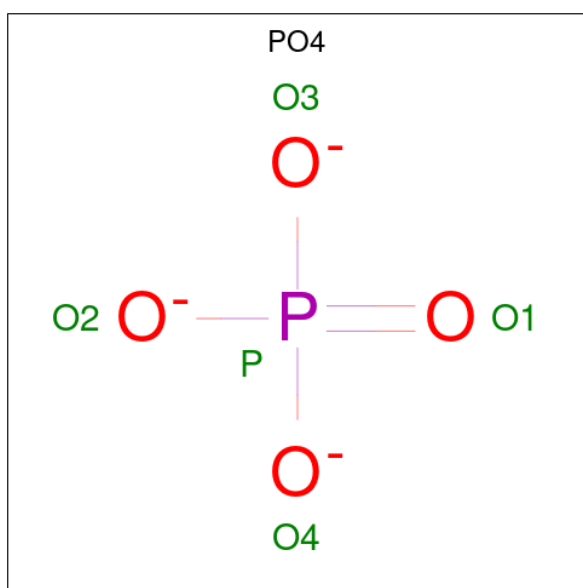
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
8	R	1	Total 14	8	1	5	0
8	R	1	Total 14	8	1	5	0
8	R	1	Total 14	8	1	5	0
8	R	1	Total 14	8	1	5	0
8	Q	1	Total 14	8	1	5	0
8	Q	1	Total 14	8	1	5	0
8	Q	1	Total 14	8	1	5	0
8	Q	1	Total 14	8	1	5	0

- Molecule 9 is CYCLOMETHYLTRYPTOPHAN (three-letter code: TCR) (formula: $C_{12}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms			AltConf	
9	R	1	Total	C	N	O	0
			16	12	2	2	
9	Q	1	Total	C	N	O	0
			16	12	2	2	

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

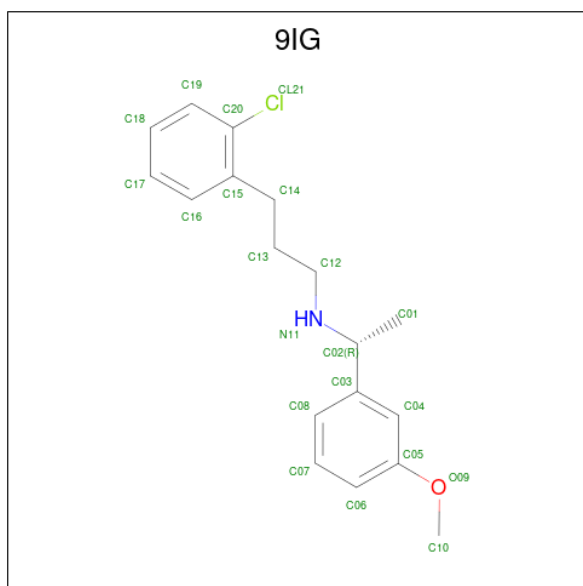


Mol	Chain	Residues	Atoms		AltConf	
10	R	1	Total	O	P	0
			5	4	1	
10	Q	1	Total	O	P	0
			5	4	1	

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

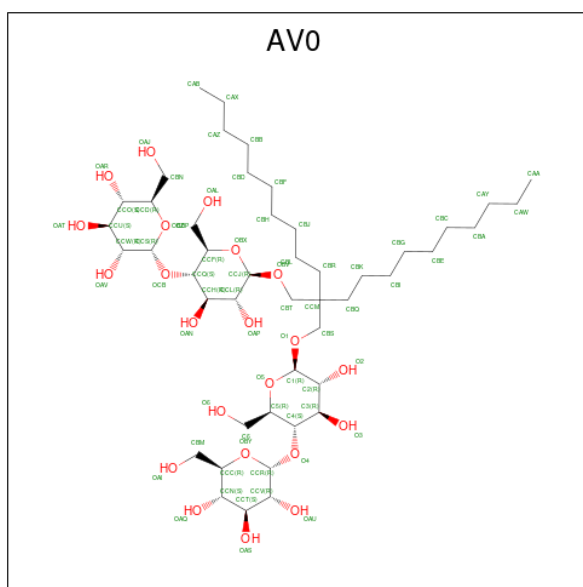
Mol	Chain	Residues	Atoms		AltConf
11	R	3	Total	Ca	0
			3	3	
11	Q	4	Total	Ca	0
			4	4	

- Molecule 12 is 3-(2-chlorophenyl)-N-[(1R)-1-(3-methoxyphenyl)ethyl]propan-1-amine (three-letter code: 9IG) (formula: C₁₈H₂₂ClNO).



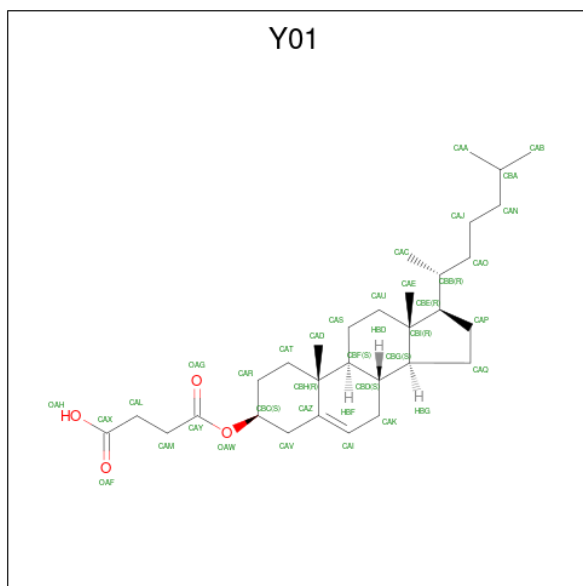
Mol	Chain	Residues	Atoms					AltConf
12	R	1	Total	C	Cl	N	O	0
			21	18	1	1	1	
12	Q	1	Total	C	Cl	N	O	0
			21	18	1	1	1	

- Molecule 13 is Lauryl Maltose Neopentyl Glycol (three-letter code: AV0) (formula: C₄₇H₈₈O₂₂).



Mol	Chain	Residues	Atoms		AltConf
13	R	1	Total	C O	0
			69	47 22	

- Molecule 14 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



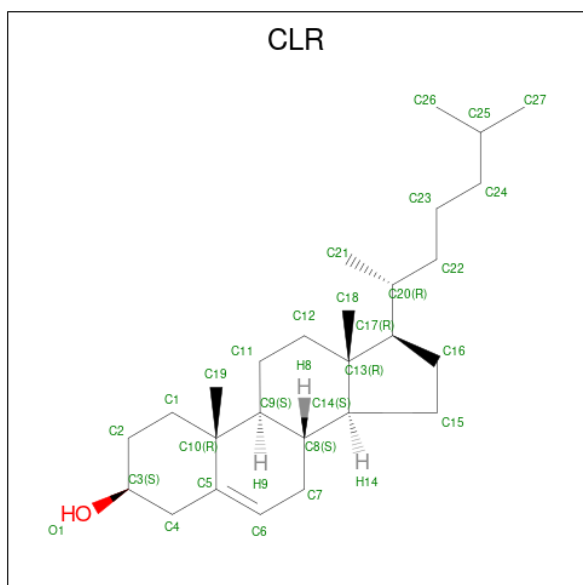
Mol	Chain	Residues	Atoms		AltConf
14	R	1	Total	C O	0
			35	31 4	
14	R	1	Total	C O	0
			35	31 4	

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Mol	Chain	Residues	Atoms			AltConf
14	R	1	Total	C	O	0
			35	31	4	
14	Q	1	Total	C	O	0
			35	31	4	

- Molecule 15 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).

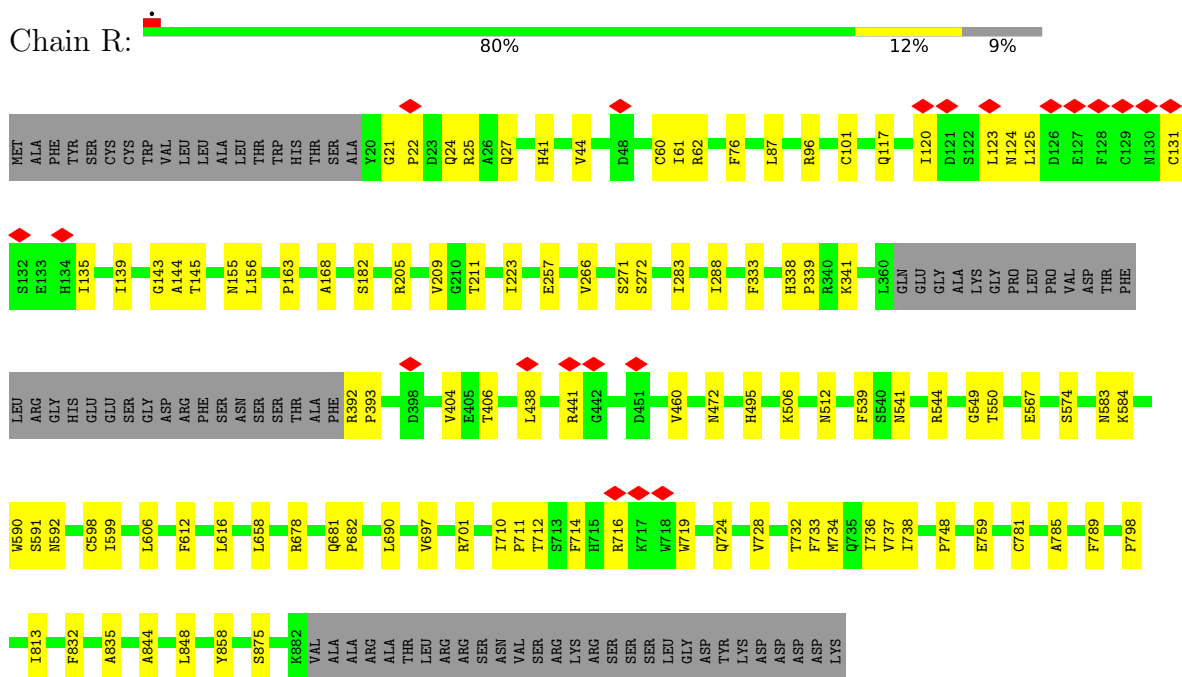


Mol	Chain	Residues	Atoms			AltConf
15	R	1	Total	C	O	0
			28	27	1	
15	R	1	Total	C	O	0
			28	27	1	
15	R	1	Total	C	O	0
			28	27	1	
15	Q	1	Total	C	O	0
			28	27	1	
15	Q	1	Total	C	O	0
			28	27	1	
15	Q	1	Total	C	O	0
			28	27	1	
15	Q	1	Total	C	O	0
			28	27	1	

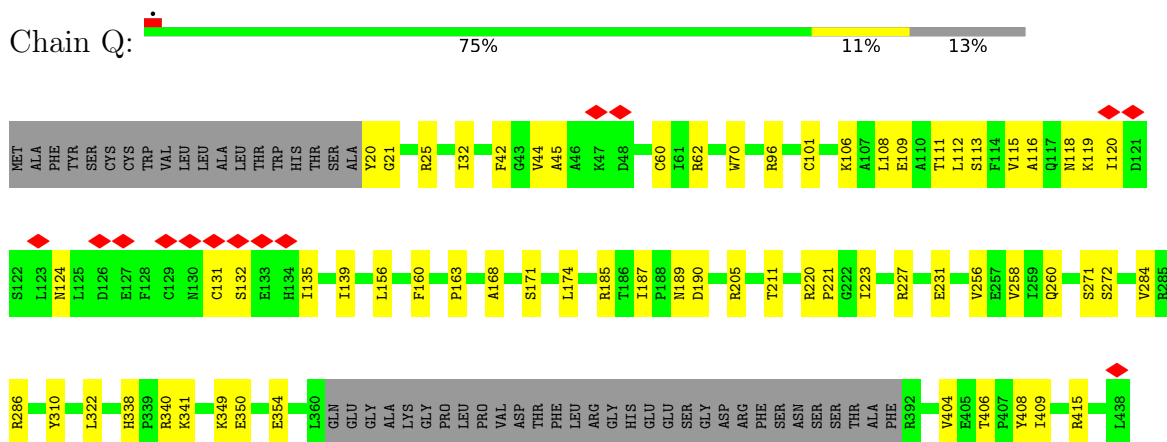
3 Residue-property plots [i](#)

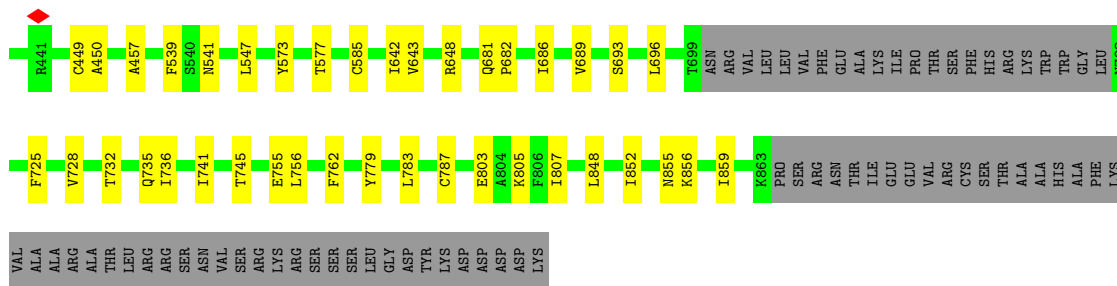
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Extracellular calcium-sensing receptor

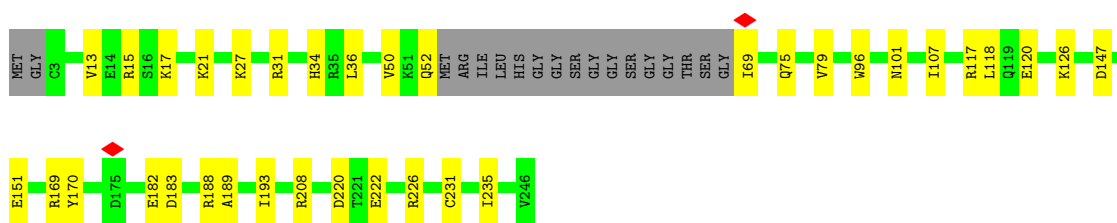
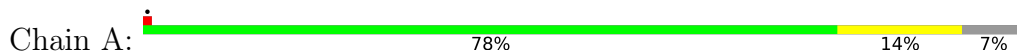


- Molecule 1: Extracellular calcium-sensing receptor

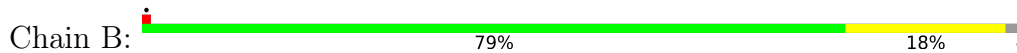




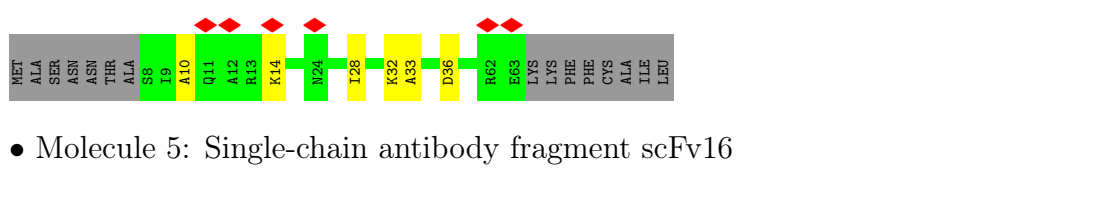
• Molecule 2: Guanine nucleotide-binding protein G(i) subunit alpha-1, Adenylate cyclase-stimulating G alpha protein



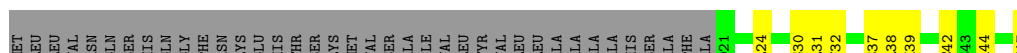
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

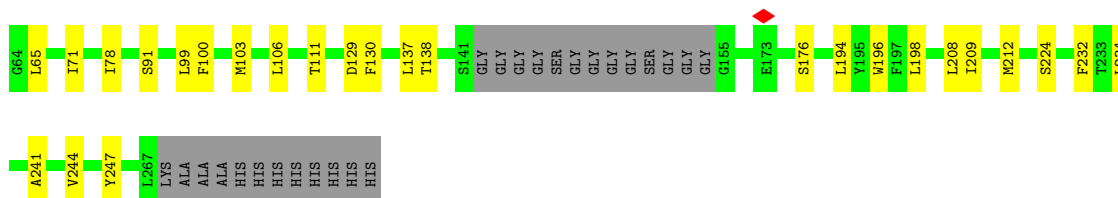


• Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

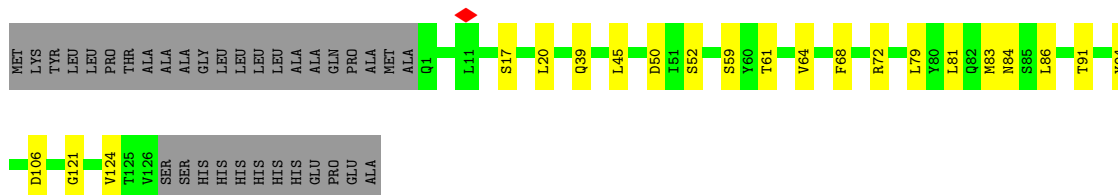


• Molecule 5: Single-chain antibody fragment scFv16





- Molecule 6: Nanobody Nb-35



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucofuranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucofuranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucofuranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucofuranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	140091	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 ($e^-/\text{\AA}^2$)	70.2	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.033	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	432.128, 432.128, 432.128	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.844, 0.844, 0.844	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: PO4, NAG, CA, TCR, 9IG, AV0, CLR, Y01

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	Q	0.28	0/6454	0.47	0/8756
1	R	0.28	0/6805	0.47	0/9234
2	A	0.27	0/1915	0.50	0/2579
3	B	0.27	0/2648	0.56	0/3589
4	G	0.24	0/439	0.44	0/592
5	H	0.27	0/1839	0.51	0/2493
6	N	0.26	0/981	0.52	0/1329
All	All	0.27	0/21081	0.49	0/28572

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	Q	6293	0	6168	71	0
1	R	6632	0	6512	71	0
2	A	1879	0	1855	27	0
3	B	2601	0	2505	40	0
4	G	433	0	442	4	0
5	H	1795	0	1724	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	N	961	0	928	13	0
7	C	28	0	25	1	0
7	D	28	0	25	0	0
7	E	28	0	25	0	0
7	F	28	0	25	1	0
8	Q	56	0	52	1	0
8	R	56	0	52	1	0
9	Q	16	0	11	1	0
9	R	16	0	11	1	0
10	Q	5	0	0	1	0
10	R	5	0	0	0	0
11	Q	4	0	0	0	0
11	R	3	0	0	0	0
12	Q	21	0	0	0	0
12	R	21	0	0	0	0
13	R	69	0	0	0	0
14	Q	35	0	49	0	0
14	R	105	0	147	7	0
15	Q	140	0	230	1	0
15	R	84	0	138	3	0
All	All	21342	0	20924	239	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 6.

The worst 5 of 239 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)
3:B:54:HIS:HE2	3:B:72:SER:HG	1.20	0.88
2:A:15:ARG:NH1	3:B:90:VAL:O	2.16	0.78
1:R:712:THR:HG22	1:R:714:PHE:H	1.48	0.77
1:Q:689:VAL:HG21	1:Q:735:GLN:HG3	1.72	0.72
3:B:215:GLU:OE1	3:B:219:ARG:NH2	2.25	0.69

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	785/911 (86%)	766 (98%)	19 (2%)	0	100	100
1	R	828/911 (91%)	806 (97%)	22 (3%)	0	100	100
2	A	224/246 (91%)	216 (96%)	8 (4%)	0	100	100
3	B	336/348 (97%)	328 (98%)	8 (2%)	0	100	100
4	G	54/71 (76%)	54 (100%)	0	0	100	100
5	H	230/297 (77%)	226 (98%)	4 (2%)	0	100	100
6	N	124/160 (78%)	123 (99%)	1 (1%)	0	100	100
All	All	2581/2944 (88%)	2519 (98%)	62 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	688/790 (87%)	687 (100%)	1 (0%)	93	98
1	R	724/790 (92%)	723 (100%)	1 (0%)	93	98
2	A	205/215 (95%)	205 (100%)	0	100	100
3	B	281/291 (97%)	281 (100%)	0	100	100
4	G	46/58 (79%)	46 (100%)	0	100	100
5	H	198/239 (83%)	198 (100%)	0	100	100
6	N	104/129 (81%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2246/2512 (89%)	2244 (100%)	2 (0%)	93 98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	205	ARG
1	Q	124	ASN

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

Mol	Chain	Res	Type
1	Q	338	HIS
2	A	130	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](#)

8 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	$\# Z > 2$
7	NAG	C	1	7,1	14,14,15	0.24	0	17,19,21	0.50	0
7	NAG	C	2	7	14,14,15	0.22	0	17,19,21	0.39	0
7	NAG	D	1	7,1	14,14,15	0.22	0	17,19,21	0.46	0
7	NAG	D	2	7	14,14,15	0.18	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	E	1	7,1	14,14,15	0.22	0	17,19,21	0.52	0
7	NAG	E	2	7	14,14,15	0.23	0	17,19,21	0.39	0
7	NAG	F	1	7,1	14,14,15	0.30	0	17,19,21	0.45	0
7	NAG	F	2	7	14,14,15	0.18	0	17,19,21	0.50	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
7	NAG	C	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	C	2	7	-	2/6/23/26	0/1/1/1
7	NAG	D	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	D	2	7	-	3/6/23/26	0/1/1/1
7	NAG	E	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	E	2	7	-	2/6/23/26	0/1/1/1
7	NAG	F	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	F	2	7	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

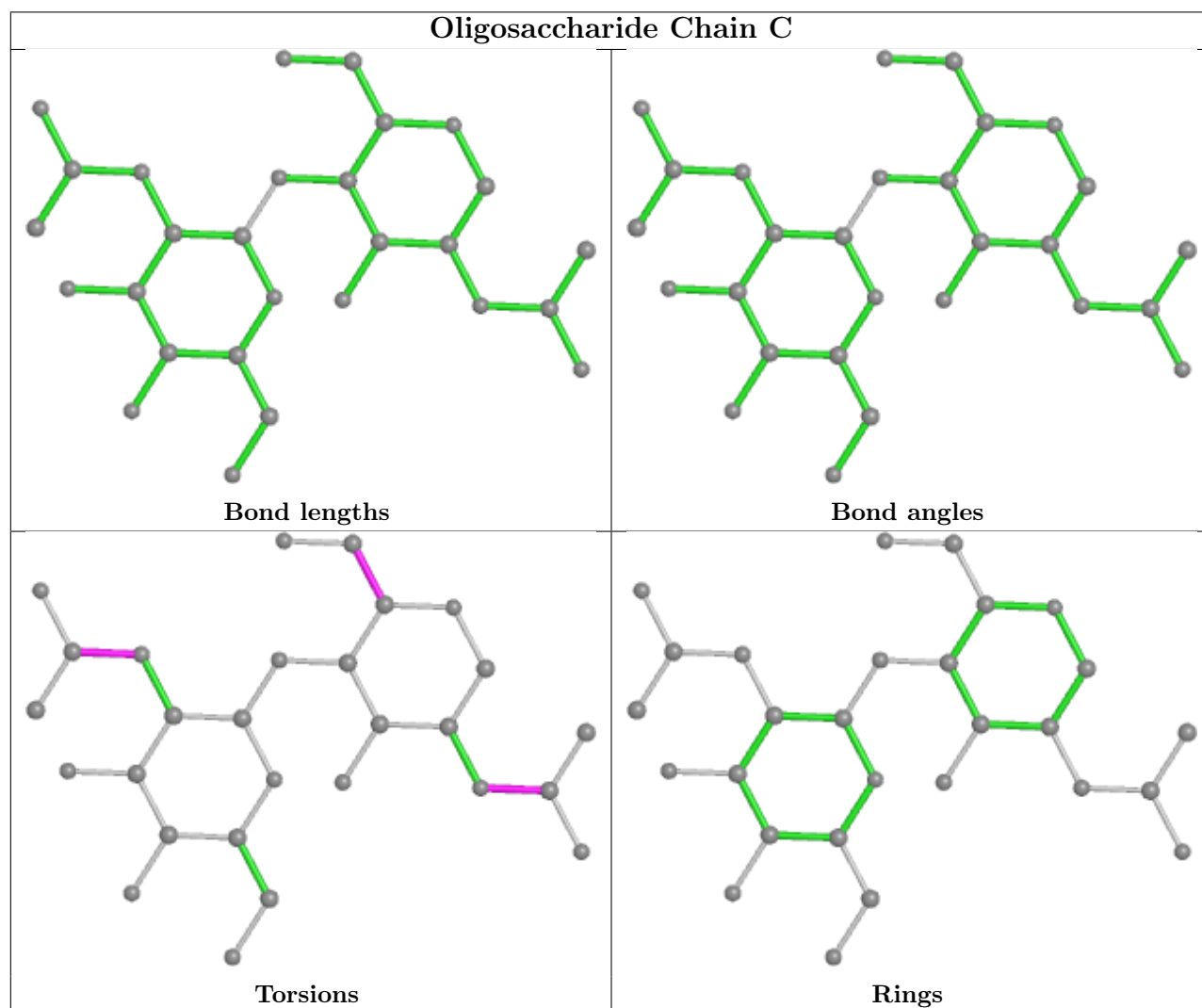
Mol	Chain	Res	Type	Atoms
7	F	2	NAG	O5-C5-C6-O6
7	D	1	NAG	O5-C5-C6-O6
7	D	1	NAG	C4-C5-C6-O6
7	F	2	NAG	C4-C5-C6-O6
7	C	1	NAG	C8-C7-N2-C2

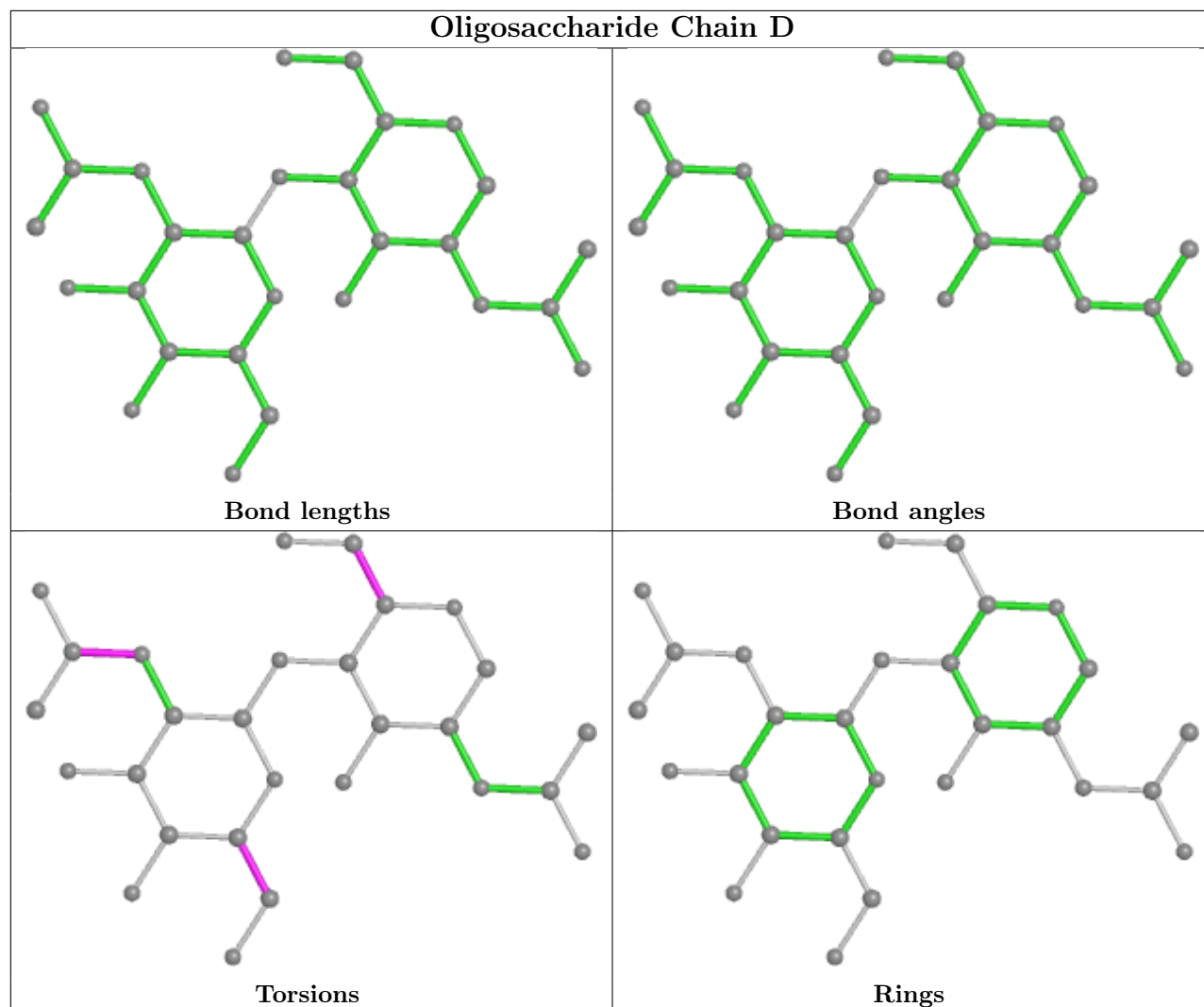
There are no ring outliers.

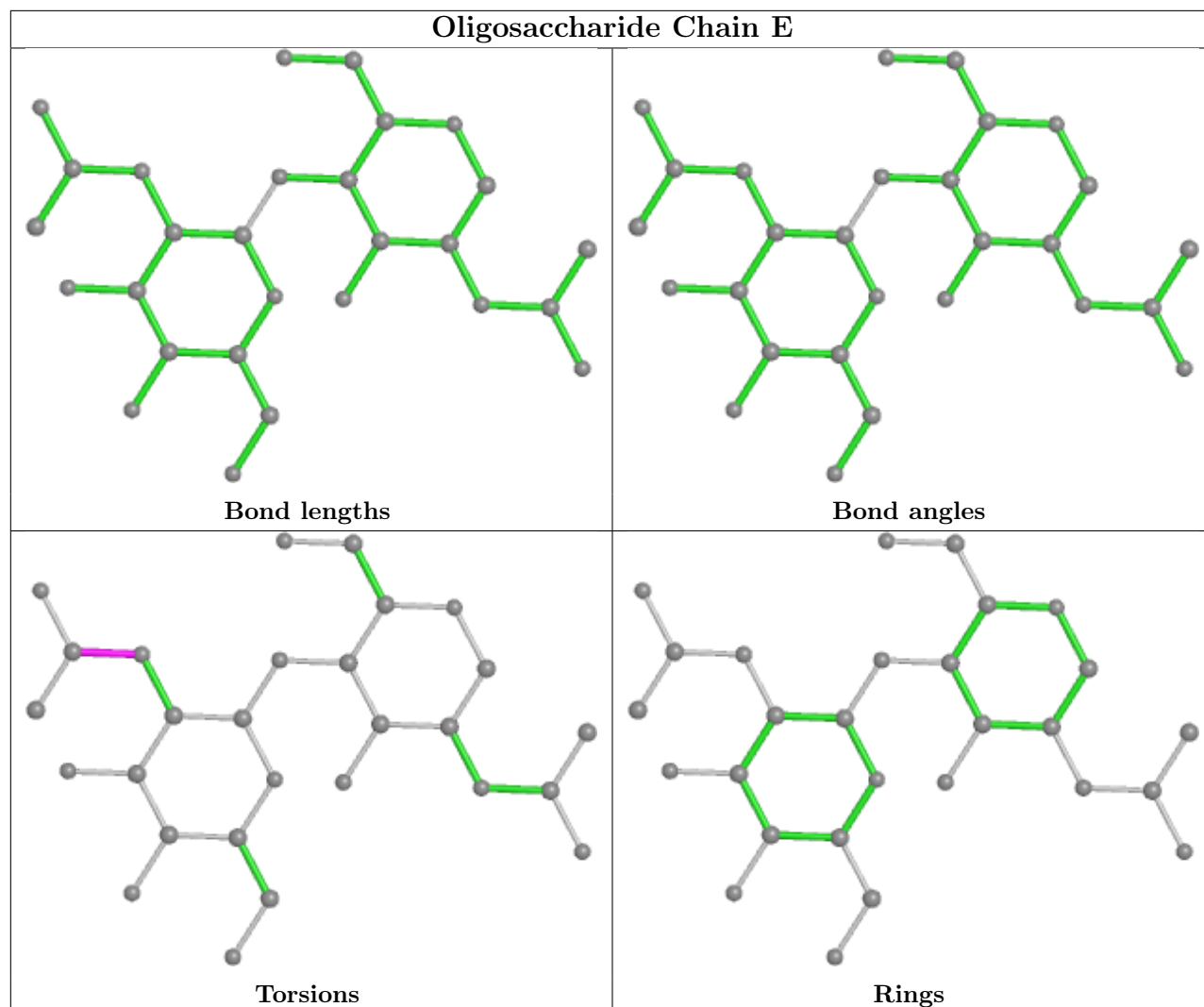
2 monomers are involved in 2 short contacts:

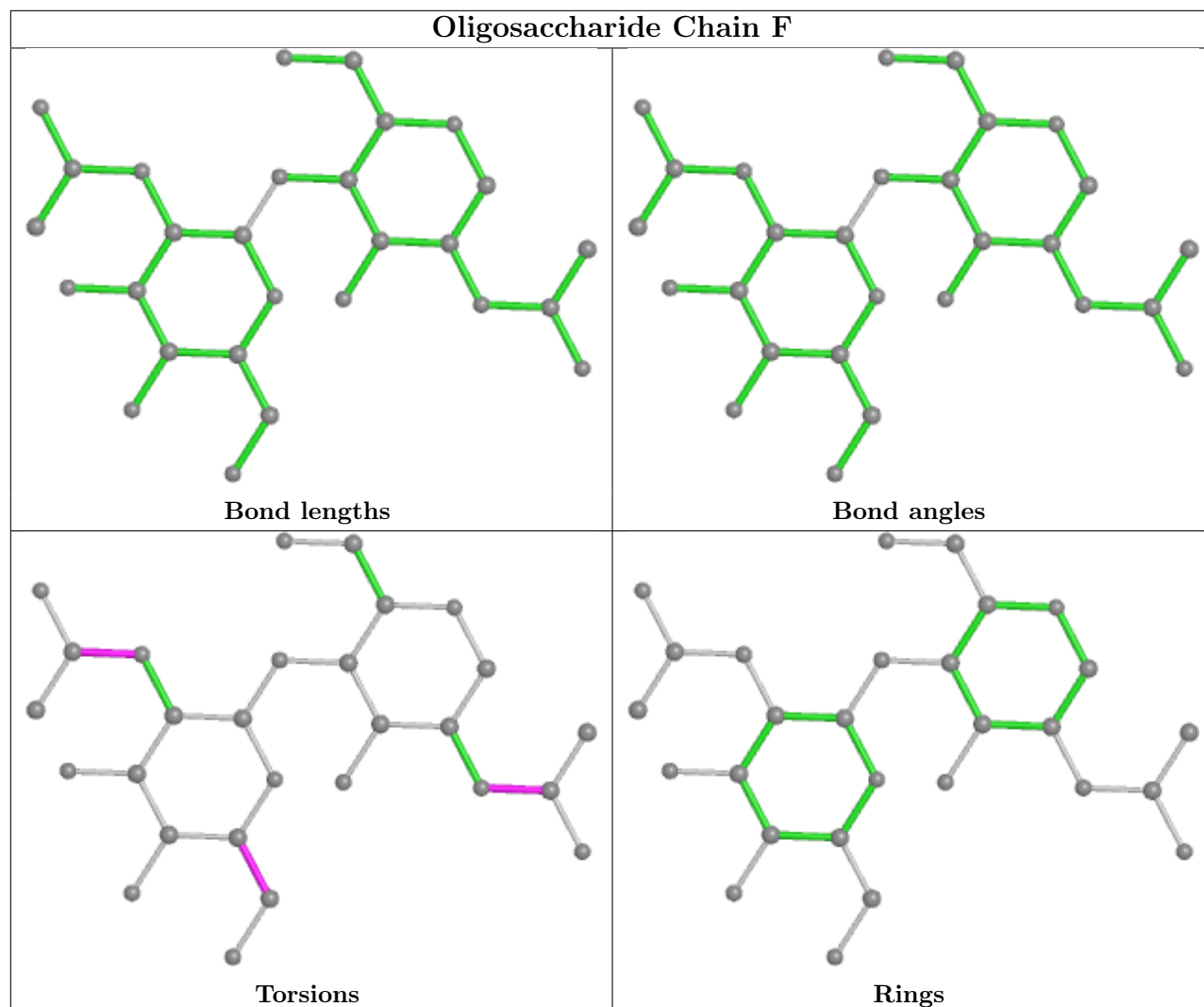
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1	NAG	1	0
7	F	1	NAG	1	0

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](#)

Of 34 ligands modelled in this entry, 7 are monoatomic - leaving 27 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	R	1004	1	14,14,15	0.21	0	17,19,21	0.42	0
10	PO4	R	1006	-	4,4,4	1.02	0	6,6,6	0.44	0
9	TCR	Q	1005	-	16,18,18	1.91	2 (12%)	16,26,26	1.25	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	R	1002	1	14,14,15	0.19	0	17,19,21	0.40	0
8	NAG	Q	1002	1	14,14,15	0.19	0	17,19,21	0.37	0
8	NAG	Q	1004	1	14,14,15	0.25	0	17,19,21	0.37	0
15	CLR	R	1015	-	31,31,31	1.06	1 (3%)	48,48,48	1.34	6 (12%)
8	NAG	R	1001	1	14,14,15	0.26	0	17,19,21	0.49	0
8	NAG	Q	1001	1	14,14,15	0.18	0	17,19,21	0.43	0
14	Y01	R	1014	-	38,38,38	1.19	3 (7%)	57,57,57	1.99	11 (19%)
9	TCR	R	1005	-	16,18,18	1.91	2 (12%)	16,26,26	1.20	2 (12%)
15	CLR	R	1017	-	31,31,31	1.08	2 (6%)	48,48,48	1.31	7 (14%)
14	Y01	R	1013	-	38,38,38	1.27	5 (13%)	57,57,57	1.88	10 (17%)
15	CLR	Q	1014	-	31,31,31	1.04	3 (9%)	48,48,48	1.37	10 (20%)
15	CLR	R	1016	-	31,31,31	1.09	2 (6%)	48,48,48	1.32	6 (12%)
15	CLR	Q	1013	-	31,31,31	1.03	2 (6%)	48,48,48	1.37	7 (14%)
15	CLR	Q	1016	-	31,31,31	1.05	2 (6%)	48,48,48	1.36	7 (14%)
15	CLR	Q	1017	-	31,31,31	1.06	2 (6%)	48,48,48	1.32	8 (16%)
12	9IG	R	1010	-	22,22,22	0.77	0	26,28,28	1.08	2 (7%)
8	NAG	Q	1003	1	14,14,15	0.24	0	17,19,21	0.44	0
14	Y01	R	1012	-	38,38,38	1.21	3 (7%)	57,57,57	1.97	12 (21%)
14	Y01	Q	1012	-	38,38,38	1.18	2 (5%)	57,57,57	1.96	11 (19%)
10	PO4	Q	1006	-	4,4,4	1.01	0	6,6,6	0.43	0
12	9IG	Q	1011	-	22,22,22	0.73	0	26,28,28	1.06	2 (7%)
13	AV0	R	1011	-	72,72,72	0.84	0	96,98,98	1.34	8 (8%)
8	NAG	R	1003	1	14,14,15	0.23	0	17,19,21	0.45	0
15	CLR	Q	1015	-	31,31,31	1.08	2 (6%)	48,48,48	1.36	6 (12%)

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	R	1004	1	-	2/6/23/26	0/1/1/1
9	TCR	Q	1005	-	-	3/4/13/13	0/3/3/3
8	NAG	R	1002	1	-	2/6/23/26	0/1/1/1
8	NAG	Q	1002	1	-	2/6/23/26	0/1/1/1
8	NAG	Q	1004	1	-	4/6/23/26	0/1/1/1
15	CLR	R	1015	-	-	6/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	R	1001	1	-	0/6/23/26	0/1/1/1
8	NAG	Q	1001	1	-	0/6/23/26	0/1/1/1
14	Y01	R	1014	-	-	8/19/77/77	0/4/4/4
9	TCR	R	1005	-	-	0/4/13/13	0/3/3/3
15	CLR	R	1017	-	-	5/10/68/68	0/4/4/4
14	Y01	R	1013	-	-	14/19/77/77	0/4/4/4
15	CLR	Q	1014	-	-	1/10/68/68	0/4/4/4
15	CLR	R	1016	-	-	2/10/68/68	0/4/4/4
15	CLR	Q	1013	-	-	6/10/68/68	0/4/4/4
15	CLR	Q	1016	-	-	1/10/68/68	0/4/4/4
15	CLR	Q	1017	-	-	0/10/68/68	0/4/4/4
12	9IG	R	1010	-	-	6/13/13/13	0/2/2/2
8	NAG	Q	1003	1	-	2/6/23/26	0/1/1/1
14	Y01	R	1012	-	-	8/19/77/77	0/4/4/4
14	Y01	Q	1012	-	-	6/19/77/77	0/4/4/4
12	9IG	Q	1011	-	-	3/13/13/13	0/2/2/2
13	AV0	R	1011	-	-	30/50/130/130	0/4/4/4
8	NAG	R	1003	1	-	2/6/23/26	0/1/1/1
15	CLR	Q	1015	-	-	2/10/68/68	0/4/4/4

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Q	1005	TCR	CB-CG	-6.06	1.44	1.51
9	R	1005	TCR	CB-CG	-5.89	1.44	1.51
14	R	1013	Y01	CAK-CAI	-4.32	1.40	1.50
14	R	1014	Y01	CAK-CAI	-4.24	1.41	1.50
14	Q	1012	Y01	CAK-CAI	-4.18	1.41	1.50

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	R	1014	Y01	CAV-CAZ-CBH	7.96	127.00	116.42
14	Q	1012	Y01	CAV-CAZ-CBH	7.93	126.96	116.42
14	R	1012	Y01	CAV-CAZ-CBH	7.77	126.74	116.42
14	R	1013	Y01	CAV-CAZ-CBH	7.17	125.95	116.42
14	Q	1012	Y01	OAW-CAY-CAM	5.34	123.02	111.50

There are no chirality outliers.

5 of 115 torsion outliers are listed below:

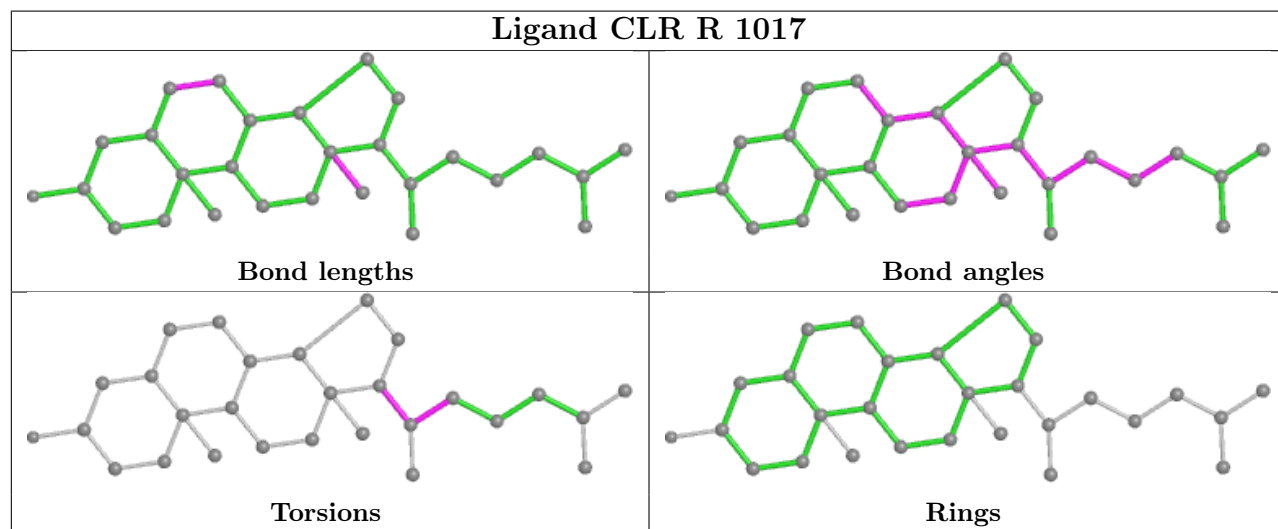
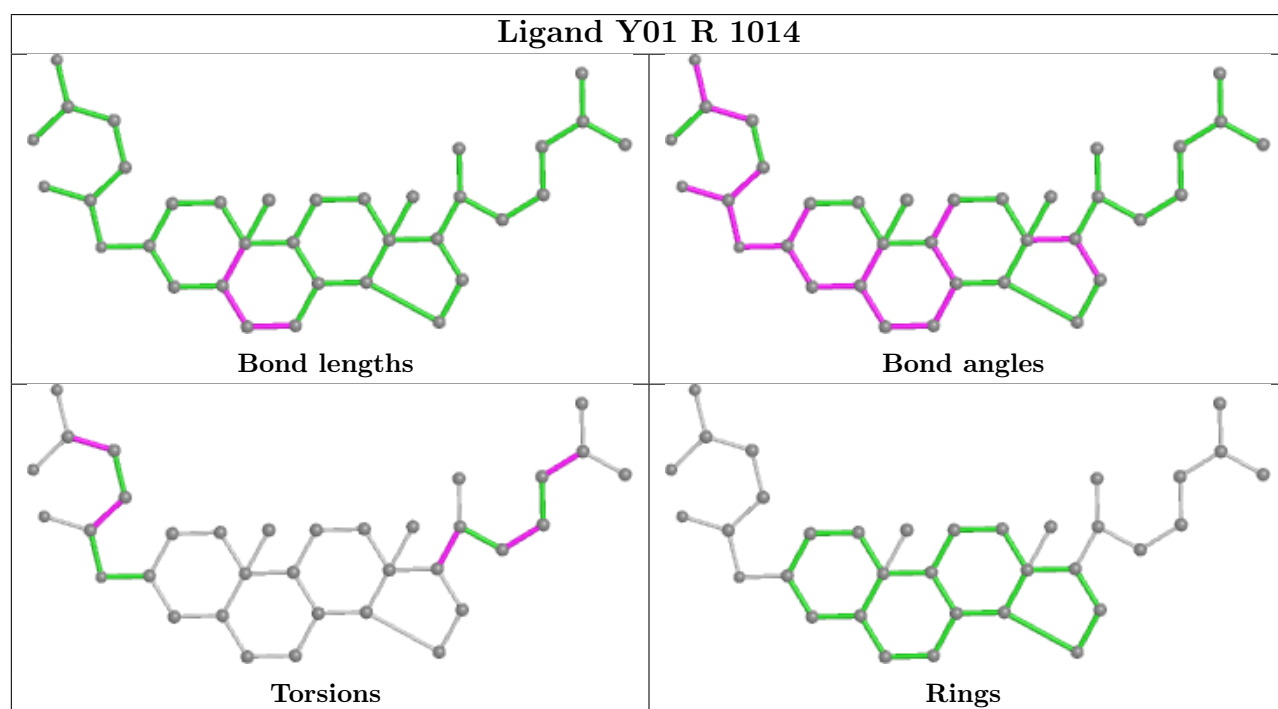
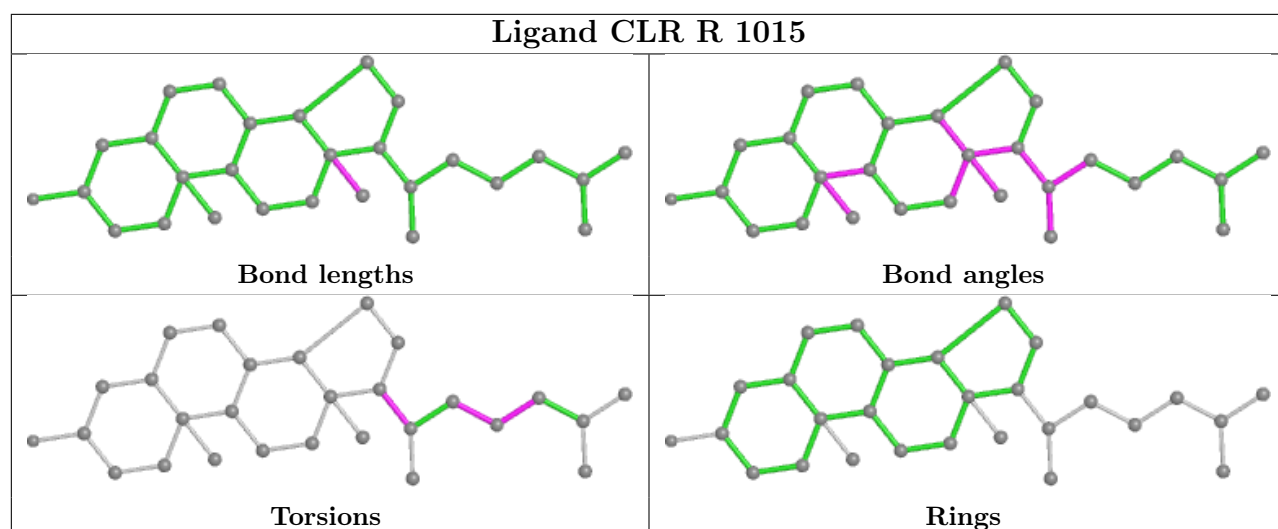
Mol	Chain	Res	Type	Atoms
13	R	1011	AV0	CBK-CBQ-CCM-CBT
13	R	1011	AV0	CBL-CBR-CCM-CBQ
13	R	1011	AV0	CBL-CBR-CCM-CBS
13	R	1011	AV0	CBL-CBR-CCM-CBT
13	R	1011	AV0	OBV-CBT-CCM-CBQ

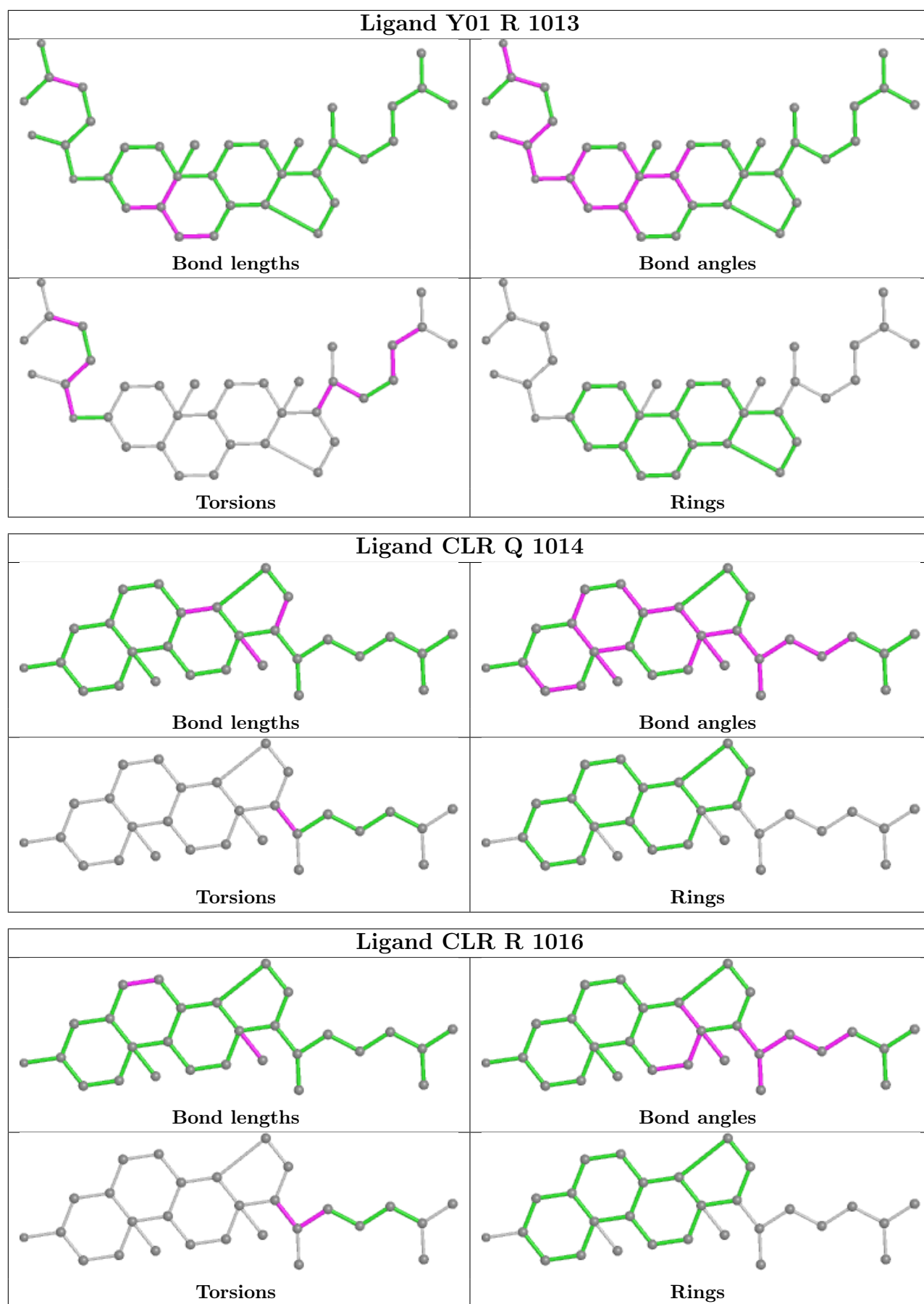
There are no ring outliers.

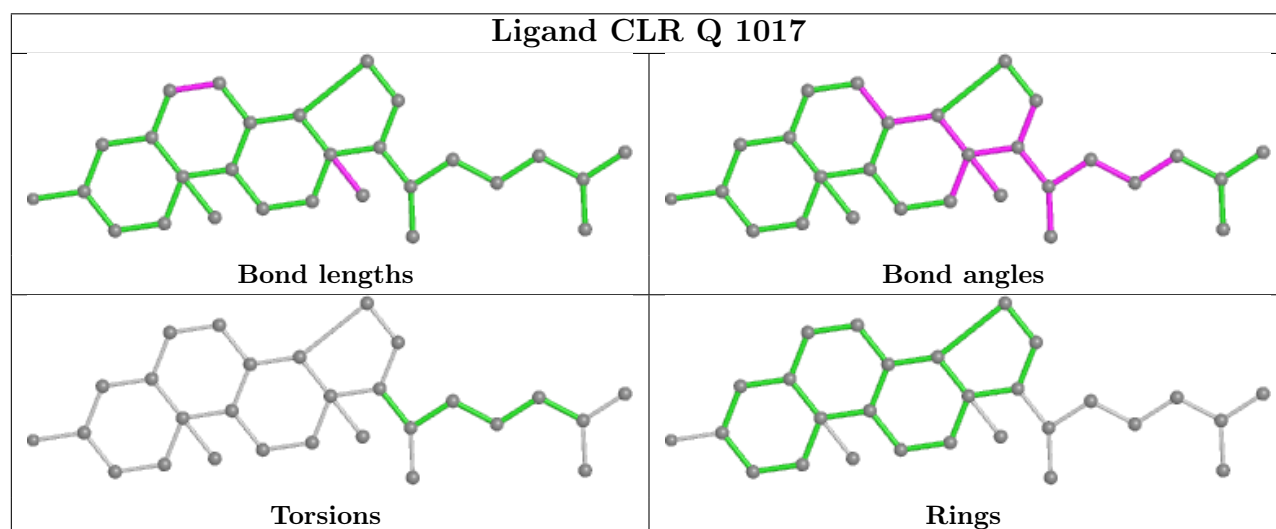
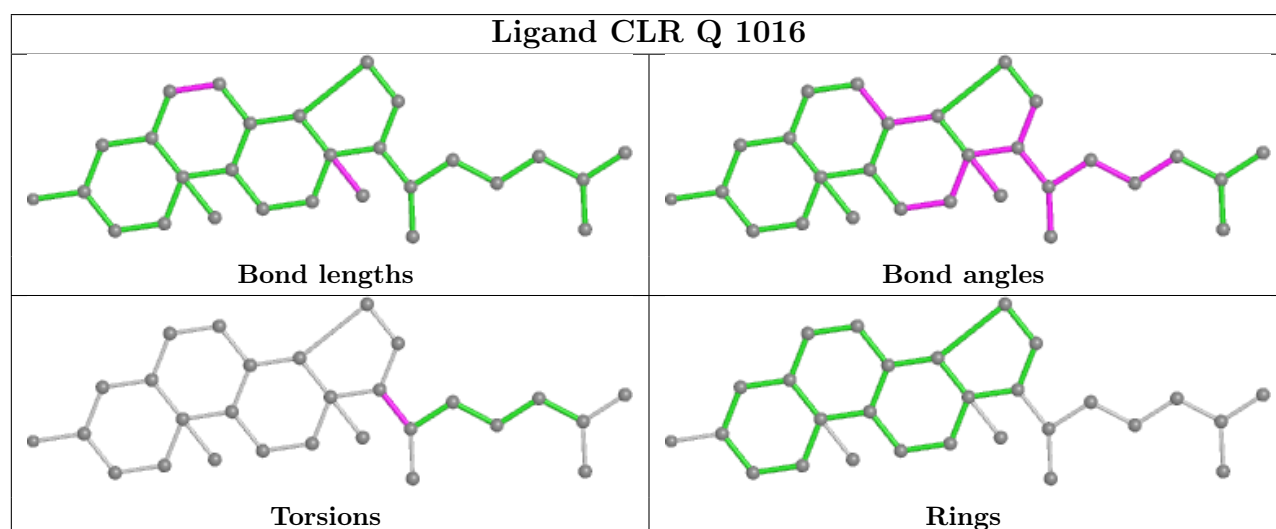
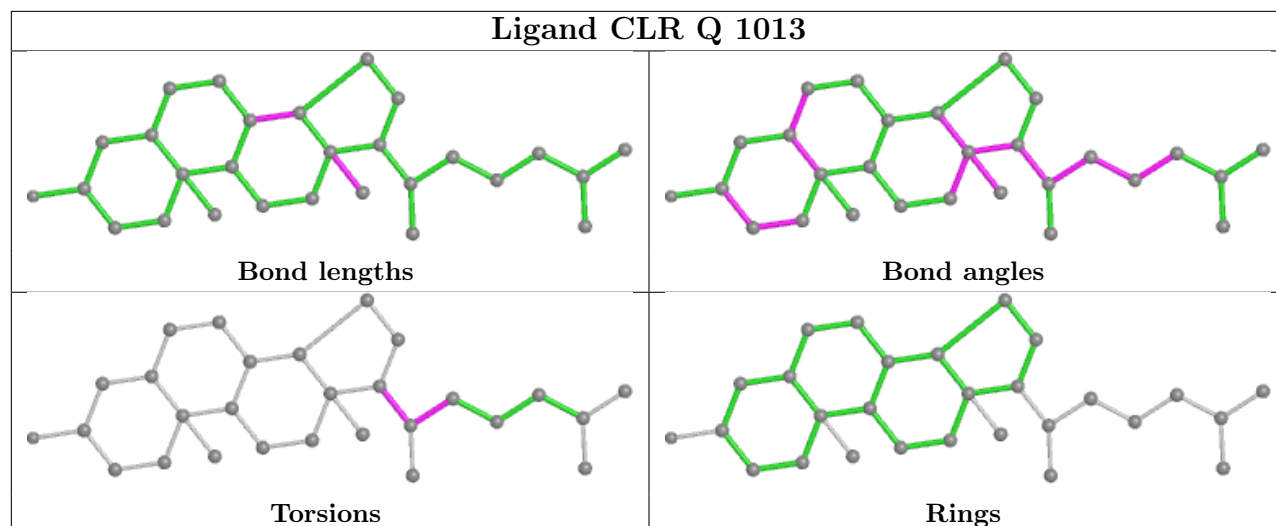
11 monomers are involved in 15 short contacts:

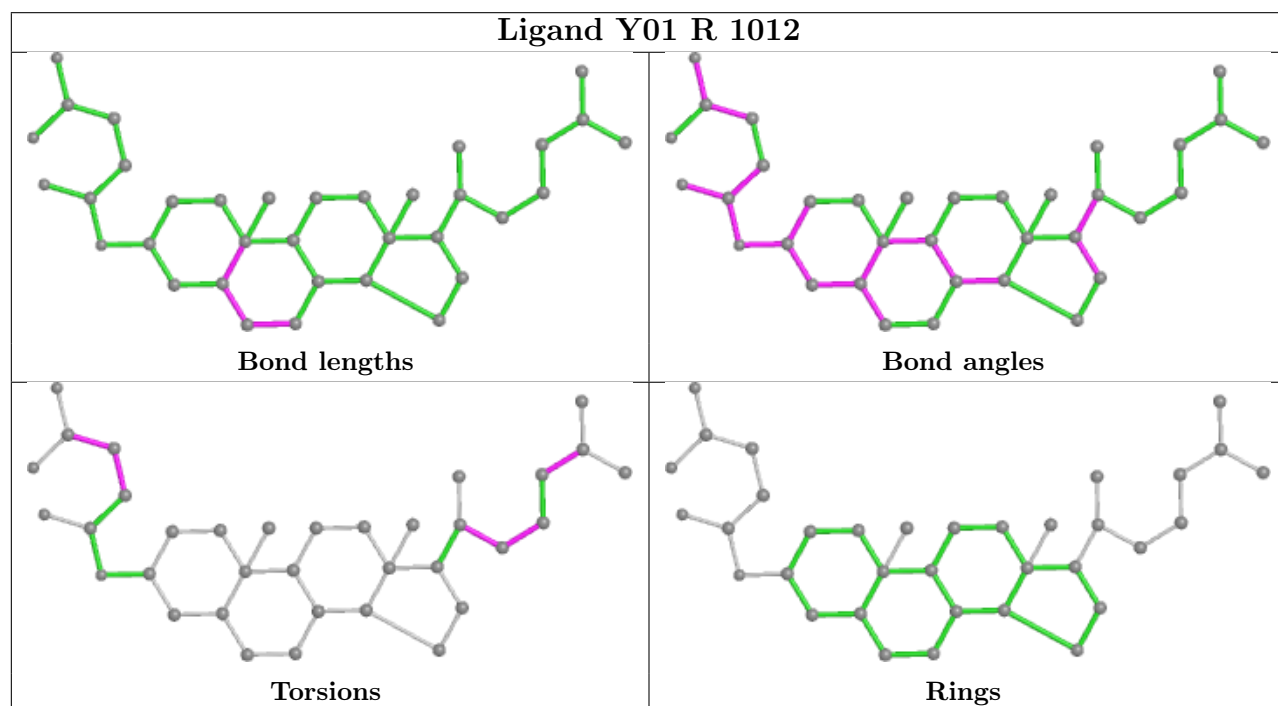
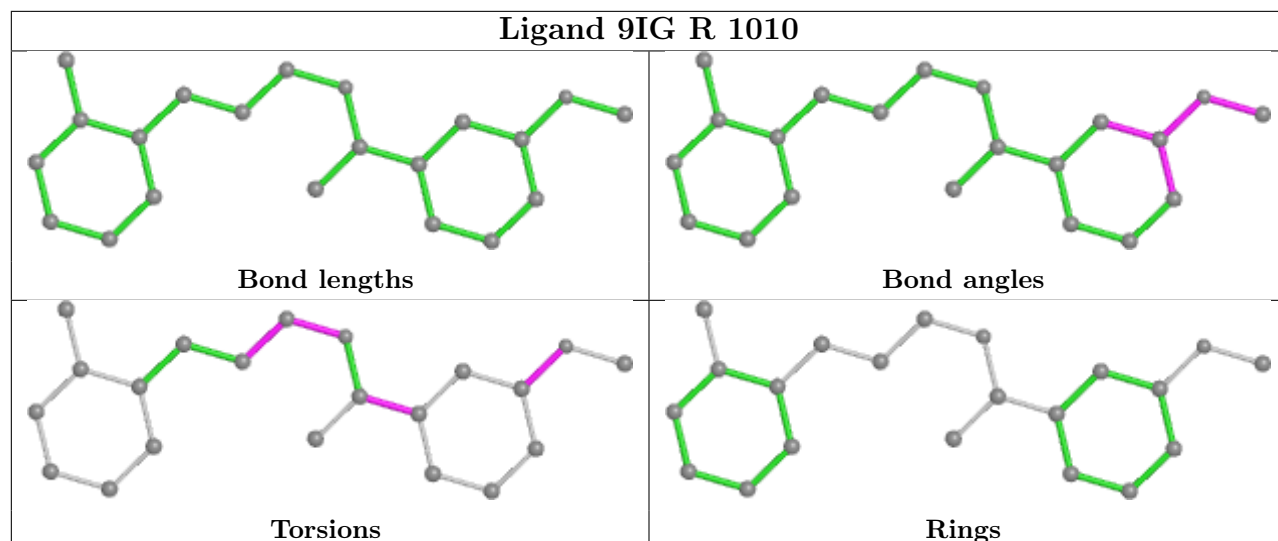
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	Q	1005	TCR	1	0
15	R	1015	CLR	1	0
8	R	1001	NAG	1	0
8	Q	1001	NAG	1	0
14	R	1014	Y01	4	0
9	R	1005	TCR	1	0
15	R	1017	CLR	1	0
14	R	1013	Y01	4	0
15	R	1016	CLR	1	0
10	Q	1006	PO4	1	0
15	Q	1015	CLR	1	0

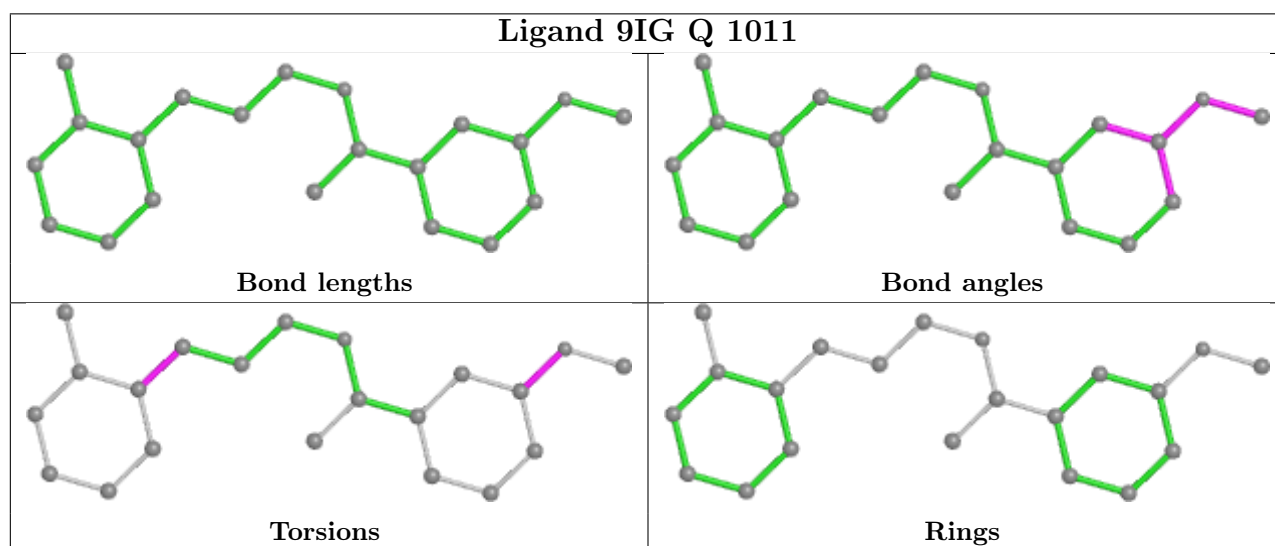
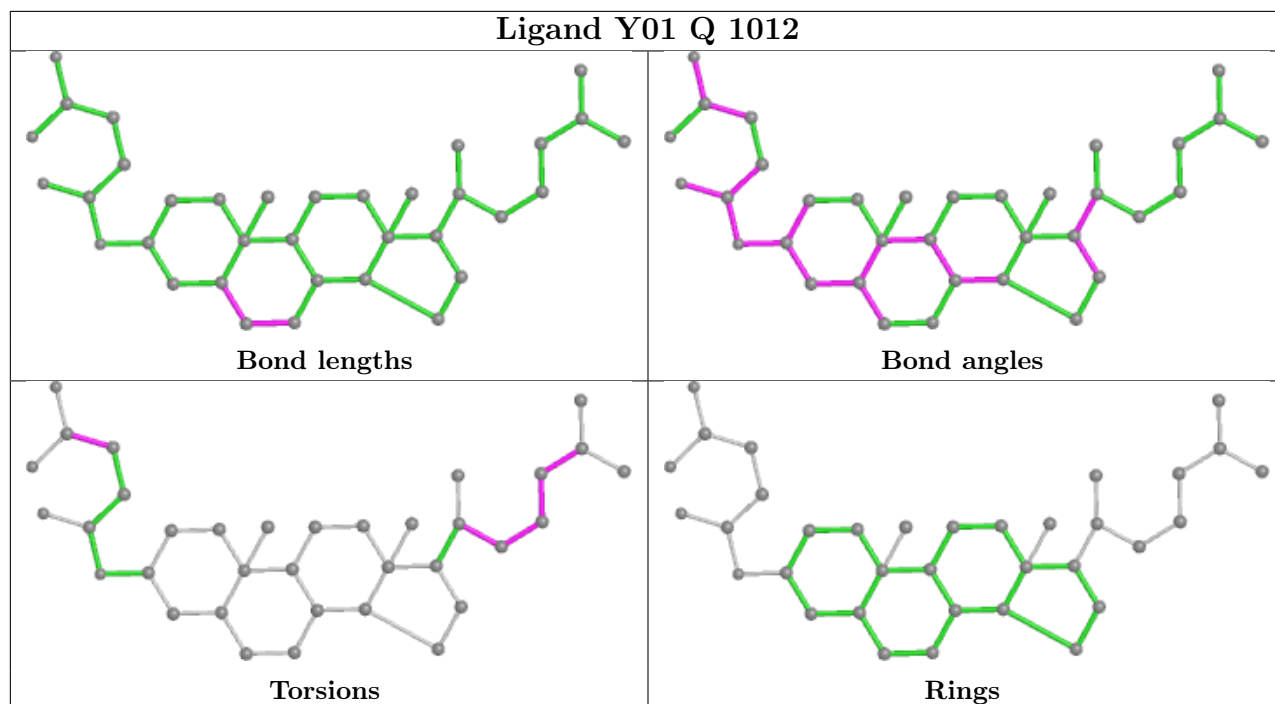
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

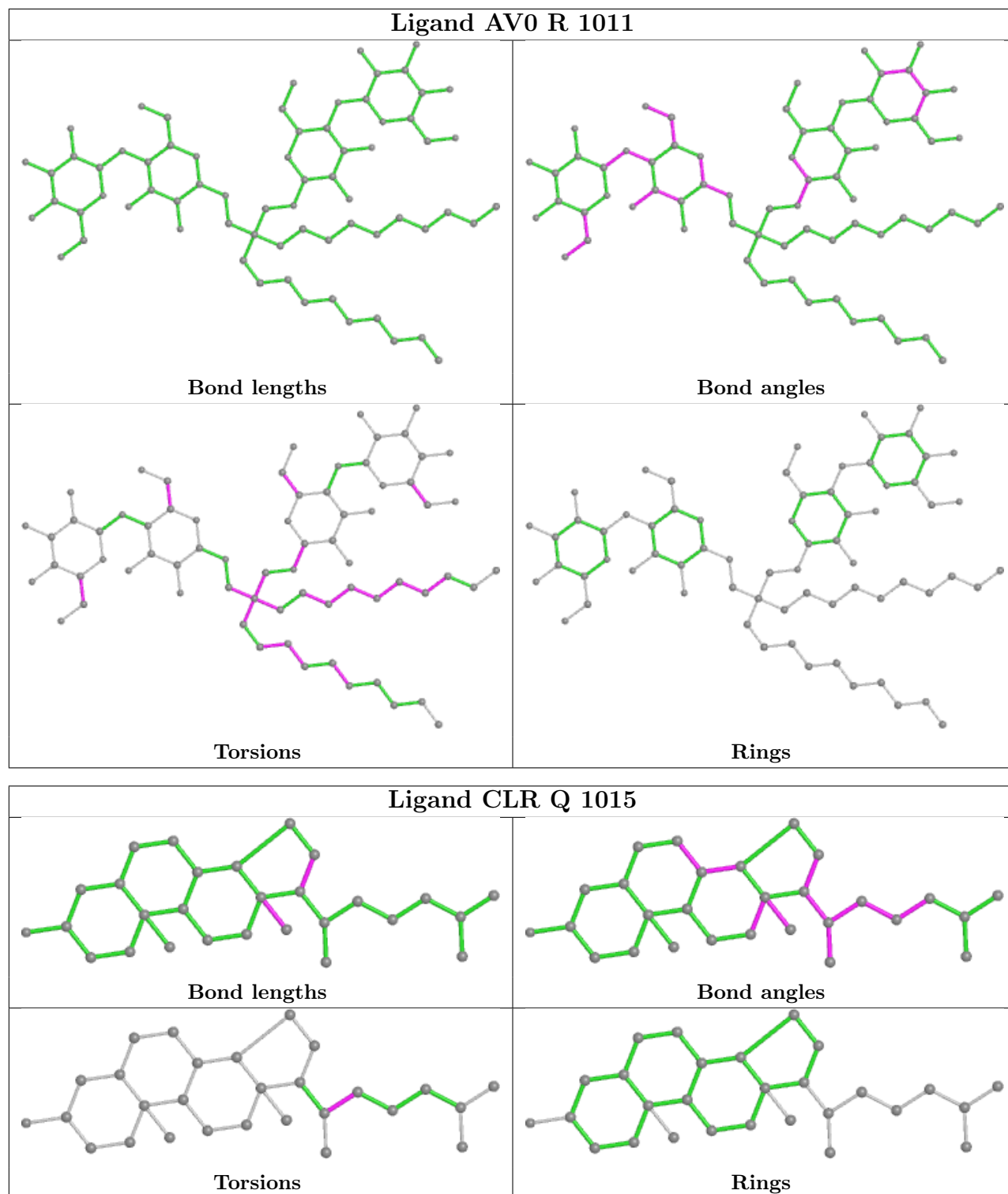












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

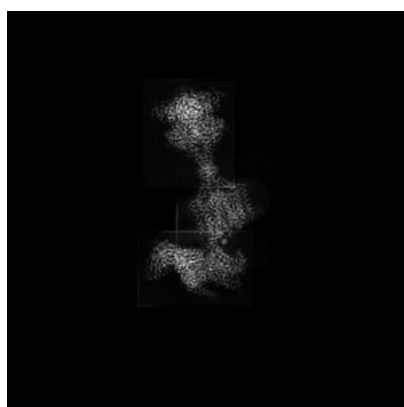
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43966. These allow visual inspection of the internal detail of the map and identification of artifacts.

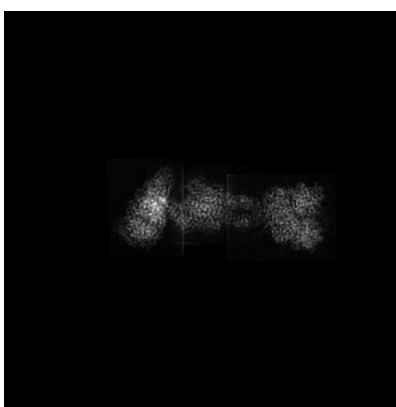
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

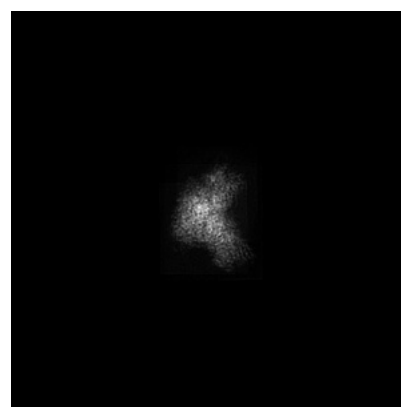
6.1.1 Primary map



X



Y

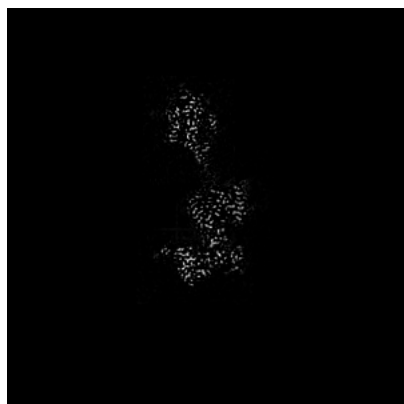


Z

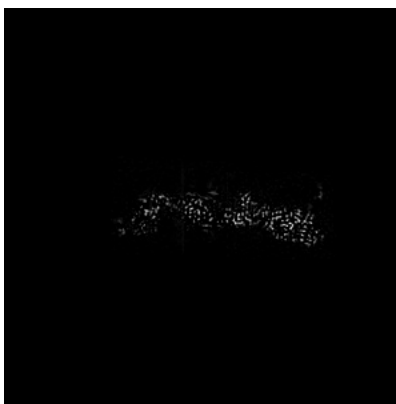
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

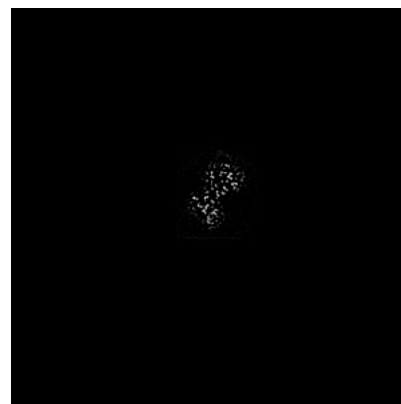
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

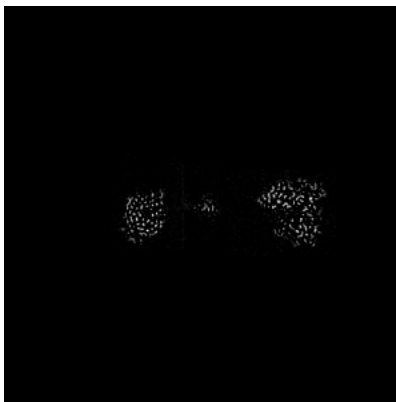
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

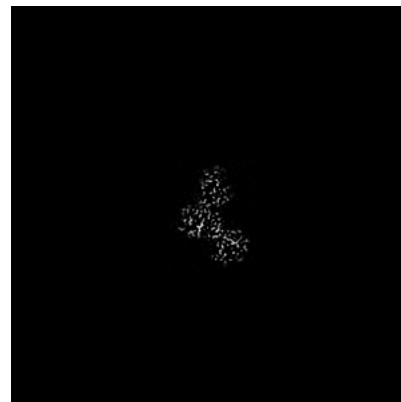
6.3.1 Primary map



X Index: 260



Y Index: 237

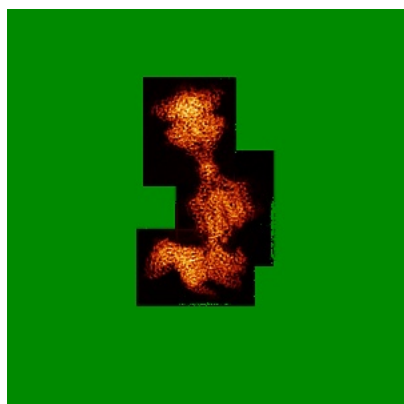


Z Index: 194

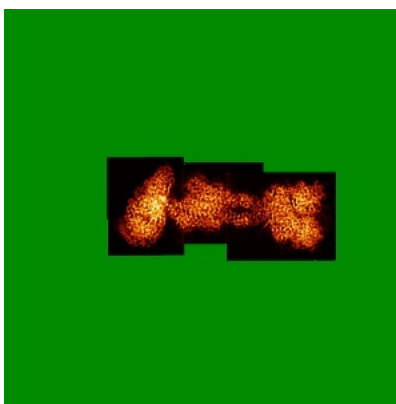
The images above show the largest variance slices of the map in three orthogonal directions.

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

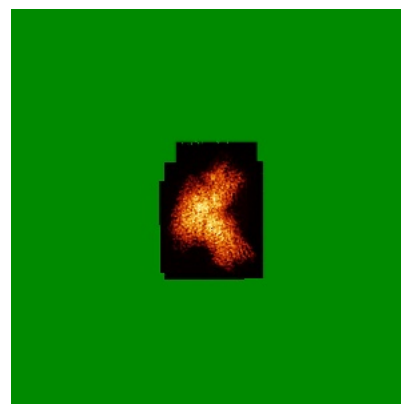
6.4.1 Primary map



X



Y

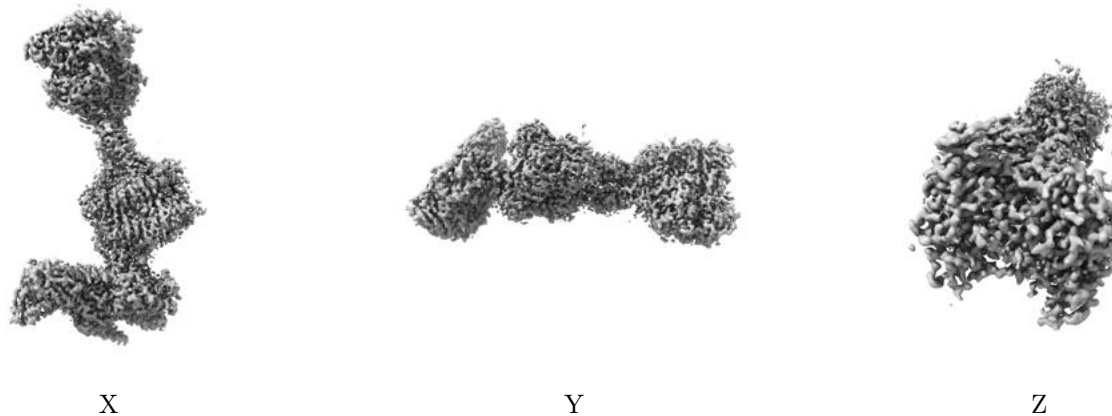


Z

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

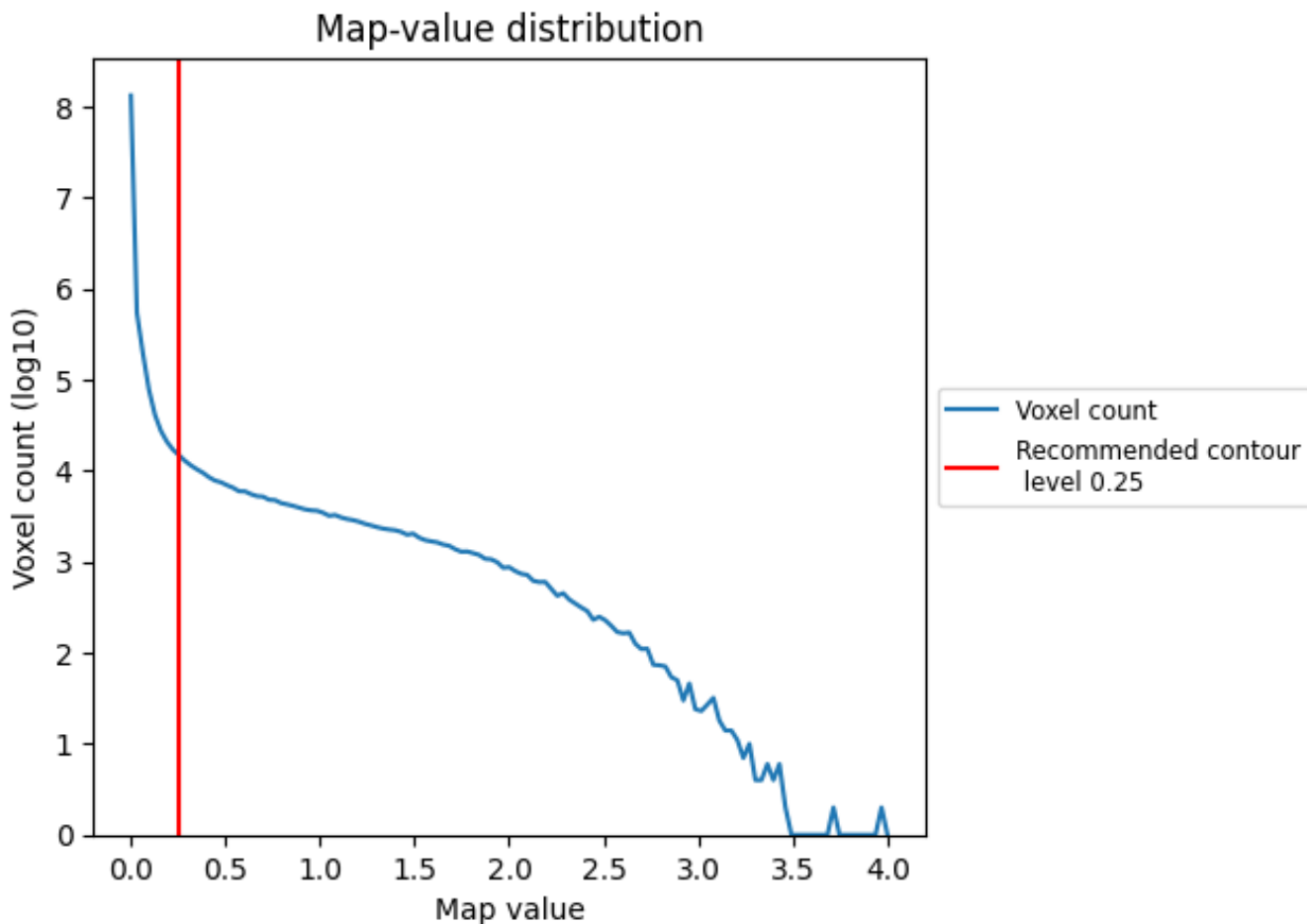
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

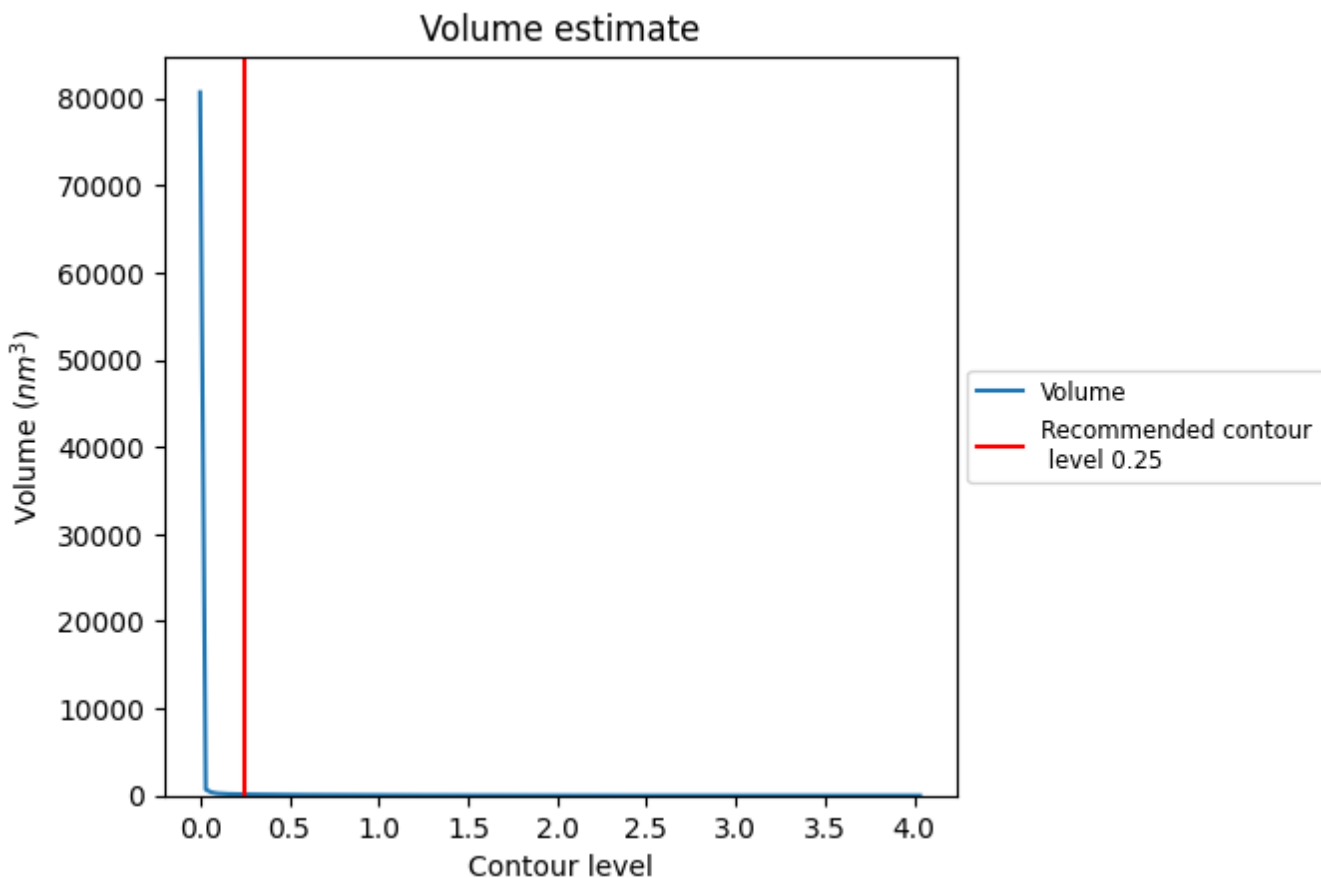
This section contains the results of statistical analysis of the map.

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.

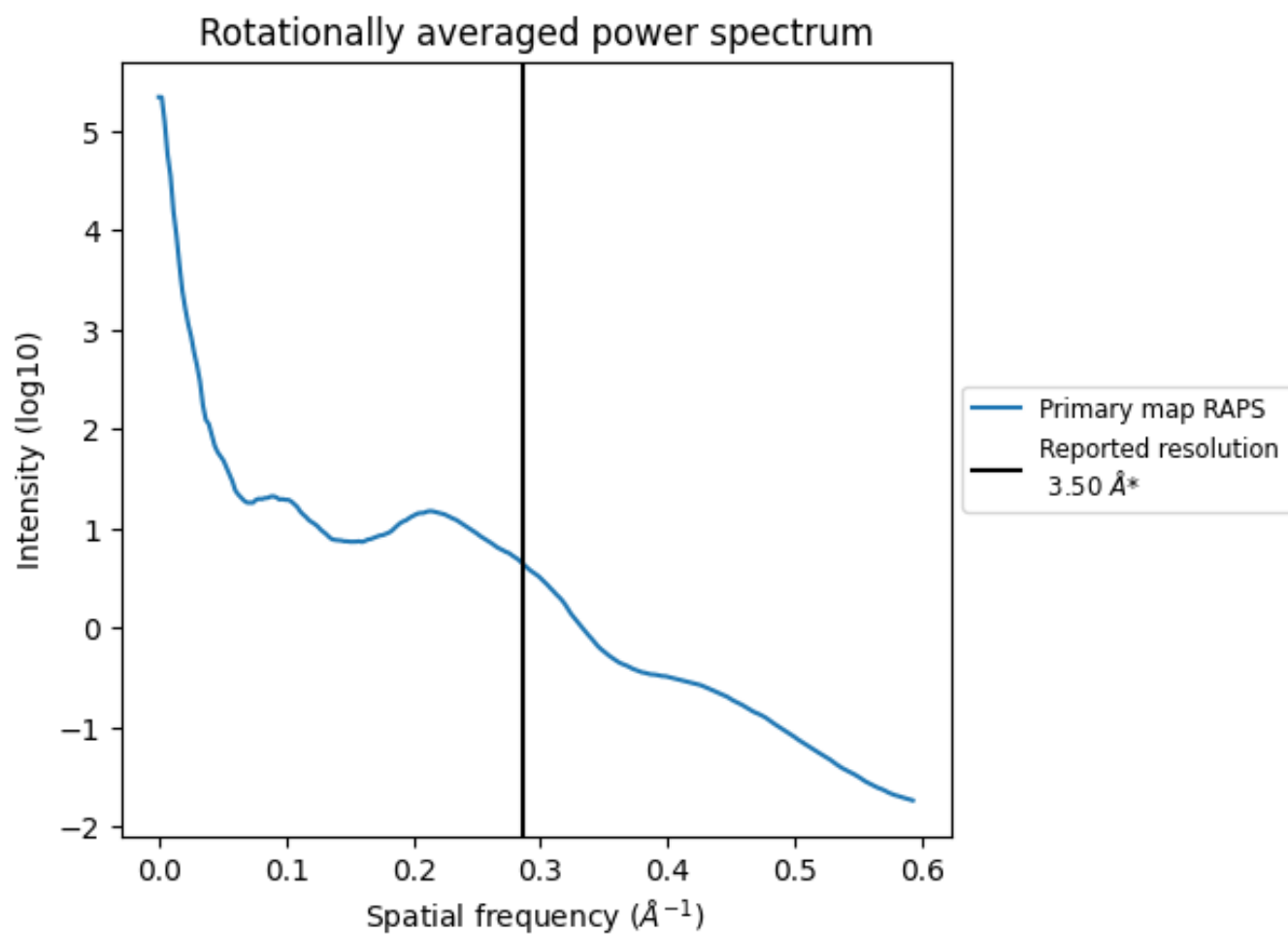
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 142 nm^3 ; this corresponds to an approximate mass of 128 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

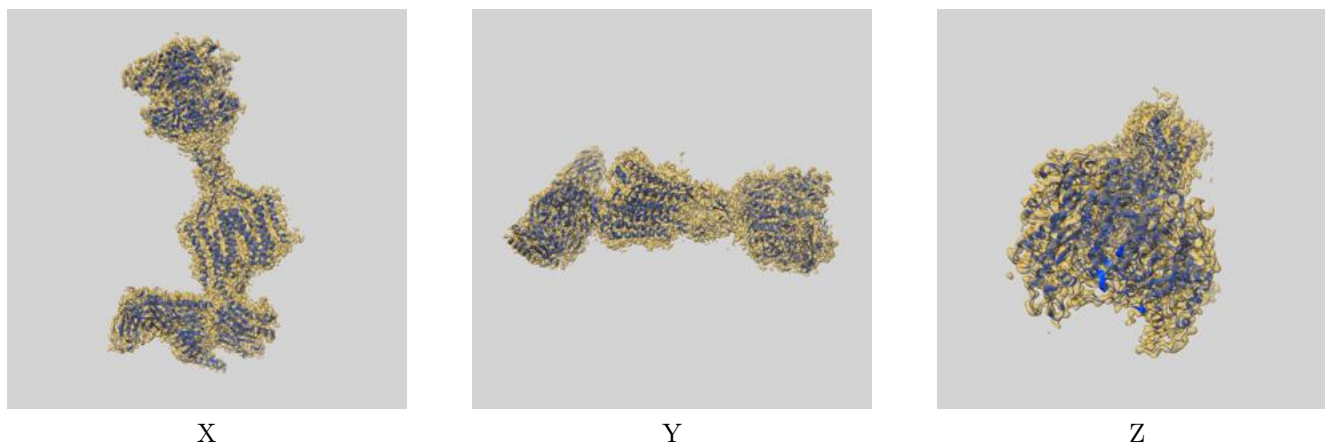
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

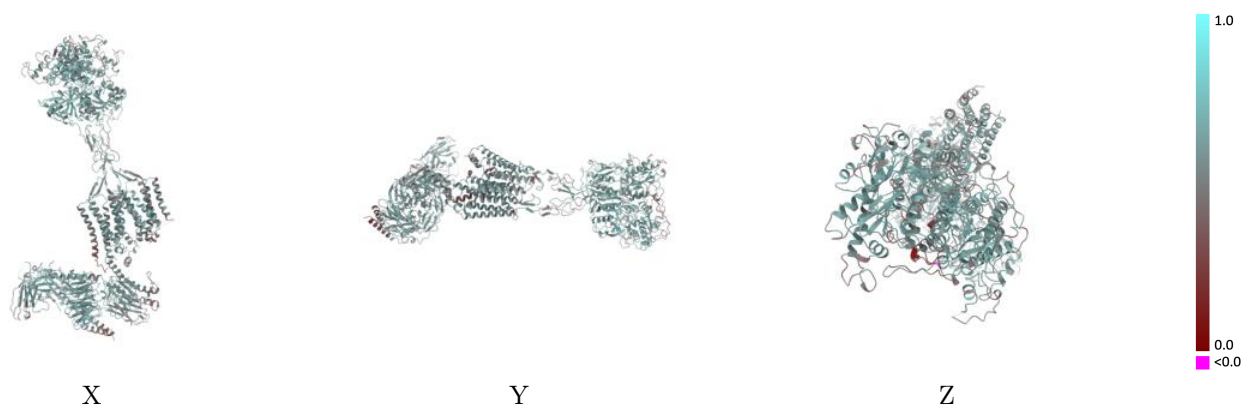
This section contains information regarding the fit between EMDB map EMD-43966 and PDB model 9AXF. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



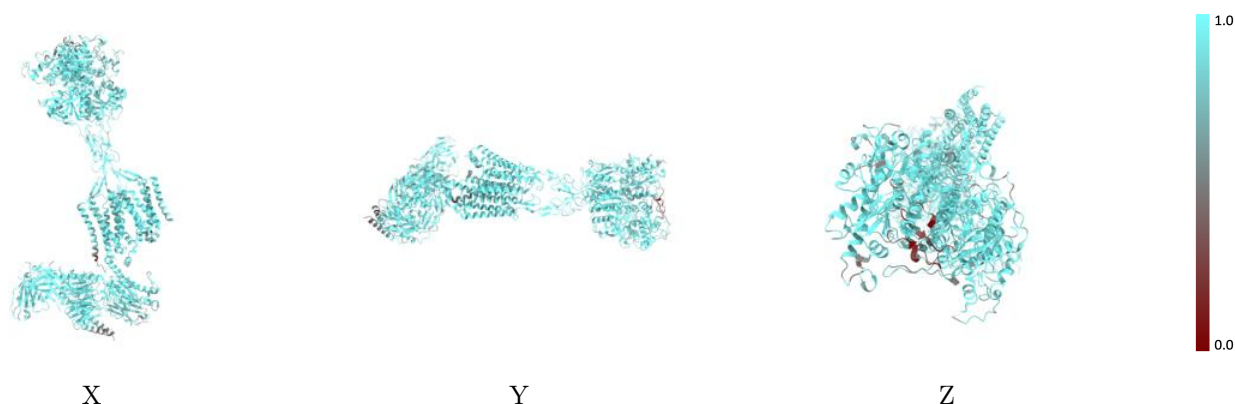
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



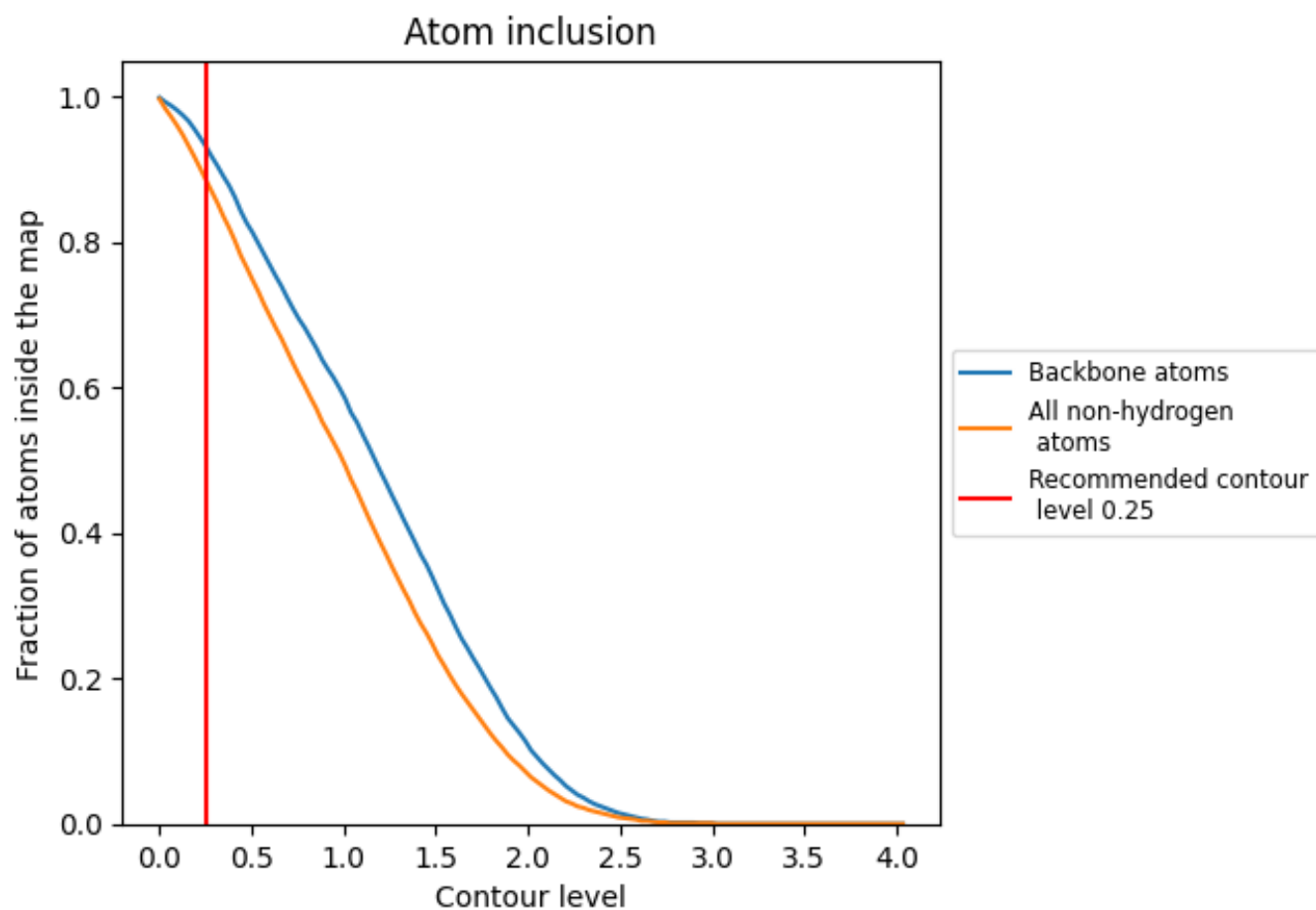
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

























9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 89% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8860	 0.5600
A	 0.8890	 0.5390
B	 0.9350	 0.6020
C	 0.6070	 0.4420
D	 0.8570	 0.5060
E	 0.6070	 0.4180
F	 0.7860	 0.4870
G	 0.7390	 0.4620
H	 0.9100	 0.5720
N	 0.8350	 0.5500
Q	 0.8870	 0.5600
R	 0.8790	 0.5560

