



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 04:02 PM EDT

PDB ID : 8TS0
Title : Crystal Structure of human ASGR1 CRD (Carbohydrate Recognition Domain)
bound to 8M24 Fab
Authors : Sampathkumar, P.; Li, Y.
Deposited on : 2023-08-10
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

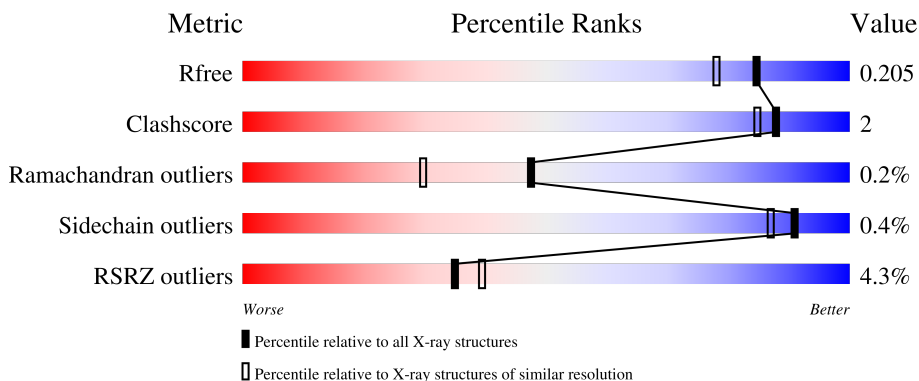
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	236	 2% 89% 9%
2	L	214	 8% 90% 9%
3	A	169	 % 74% 24%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4848 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 8M24 Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	215	1651	1045	273	327	6	0	4	0

- Molecule 2 is a protein called 8M24 Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	212	1659	1048	276	330	5	0	4	0

- Molecule 3 is a protein called Asialoglycoprotein receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	129	1083	682	193	201	7	0	1	0

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	HIS	-	expression tag	UNP P07306
A	124	HIS	-	expression tag	UNP P07306
A	125	HIS	-	expression tag	UNP P07306
A	126	HIS	-	expression tag	UNP P07306
A	127	HIS	-	expression tag	UNP P07306
A	128	HIS	-	expression tag	UNP P07306
A	129	HIS	-	expression tag	UNP P07306
A	130	HIS	-	expression tag	UNP P07306
A	131	GLY	-	expression tag	UNP P07306
A	132	SER	-	expression tag	UNP P07306
A	133	GLY	-	expression tag	UNP P07306
A	134	SER	-	expression tag	UNP P07306
A	135	GLY	-	expression tag	UNP P07306
A	136	LEU	-	expression tag	UNP P07306

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Chain	Residue	Modelled	Actual	Comment	Reference
A	137	ASN	-	expression tag	UNP P07306
A	138	ASP	-	expression tag	UNP P07306
A	139	ILE	-	expression tag	UNP P07306
A	140	PHE	-	expression tag	UNP P07306
A	141	GLU	-	expression tag	UNP P07306
A	142	ALA	-	expression tag	UNP P07306
A	143	GLN	-	expression tag	UNP P07306
A	144	LYS	-	expression tag	UNP P07306
A	145	ILE	-	expression tag	UNP P07306
A	146	GLU	-	expression tag	UNP P07306
A	147	TRP	-	expression tag	UNP P07306
A	148	HIS	-	expression tag	UNP P07306
A	149	GLU	-	expression tag	UNP P07306
A	150	SER	-	expression tag	UNP P07306
A	151	GLY	-	expression tag	UNP P07306
A	152	SER	-	expression tag	UNP P07306
A	153	GLY	-	expression tag	UNP P07306

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Ca 3 3	0	0

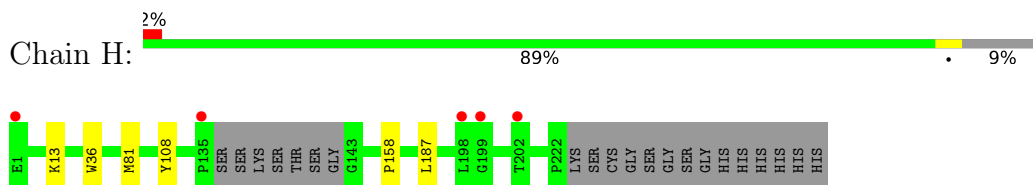
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	140	Total O 140 140	0	0
6	L	148	Total O 148 148	0	0
6	A	128	Total O 128 128	0	0

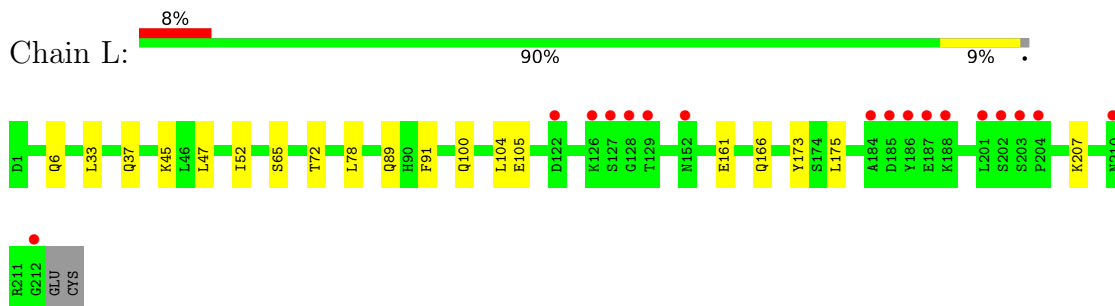
3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

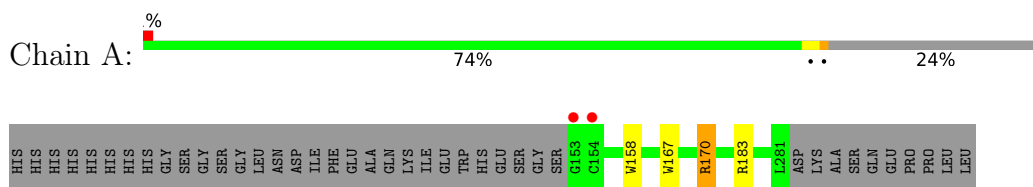
- Molecule 1: 8M24 Fab Heavy chain



- Molecule 2: 8M24 Fab Light chain



- Molecule 3: Asialoglycoprotein receptor 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	38.91Å 90.32Å 167.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.05 – 1.70 38.05 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.05-1.70) 100.0 (38.05-1.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 1.70Å)	Xtrriage
Refinement program	PHENIX 1.14rc1_3177	Depositor
R, R_{free}	0.173 , 0.205 0.173 , 0.205	Depositor DCC
R_{free} test set	3233 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtrriage
Anisotropy	0.287	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4848	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: GOL, CA

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	H	0.38	0/1704	0.59	1/2320 (0.0%)
2	L	0.39	0/1709	0.60	0/2322
3	A	0.40	0/1129	0.56	0/1542
All	All	0.39	0/4542	0.58	1/6184 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	H	187	LEU	CA-CB-CG	5.09	127.02	115.30

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	H	1651	0	1609	3	0
2	L	1659	0	1626	12	0
3	A	1083	0	940	3	0
4	A	6	0	6	0	0
4	H	18	0	24	0	0
4	L	12	0	16	2	0
5	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	128	0	0	1	0
6	H	140	0	0	1	0
6	L	148	0	0	1	0
All	All	4848	0	4221	17	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 2.

All (17) 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)
2:L:166:GLN:HG3	2:L:173:TYR:CZ	2.38	0.59
2:L:161:GLU:HG2	2:L:175:LEU:HD21	1.87	0.57
2:L:78:LEU:HD11	2:L:104[A]:LEU:HD21	1.88	0.56
2:L:37:GLN:OE1	4:L:302:GOL:H12	2.13	0.49
3:A:170:ARG:NH2	6:A:402:HOH:O	2.34	0.49
2:L:72[B]:THR:HG23	6:L:469:HOH:O	2.14	0.48
2:L:45:LYS:NZ	4:L:302:GOL:H11	2.29	0.47
2:L:52:ILE:HG22	2:L:65:SER:HA	1.99	0.45
1:H:36:TRP:CE2	1:H:81:MET:HB2	2.53	0.44
2:L:207:LYS:HD3	2:L:207:LYS:HA	1.73	0.44
2:L:6:GLN:O	2:L:100:GLN:NE2	2.33	0.43
3:A:183:ARG:HD3	3:A:183:ARG:HA	1.80	0.43
2:L:37:GLN:HB2	2:L:47:LEU:HD11	2.00	0.42
2:L:33:LEU:HD22	2:L:89:GLN:O	2.20	0.42
1:H:13:LYS:HG2	6:H:464:HOH:O	2.20	0.41
1:H:108:TYR:HA	2:L:91:PHE:CZ	2.56	0.41
3:A:158:TRP:CD2	3:A:167:TRP:HB2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	H	215/236 (91%)	211 (98%)	3 (1%)	1 (0%)	29	13
2	L	214/214 (100%)	207 (97%)	7 (3%)	0	100	100
3	A	128/169 (76%)	125 (98%)	3 (2%)	0	100	100
All	All	557/619 (90%)	543 (98%)	13 (2%)	1 (0%)	47	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	158	PRO

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 X-ray entries followed by that with respect to entries of similar resolution.

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	H	186/199 (94%)	186 (100%)	0	100	100
2	L	189/187 (101%)	188 (100%)	1 (0%)	88	83
3	A	112/145 (77%)	111 (99%)	1 (1%)	78	70
All	All	487/531 (92%)	485 (100%)	2 (0%)	91	87

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

Mol	Chain	Res	Type
2	L	105	GLU
3	A	170	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	62	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	$\# Z > 2$
4	GOL	L	301	-	5,5,5	0.90	0	5,5,5	0.99	0
4	GOL	H	302	-	5,5,5	1.00	0	5,5,5	0.96	0
4	GOL	A	304	5	5,5,5	1.02	0	5,5,5	1.00	0
4	GOL	H	303	-	5,5,5	0.94	0	5,5,5	0.94	0
4	GOL	L	302	-	5,5,5	1.13	0	5,5,5	0.71	0
4	GOL	H	301	-	5,5,5	0.59	0	5,5,5	1.19	1 (20%)

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
4	GOL	L	301	-	-	4/4/4/4	-
4	GOL	H	302	-	-	2/4/4/4	-
4	GOL	A	304	5	-	0/4/4/4	-
4	GOL	H	303	-	-	4/4/4/4	-
4	GOL	L	302	-	-	1/4/4/4	-
4	GOL	H	301	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	301	GOL	C3-C2-C1	-2.18	103.23	111.70

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	302	GOL	O1-C1-C2-C3
4	H	303	GOL	O1-C1-C2-C3
4	H	303	GOL	C1-C2-C3-O3
4	L	301	GOL	O1-C1-C2-O2
4	L	301	GOL	O1-C1-C2-C3
4	L	301	GOL	C1-C2-C3-O3
4	L	302	GOL	O1-C1-C2-C3
4	H	302	GOL	O1-C1-C2-O2
4	H	303	GOL	O1-C1-C2-O2
4	L	301	GOL	O2-C2-C3-O3
4	H	303	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	302	GOL	2	0

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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	H	215/236 (91%)	0.16	5 (2%) 60 65	20, 33, 50, 65	0
2	L	212/214 (99%)	0.43	17 (8%) 12 14	19, 32, 56, 68	0
3	A	129/169 (76%)	0.25	2 (1%) 72 76	18, 26, 45, 63	0
All	All	556/619 (89%)	0.28	24 (4%) 35 39	18, 31, 53, 68	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	187	GLU	4.0
2	L	202	SER	3.9
2	L	203	SER	3.6
2	L	184	ALA	3.5
2	L	126	LYS	3.4
2	L	122	ASP	3.3
3	A	153	GLY	3.2
2	L	212	GLY	3.2
2	L	152	ASN	3.1
1	H	1	GLU	3.1
2	L	127	SER	3.1
2	L	129	THR	3.0
3	A	154	CYS	2.9
1	H	198	LEU	2.7
2	L	185	ASP	2.5
1	H	135	PRO	2.5
2	L	186	TYR	2.4
2	L	210	ASN	2.4
1	H	199	GLY	2.4
2	L	188	LYS	2.2
2	L	201	LEU	2.2
2	L	204	PRO	2.1
2	L	128	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	202	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

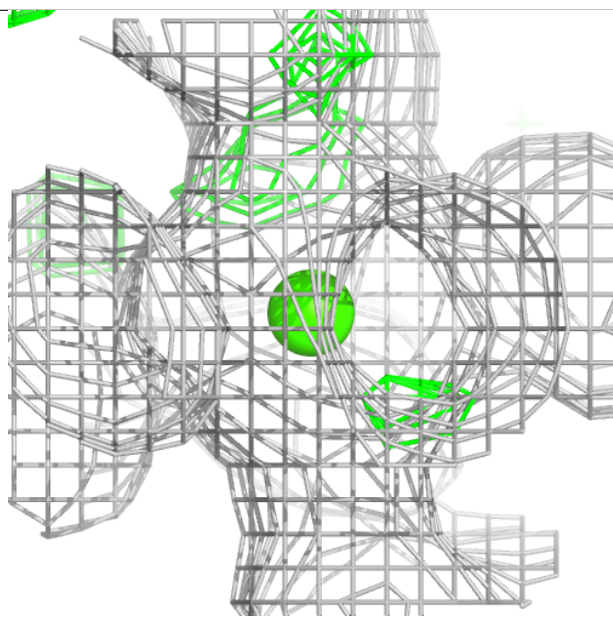
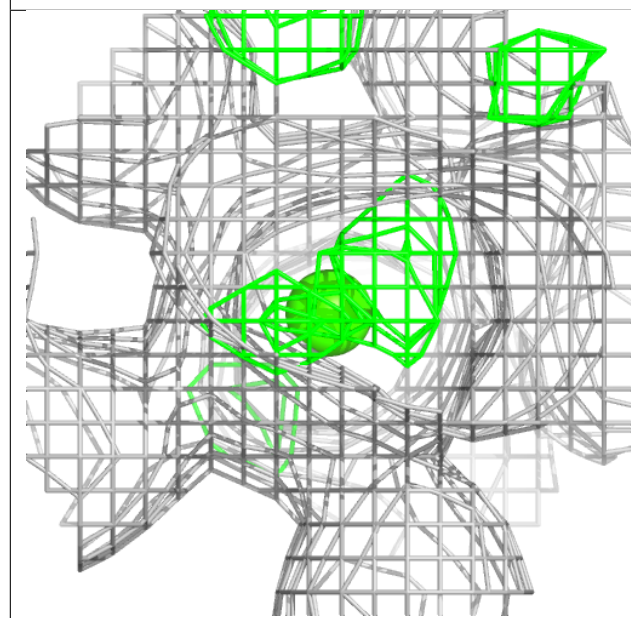
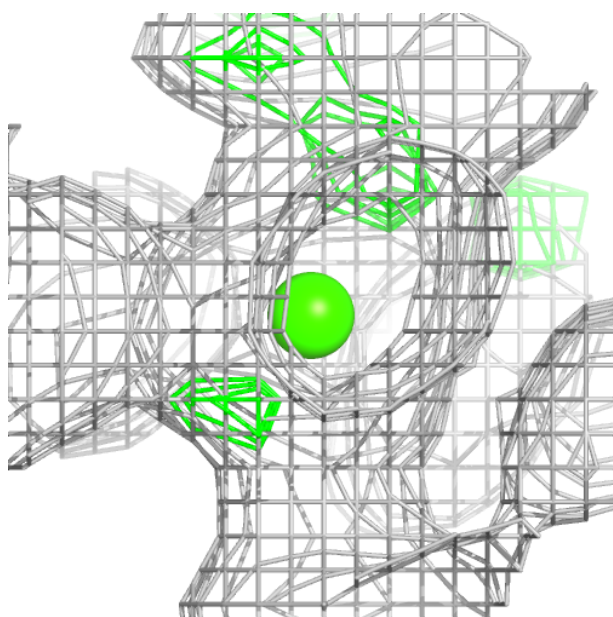
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	L	302	6/6	0.76	0.26	32,57,61,65	0
4	GOL	L	301	6/6	0.80	0.20	39,56,59,60	0
4	GOL	H	303	6/6	0.84	0.17	38,52,61,68	0
4	GOL	H	302	6/6	0.88	0.14	55,61,63,64	0
4	GOL	H	301	6/6	0.94	0.15	27,39,46,56	0
4	GOL	A	304	6/6	0.94	0.09	24,30,40,41	0
5	CA	A	301	1/1	0.96	0.09	27,27,27,27	0
5	CA	A	302	1/1	0.98	0.12	25,25,25,25	0
5	CA	A	303	1/1	1.00	0.07	23,23,23,23	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

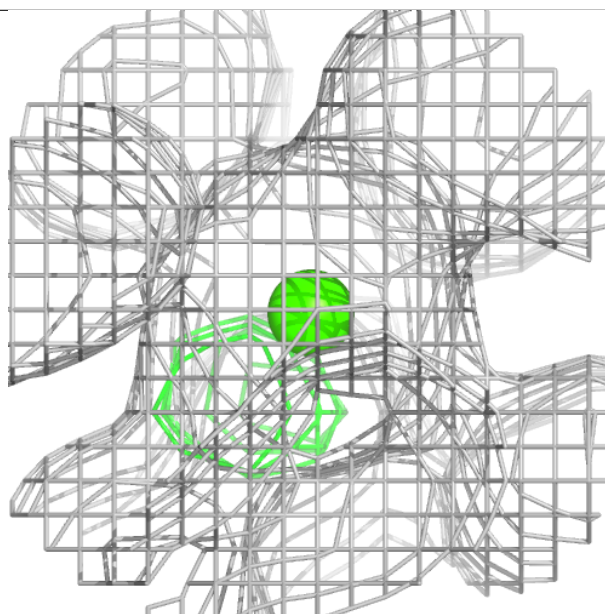
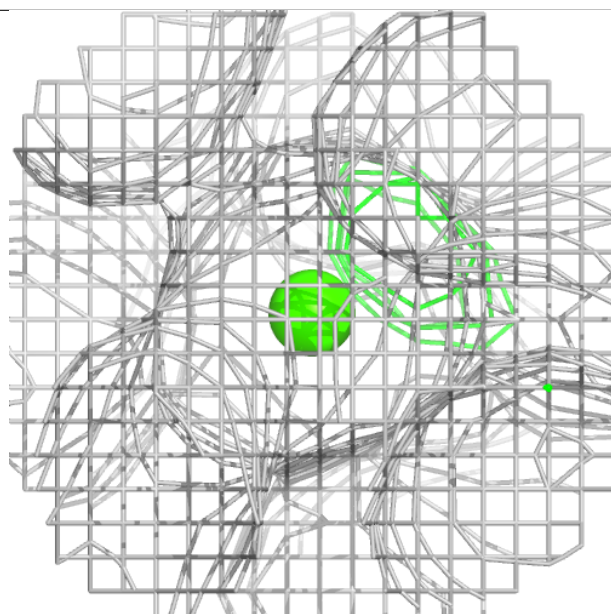
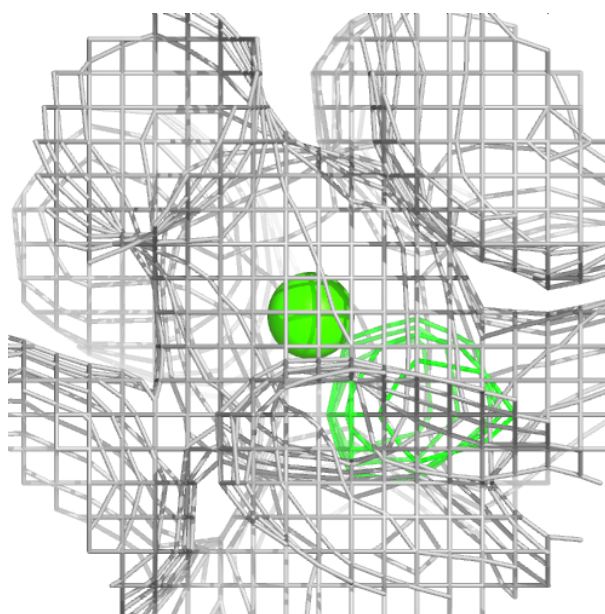
Electron density around CA A 301:

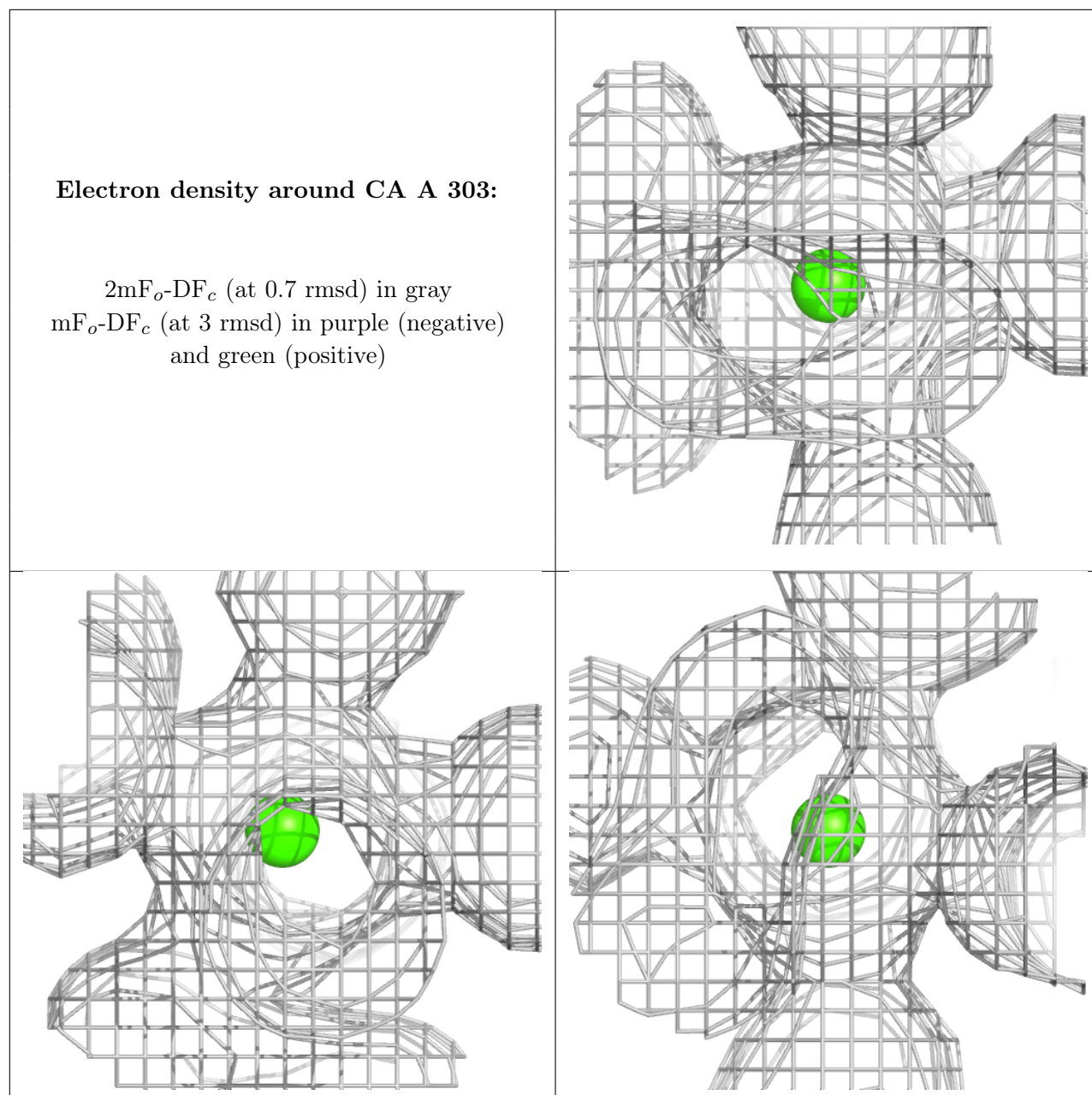
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA A 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.