Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2025 – 12:13 PM JST

PDB ID	:	8ZCA / pdb_00008zca
Title	:	Crystal structure of human CD47 ECD bound to Fab of Hu1C8
Authors	:	Chen, Z.; Ding, J.
Deposited on	:	2024-04-29
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

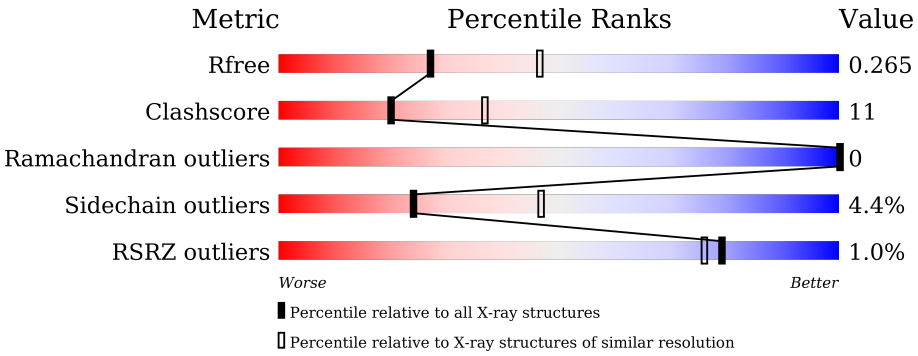
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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 <=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	A	218	77% 20%
1	B	218	72% 24%
2	C	225	74% 21% 5%
2	D	225	69% 24% 5%
3	E	131	69% 20% 10%
3	F	131	66% 19% 12%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8567 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 1C8 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1659	1042	273	339	5			
1	B	215	Total	C	N	O	S	0	0	0
			1650	1037	272	336	5			

- Molecule 2 is a protein called 1C8 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	214	Total	C	N	O	S	0	0	0
			1590	1006	265	314	5			
2	C	213	Total	C	N	O	S	0	0	0
			1581	1000	263	313	5			

- Molecule 3 is a protein called Leukocyte surface antigen CD47.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	118	Total	C	N	O	S	0	0	0
			937	597	150	186	4			
3	F	115	Total	C	N	O	S	0	0	0
			910	578	146	182	4			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	15	GLY	CYS	conflict	UNP Q08722
E	122	GLY	-	expression tag	UNP Q08722
E	123	SER	-	expression tag	UNP Q08722
E	124	HIS	-	expression tag	UNP Q08722
E	125	HIS	-	expression tag	UNP Q08722
E	126	HIS	-	expression tag	UNP Q08722
E	127	HIS	-	expression tag	UNP Q08722
E	128	HIS	-	expression tag	UNP Q08722

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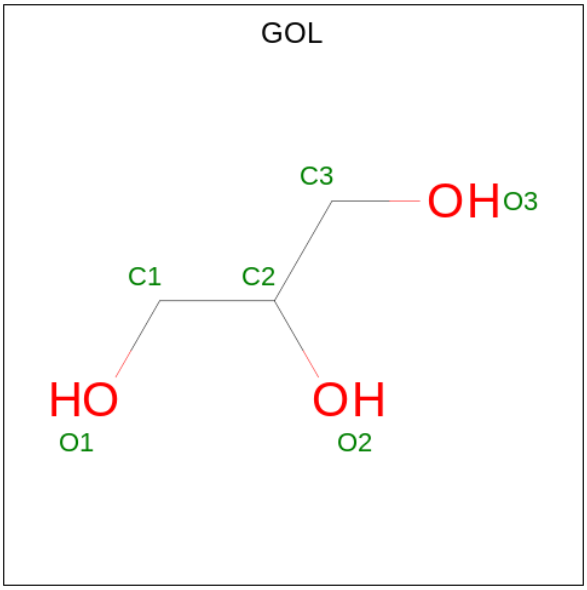
Chain	Residue	Modelled	Actual	Comment	Reference
E	129	HIS	-	expression tag	UNP Q08722
E	130	HIS	-	expression tag	UNP Q08722
E	131	HIS	-	expression tag	UNP Q08722
F	15	GLY	CYS	conflict	UNP Q08722
F	122	GLY	-	expression tag	UNP Q08722
F	123	SER	-	expression tag	UNP Q08722
F	124	HIS	-	expression tag	UNP Q08722
F	125	HIS	-	expression tag	UNP Q08722
F	126	HIS	-	expression tag	UNP Q08722
F	127	HIS	-	expression tag	UNP Q08722
F	128	HIS	-	expression tag	UNP Q08722
F	129	HIS	-	expression tag	UNP Q08722
F	130	HIS	-	expression tag	UNP Q08722
F	131	HIS	-	expression tag	UNP Q08722

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

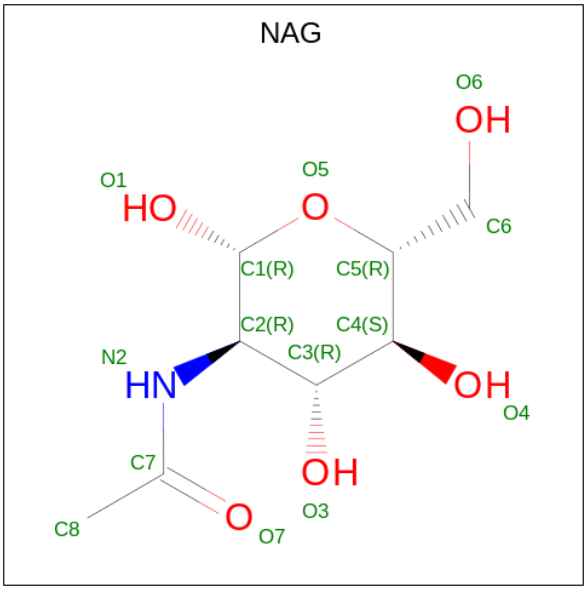
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0
6	F	1	Total C N O 14 8 1 5	0	0
6	F	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	31	Total O 31 31	0	0
7	D	33	Total O 33 33	0	0
7	B	29	Total O 29 29	0	0

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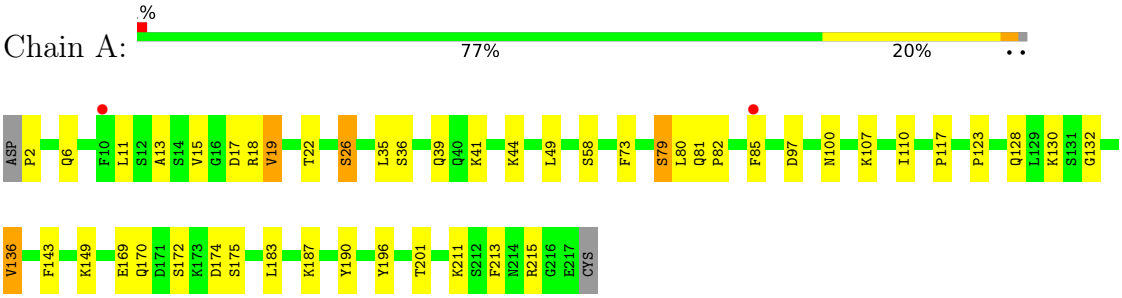
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	39	Total O 39 39	0	0
7	E	21	Total O 21 21	0	0
7	F	17	Total O 17 17	0	0

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.

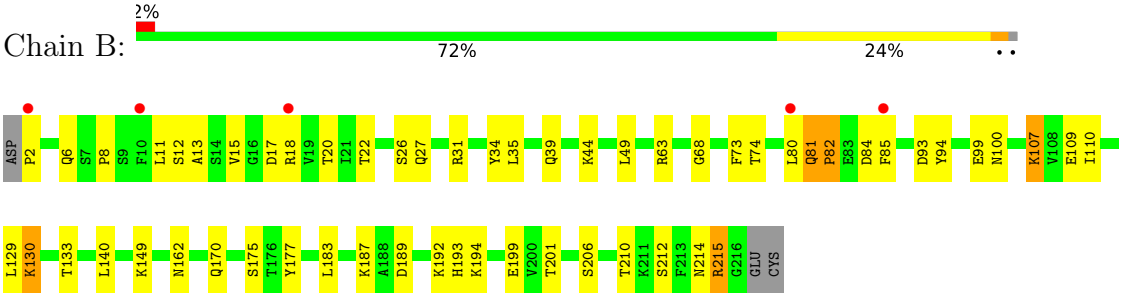
• Molecule 1: 1C8 Fab light chain

Chain A:



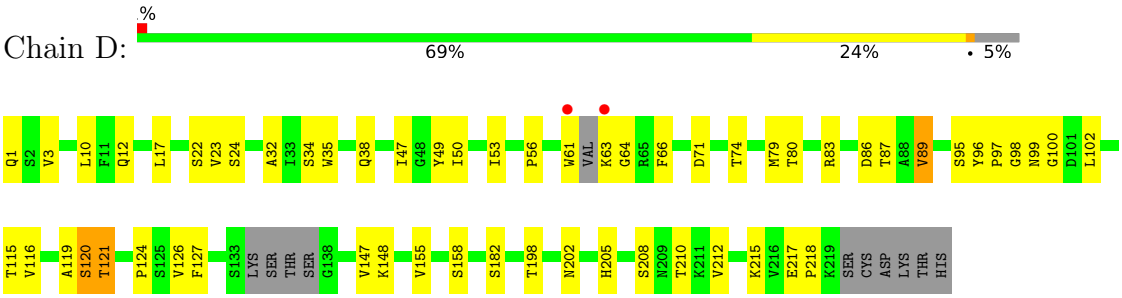
• Molecule 1: 1C8 Fab light chain

Chain B:



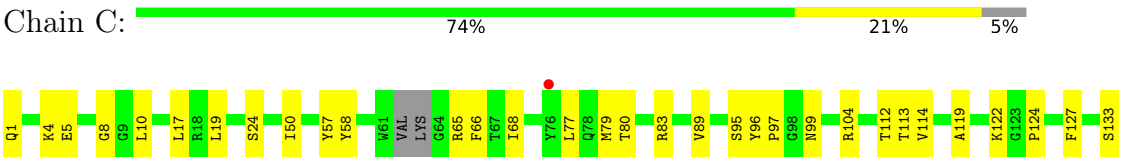
• Molecule 2: 1C8 Fab heavy chain

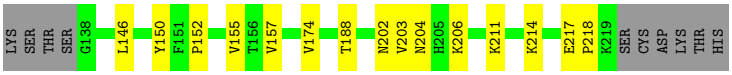
Chain D:



• Molecule 2: 1C8 Fab heavy chain

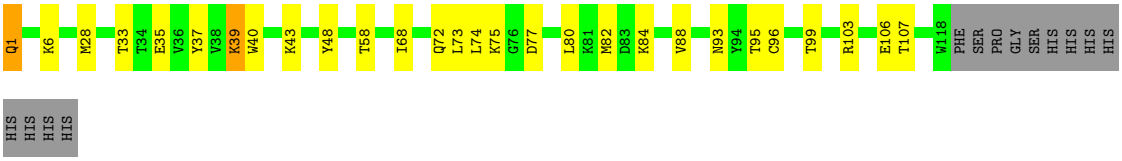
Chain C:





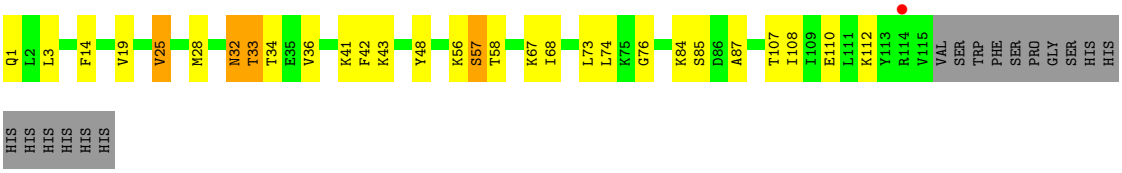
• Molecule 3: Leukocyte surface antigen CD47

Chain E:



• Molecule 3: Leukocyte surface antigen CD47

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	45.22Å 79.93Å 92.75Å 112.50° 96.61° 103.16°	Depositor
Resolution (Å)	38.52 – 2.50 38.52 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.1 (38.52-2.50) 92.0 (38.52-2.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.215 , 0.266 0.215 , 0.265	Depositor DCC
R_{free} test set	37385 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å^2)	41.0	Xtriage
Anisotropy	0.709	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 21.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,h+k+l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8567	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GOL, NAG, PCA

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	0.38	0/1696	0.54	0/2301
1	B	0.40	0/1687	0.64	1/2289 (0.0%)
2	C	0.39	0/1619	0.60	0/2203
2	D	0.38	0/1628	0.63	0/2214
3	E	0.46	0/947	0.64	0/1283
3	F	0.42	0/918	0.65	0/1242
All	All	0.40	0/8495	0.61	1/11532 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	82	PRO	CA-N-CD	-5.02	104.98	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	8	PRO	Peptide

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	1659	0	1602	41	0
1	B	1650	0	1596	45	0
2	C	1581	0	1542	27	0
2	D	1590	0	1555	43	0
3	E	937	0	923	20	0
3	F	910	0	899	23	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	C	6	0	8	1	0
5	D	6	0	8	3	0
6	E	28	0	24	1	0
6	F	28	0	26	0	0
7	A	31	0	0	0	0
7	B	29	0	0	2	0
7	C	39	0	0	2	0
7	D	33	0	0	0	0
7	E	21	0	0	0	0
7	F	17	0	0	0	0
All	All	8567	0	8183	186	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 11.

All (186) 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:E:33:THR:HG22	3:E:74:LEU:HD21	1.51	0.93
3:F:67:LYS:HE3	3:F:68:ILE:H	1.34	0.92
2:C:122:LYS:HB2	5:C:301:GOL:H32	1.57	0.87
2:D:1:GLN:OE1	2:D:1:GLN:N	2.10	0.84
2:C:1:GLN:OE1	2:C:1:GLN:N	2.12	0.82
3:F:110:GLU:HG2	3:F:112:LYS:HG3	1.60	0.81
2:D:119:ALA:HB1	5:D:301:GOL:H32	1.63	0.80
3:F:19:VAL:HG21	3:F:87:ALA:HB2	1.67	0.76
1:B:2:PRO:HA	1:B:26:SER:HB2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:TYR:H	1:B:100:ASN:HD21	1.35	0.74
1:A:17:ASP:C	1:A:18:ARG:HD2	2.13	0.74
2:D:10:LEU:HD23	2:D:121:THR:HG22	1.70	0.73
2:D:120:SER:H	5:D:301:GOL:H11	1.53	0.73
1:B:13:ALA:HB1	1:B:17:ASP:HB3	1.75	0.67
2:D:71:ASP:OD1	2:D:74:THR:OG1	2.11	0.67
1:A:13:ALA:HB1	1:A:17:ASP:HB3	1.78	0.66
2:D:64:GLY:HA3	2:D:66:PHE:CE1	2.31	0.65
2:D:87:THR:HG23	2:D:115:THR:HA	1.79	0.65
1:B:2:PRO:HB3	1:B:27:GLN:HG2	1.79	0.64
3:E:6:LYS:HE2	3:E:107:THR:OG1	1.96	0.64
3:F:48:TYR:HH	3:F:57:SER:HG	1.46	0.64
1:A:85:PHE:CG	1:A:170:GLN:HB3	2.33	0.64
2:D:12:GLN:OE1	2:D:12:GLN:N	2.24	0.64
1:B:31:ARG:HH12	3:E:99:THR:HG21	1.63	0.63
1:B:149:LYS:HB3	1:B:201:THR:HG22	1.80	0.63
2:D:10:LEU:HD21	2:D:119:ALA:O	1.99	0.62
1:A:80:LEU:HD21	1:A:110:ILE:HG13	1.82	0.62
1:A:2:PRO:N	1:A:26:SER:HG	1.97	0.62
1:B:2:PRO:HD3	1:B:99:GLU:HB3	1.81	0.62
2:D:148:LYS:HA	2:D:182:SER:HB2	1.82	0.62
2:C:204:ASN:HD22	2:C:211:LYS:HG2	1.65	0.62
1:B:85:PHE:CE2	1:B:109:GLU:HA	2.35	0.61
2:C:217:GLU:HG2	2:C:218:PRO:HD2	1.82	0.61
3:E:1:PCA:HG2	3:E:103:ARG:HG2	1.83	0.61
1:B:162:ASN:HB3	1:B:183:LEU:HD12	1.83	0.60
2:C:17:LEU:HD11	2:C:19:LEU:HD21	1.84	0.60
1:A:100:ASN:HB3	2:D:102:LEU:HD12	1.83	0.59
1:A:85:PHE:CE1	1:A:107:LYS:HD2	2.36	0.59
2:D:198:THR:HG23	2:D:215:LYS:HE3	1.85	0.59
3:F:14:PHE:O	3:F:84:LYS:NZ	2.31	0.59
1:B:85:PHE:CZ	1:B:107:LYS:HD2	2.38	0.58
2:D:32:ALA:HB3	2:D:95:SER:HB2	1.86	0.58
1:B:82:PRO:HB3	1:B:175:SER:OG	2.02	0.58
1:A:18:ARG:HD2	1:A:18:ARG:N	2.18	0.57
2:D:124:PRO:HD2	2:D:210:THR:HG21	1.86	0.57
2:D:158:SER:HB3	2:D:202:ASN:HB2	1.85	0.57
3:E:40:TRP:CD1	3:E:80:LEU:HD13	2.39	0.57
3:F:67:LYS:HE3	3:F:68:ILE:N	2.12	0.57
2:D:63:LYS:O	2:D:83:ARG:NH2	2.37	0.57
1:B:170:GLN:HG3	1:B:177:TYR:CZ	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:57:TYR:OH	3:E:43:LYS:HA	2.05	0.56
3:F:110:GLU:HG2	3:F:112:LYS:CG	2.32	0.56
1:B:44:LYS:NZ	7:B:405:HOH:O	2.38	0.56
2:D:1:GLN:HA	2:D:24:SER:O	2.06	0.56
2:D:53:ILE:HG21	3:F:108:ILE:HG12	1.87	0.55
1:B:2:PRO:CD	1:B:99:GLU:HB3	2.36	0.55
3:F:48:TYR:OH	3:F:57:SER:OG	2.21	0.55
1:A:82:PRO:HB3	1:A:175:SER:OG	2.07	0.55
3:E:74:LEU:HD22	3:E:74:LEU:H	1.72	0.55
2:D:96:TYR:O	2:D:98:GLY:N	2.42	0.53
1:A:149:LYS:HB3	1:A:201:THR:HG23	1.91	0.52
2:D:3:VAL:HG12	2:D:23:VAL:HG12	1.91	0.52
2:C:99:ASN:HB3	3:E:95:THR:HG21	1.90	0.52
1:A:82:PRO:HD2	1:B:81:GLN:HE22	1.74	0.52
1:B:39:GLN:HB2	1:B:49:LEU:HD11	1.93	0.51
2:D:35:TRP:O	2:D:47:ILE:HB	2.10	0.51
1:B:85:PHE:CD2	1:B:109:GLU:HA	2.45	0.51
1:A:81:GLN:OE1	1:B:82:PRO:HD2	2.09	0.51
2:D:96:TYR:O	2:D:97:PRO:C	2.51	0.51
2:D:61:TRP:HE3	2:D:63:LYS:N	2.08	0.51
1:A:149:LYS:HB3	1:A:201:THR:CG2	2.41	0.51
3:E:48:TYR:CE2	3:E:68:ILE:HD12	2.46	0.51
2:D:120:SER:N	5:D:301:GOL:H11	2.25	0.51
1:A:190:TYR:O	1:A:196:TYR:OH	2.28	0.50
1:B:82:PRO:HA	1:B:110:ILE:HG13	1.93	0.50
1:A:18:ARG:HE	1:A:79:SER:H	1.58	0.50
1:A:39:GLN:HB2	1:A:49:LEU:HD11	1.93	0.50
2:C:66:PHE:CD1	2:C:77:LEU:HD11	2.46	0.50
2:D:99:ASN:HB2	3:F:41:LYS:HD3	1.94	0.50
1:B:85:PHE:CE1	1:B:107:LYS:HD2	2.47	0.50
1:B:6:GLN:HA	1:B:22:THR:O	2.11	0.50
1:A:11:LEU:HD12	1:A:19:VAL:HG22	1.92	0.50
2:D:64:GLY:HA2	2:D:83:ARG:NH2	2.27	0.50
1:A:85:PHE:CD2	1:A:170:GLN:HB3	2.47	0.49
1:A:41:LYS:HD2	1:A:44:LYS:HE2	1.94	0.49
7:C:403:HOH:O	6:E:201:NAG:H83	2.12	0.49
1:B:187:LYS:NZ	7:B:407:HOH:O	2.45	0.49
1:A:128:GLN:HG3	2:D:127:PHE:CE2	2.48	0.48
2:C:95:SER:HA	2:C:104:ARG:O	2.13	0.48
1:B:94:TYR:N	1:B:100:ASN:HD21	2.05	0.48
1:A:17:ASP:CG	1:A:18:ARG:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ASP:O	1:B:192:LYS:HG2	2.12	0.48
2:C:96:TYR:O	2:C:97:PRO:C	2.55	0.48
2:C:127:PHE:HD2	2:C:146:LEU:HD23	1.78	0.48
2:D:64:GLY:HA2	2:D:83:ARG:HH22	1.79	0.47
3:E:37:TYR:HB3	3:E:99:THR:HB	1.96	0.47
1:A:82:PRO:CD	1:B:81:GLN:HE22	2.27	0.47
2:C:89:VAL:HG22	2:C:113:THR:OG1	2.14	0.47
1:A:35:LEU:HD22	1:A:73:PHE:CG	2.49	0.47
1:A:85:PHE:CZ	1:A:107:LYS:HD2	2.50	0.47
1:B:15:VAL:HA	1:B:80:LEU:O	2.14	0.47
3:E:75:LYS:HA	3:E:75:LYS:HD2	1.52	0.47
1:A:80:LEU:CD2	1:A:110:ILE:HG13	2.45	0.47
3:E:84:LYS:HE3	3:E:84:LYS:HB2	1.55	0.47
1:A:117:PRO:HB3	1:A:143:PHE:HB3	1.97	0.47
1:B:63:ARG:NH2	1:B:84:ASP:OD1	2.42	0.47
1:B:170:GLN:NE2	1:B:175:SER:O	2.47	0.47
1:A:132:GLY:HA2	1:A:187:LYS:HE2	1.95	0.47
2:D:102:LEU:HD23	2:D:102:LEU:HA	1.68	0.46
2:D:10:LEU:CD2	2:D:121:THR:HG22	2.42	0.46
1:B:12:SER:HB3	1:B:109:GLU:HB3	1.98	0.46
2:D:147:VAL:HG11	2:D:155:VAL:HG11	1.97	0.46
1:B:80:LEU:C	1:B:81:GLN:HG2	2.39	0.46
7:C:403:HOH:O	3:E:93:ASN:HB2	2.15	0.45
1:B:199:GLU:HG3	1:B:210:THR:OG1	2.16	0.45
1:B:85:PHE:HB2	1:B:110:ILE:HG12	1.98	0.45
2:C:65:ARG:NH2	2:C:83:ARG:HE	2.14	0.45
3:E:73:LEU:HD12	3:E:73:LEU:HA	1.76	0.45
1:B:85:PHE:CD2	1:B:170:GLN:OE1	2.70	0.45
3:F:32:ASN:OD1	3:F:33:THR:N	2.49	0.45
3:E:72:GLN:HB3	3:E:77:ASP:HB3	1.98	0.45
1:A:13:ALA:HB3	1:A:80:LEU:HD22	1.99	0.45
1:A:6:GLN:HA	1:A:22:THR:O	2.17	0.45
1:B:129:LEU:O	1:B:187:LYS:HD2	2.16	0.45
2:C:4:LYS:HB3	2:C:4:LYS:HE3	1.54	0.45
3:F:28:MET:HE2	3:F:76:GLY:HA2	1.98	0.45
2:C:1:GLN:HA	2:C:24:SER:O	2.18	0.44
3:F:32:ASN:OD1	3:F:34:THR:HG23	2.18	0.44
1:B:35:LEU:HD13	1:B:73:PHE:CD2	2.52	0.44
1:B:193:HIS:O	1:B:215:ARG:NH1	2.49	0.44
1:A:82:PRO:HD2	1:B:81:GLN:NE2	2.33	0.43
3:F:36:VAL:HG11	3:F:73:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:LYS:O	1:B:214:ASN:HA	2.17	0.43
2:C:124:PRO:HB3	2:C:150:TYR:HB3	1.99	0.43
2:C:66:PHE:HD1	2:C:77:LEU:HD11	1.83	0.43
1:B:34:TYR:HB3	1:B:93:ASP:HB3	2.00	0.43
3:F:107:THR:C	3:F:108:ILE:HD12	2.43	0.43
2:D:50:ILE:HA	2:D:56:PRO:HA	2.01	0.43
1:A:215:ARG:HG2	1:A:215:ARG:HH11	1.82	0.43
2:D:86:ASP:HB2	2:D:116:VAL:HG21	2.01	0.43
1:B:20:THR:HG23	1:B:74:THR:HG23	2.01	0.43
1:A:15:VAL:HG22	1:A:82:PRO:HD3	2.01	0.43
3:F:42:PHE:CE2	3:F:43:LYS:HG3	2.54	0.43
2:D:38:GLN:HB3	2:D:89:VAL:HG23	2.01	0.42
3:F:73:LEU:HA	3:F:73:LEU:HD23	1.79	0.42
2:D:205:HIS:ND1	2:D:208:SER:OG	2.42	0.42
3:F:28:MET:CE	3:F:76:GLY:HA2	2.49	0.42
1:A:85:PHE:HE2	1:A:169:GLU:HB3	1.85	0.42
1:A:58:SER:OG	2:C:188:THR:O	2.32	0.42
2:D:61:TRP:CE3	2:D:63:LYS:N	2.87	0.42
2:C:8:GLY:N	2:C:112:THR:OG1	2.52	0.42
2:C:157:VAL:HG22	2:C:203:VAL:HG22	2.00	0.42
2:C:204:ASN:ND2	2:C:211:LYS:HG2	2.33	0.42
3:E:96:CYS:O	3:E:106:GLU:HA	2.19	0.42
3:E:35:GLU:H	3:E:35:GLU:HG2	1.73	0.42
1:A:80:LEU:C	1:A:81:GLN:HG2	2.45	0.42
2:C:10:LEU:HB2	2:C:152:PRO:HG3	2.01	0.42
3:F:32:ASN:C	3:F:74:LEU:HD21	2.45	0.42
2:D:217:GLU:HG2	2:D:218:PRO:HD2	2.01	0.41
2:C:204:ASN:OD1	2:C:206:LYS:HG3	2.20	0.41
1:A:97:ASP:OD2	3:F:41:LYS:NZ	2.49	0.41
3:F:57:SER:OG	3:F:67:LYS:NZ	2.53	0.41
2:C:65:ARG:HG2	2:C:80:THR:O	2.21	0.41
2:D:126:VAL:HB	2:D:212:VAL:HG11	2.02	0.41
1:A:123:PRO:HB3	1:A:213:PHE:CE1	2.55	0.41
1:A:80:LEU:HG	1:A:81:GLN:N	2.35	0.41
1:A:174:ASP:OD1	1:A:174:ASP:C	2.64	0.41
3:E:39:LYS:HG2	3:E:40:TRP:N	2.35	0.41
3:E:82:MET:HE2	3:E:82:MET:HB2	1.77	0.41
1:B:130:LYS:HE3	1:B:130:LYS:HB3	1.80	0.41
2:C:10:LEU:HD21	2:C:119:ALA:O	2.21	0.41
3:F:3:LEU:O	3:F:25:VAL:HA	2.21	0.41
2:D:17:LEU:HB3	2:D:79:MET:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:TYR:CE2	2:D:100:GLY:HA3	2.56	0.40
1:B:94:TYR:HD2	1:B:100:ASN:HD22	1.68	0.40
3:E:40:TRP:HE1	3:E:68:ILE:HD11	1.85	0.40
1:A:81:GLN:HE22	1:B:82:PRO:CD	2.34	0.40
1:A:136:VAL:HB	1:A:183:LEU:HB3	2.03	0.40
2:D:198:THR:HG23	2:D:215:LYS:CE	2.51	0.40
3:F:48:TYR:OH	3:F:67:LYS:NZ	2.49	0.40
2:D:22:SER:HA	2:D:74:THR:HG22	2.04	0.40
1:B:68:GLY:HA3	1:B:73:PHE:HA	2.03	0.40
2:D:64:GLY:HA2	2:D:83:ARG:NH1	2.36	0.40
1:B:17:ASP:CG	1:B:18:ARG:H	2.29	0.40
2:C:17:LEU:HB3	2:C:79:MET:HB2	2.02	0.40
2:C:58:TYR:HE2	2:C:68:ILE:HG13	1.86	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	A	214/218 (98%)	205 (96%)	9 (4%)	0	100	100
1	B	213/218 (98%)	202 (95%)	11 (5%)	0	100	100
2	C	207/225 (92%)	197 (95%)	10 (5%)	0	100	100
2	D	208/225 (92%)	194 (93%)	14 (7%)	0	100	100
3	E	116/131 (88%)	113 (97%)	3 (3%)	0	100	100
3	F	113/131 (86%)	110 (97%)	3 (3%)	0	100	100
All	All	1071/1148 (93%)	1021 (95%)	50 (5%)	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 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	A	188/190 (99%)	180 (96%)	8 (4%)	25	48
1	B	187/190 (98%)	178 (95%)	9 (5%)	21	43
2	C	177/189 (94%)	169 (96%)	8 (4%)	23	46
2	D	178/189 (94%)	173 (97%)	5 (3%)	38	65
3	E	106/118 (90%)	102 (96%)	4 (4%)	28	53
3	F	103/118 (87%)	96 (93%)	7 (7%)	13	27
All	All	939/994 (94%)	898 (96%)	41 (4%)	24	47

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	26	SER
1	A	36	SER
1	A	79	SER
1	A	130	LYS
1	A	136	VAL
1	A	172	SER
1	A	211	LYS
2	D	34	SER
2	D	80	THR
2	D	89	VAL
2	D	120	SER
2	D	121	THR
1	B	11	LEU
1	B	81	GLN
1	B	107	LYS
1	B	130	LYS
1	B	133	THR
1	B	140	LEU
1	B	206	SER
1	B	212	SER
1	B	215	ARG

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Mol	Chain	Res	Type
2	C	5	GLU
2	C	50	ILE
2	C	114	VAL
2	C	133	SER
2	C	155	VAL
2	C	174	VAL
2	C	202	ASN
2	C	214	LYS
3	E	28	MET
3	E	39	LYS
3	E	58	THR
3	E	88	VAL
3	F	25	VAL
3	F	32	ASN
3	F	33	THR
3	F	56	LYS
3	F	57	SER
3	F	58	THR
3	F	85	SER

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

Mol	Chain	Res	Type
1	A	141	ASN
2	D	99	ASN
1	B	32	ASN
1	B	100	ASN
1	B	142	ASN
1	B	170	GLN
1	B	214	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)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
3	PCA	F	1	3	7,8,9	2.11	1 (14%)	9,10,12	2.26	4 (44%)
3	PCA	E	1	3	7,8,9	1.89	1 (14%)	9,10,12	1.97	5 (55%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCA	F	1	3	-	0/0/11/13	0/1/1/1
3	PCA	E	1	3	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	PCA	CD-N	5.18	1.48	1.34
3	E	1	PCA	CD-N	4.75	1.47	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1	PCA	CB-CA-C	-3.80	107.47	112.70
3	F	1	PCA	OE-CD-CG	-3.27	121.05	126.76
3	E	1	PCA	OE-CD-CG	-2.85	121.78	126.76
3	F	1	PCA	CA-N-CD	-2.67	104.45	113.58
3	E	1	PCA	CA-N-CD	-2.64	104.55	113.58
3	E	1	PCA	CB-CA-N	2.36	110.06	103.30
3	E	1	PCA	CB-CA-C	-2.31	109.53	112.70
3	E	1	PCA	CG-CD-N	2.29	114.33	108.39
3	F	1	PCA	CB-CA-N	2.20	109.61	103.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	PCA	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
6	NAG	E	201	3	14,14,15	0.16	0	17,19,21	1.06	1 (5%)
6	NAG	E	202	3	14,14,15	0.69	0	17,19,21	0.89	1 (5%)
5	GOL	D	301	-	5,5,5	1.32	1 (20%)	5,5,5	0.71	0
5	GOL	C	301	-	5,5,5	1.32	0	5,5,5	0.68	0
6	NAG	F	201	3	14,14,15	1.32	1 (7%)	17,19,21	0.94	1 (5%)
6	NAG	F	202	3	14,14,15	0.73	1 (7%)	17,19,21	0.84	1 (5%)

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
6	NAG	E	201	3	-	3/6/23/26	0/1/1/1
6	NAG	E	202	3	-	2/6/23/26	0/1/1/1
5	GOL	D	301	-	-	2/4/4/4	-
5	GOL	C	301	-	-	0/4/4/4	-
6	NAG	F	201	3	-	2/6/23/26	0/1/1/1
6	NAG	F	202	3	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	201	NAG	O5-C1	4.79	1.51	1.43
5	D	301	GOL	C1-C2	2.15	1.60	1.51
6	F	202	NAG	C1-C2	2.07	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	201	NAG	C1-O5-C5	3.47	116.90	112.19
6	F	201	NAG	C1-O5-C5	3.10	116.39	112.19
6	F	202	NAG	C1-O5-C5	2.84	116.04	112.19
6	E	202	NAG	C2-N2-C7	2.20	126.04	122.90

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	201	NAG	C8-C7-N2-C2
6	E	201	NAG	O7-C7-N2-C2
6	F	201	NAG	O5-C5-C6-O6
5	D	301	GOL	O2-C2-C3-O3
5	D	301	GOL	C1-C2-C3-O3
6	E	202	NAG	O5-C5-C6-O6
6	E	201	NAG	O5-C5-C6-O6
6	F	201	NAG	C4-C5-C6-O6
6	E	202	NAG	C4-C5-C6-O6

There are no ring outliers.

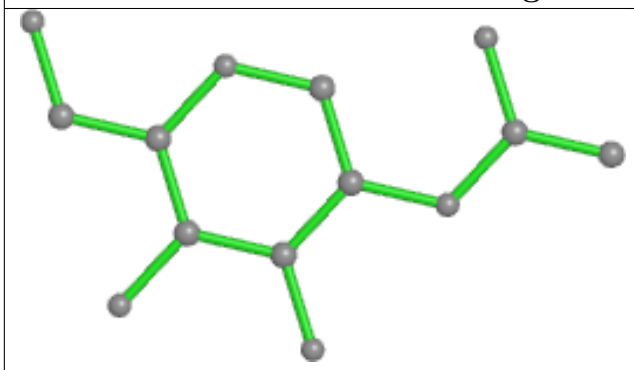
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	201	NAG	1	0
5	D	301	GOL	3	0
5	C	301	GOL	1	0

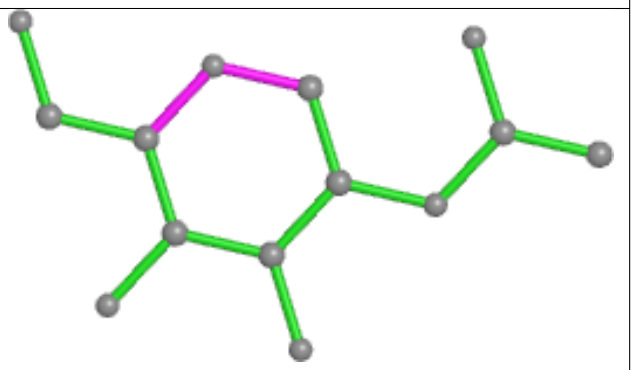
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

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

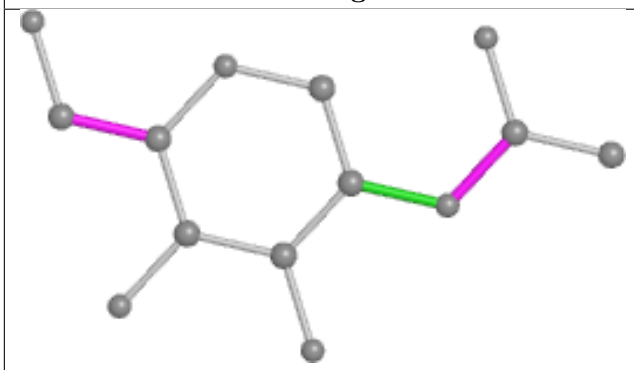
Ligand NAG E 201



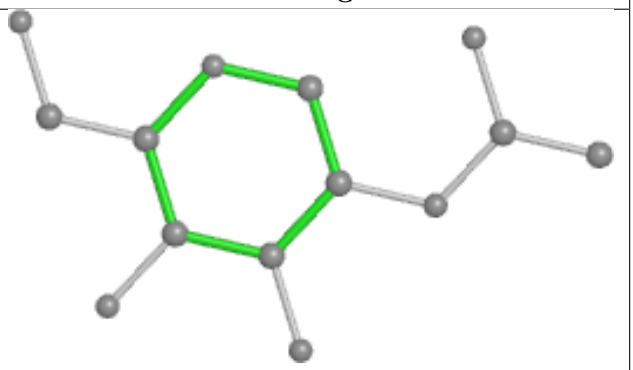
Bond lengths



Bond angles

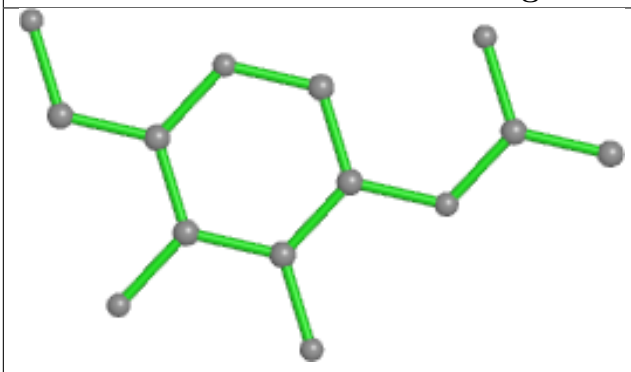


Torsions

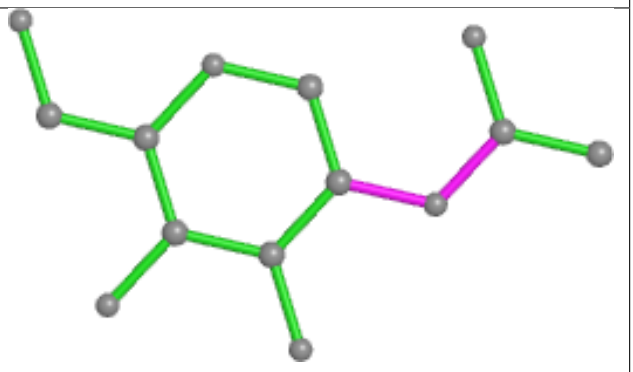


Rings

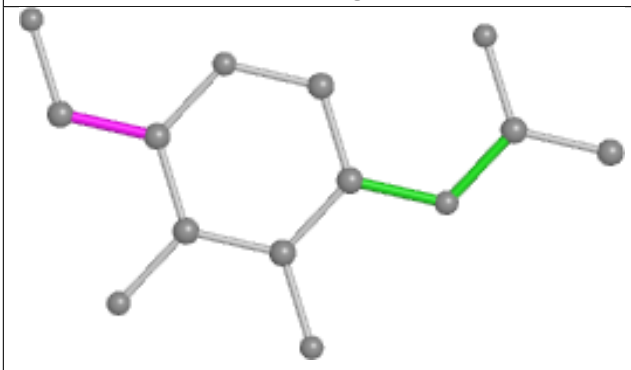
Ligand NAG E 202



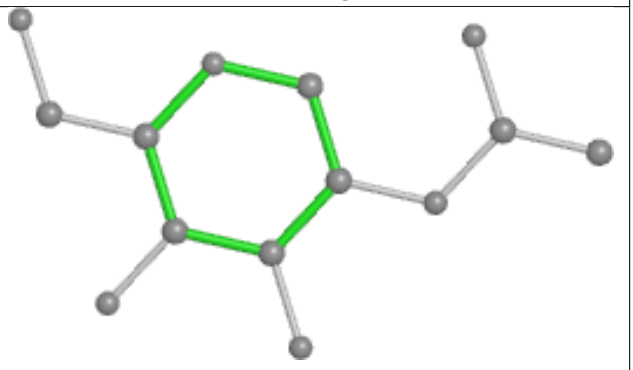
Bond lengths



Bond angles

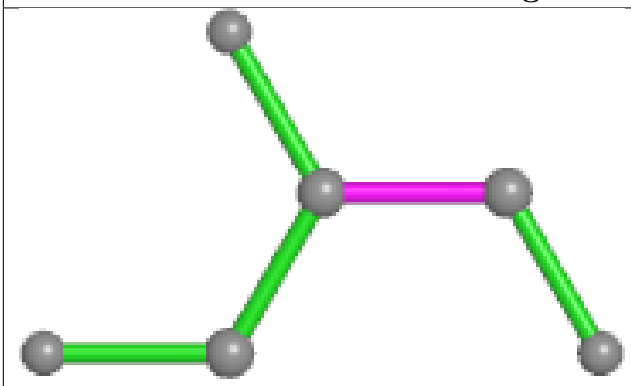


Torsions

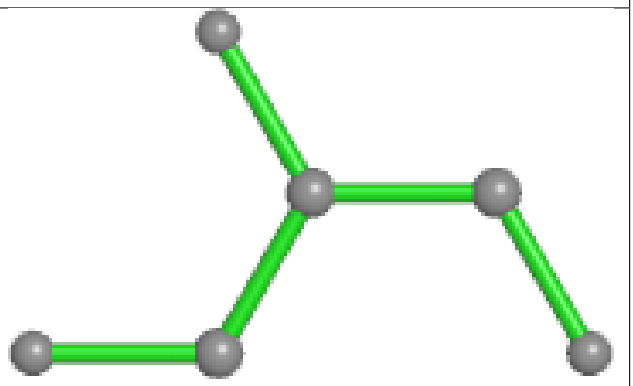


Rings

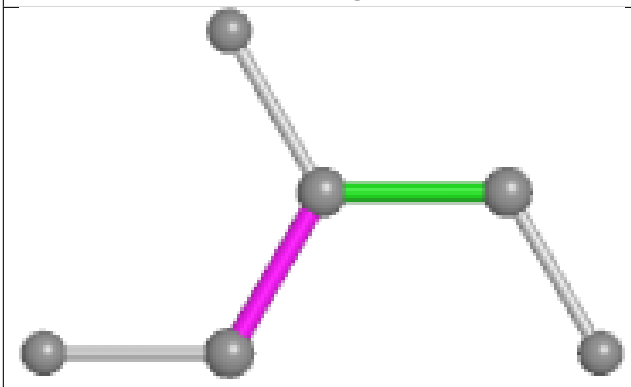
Ligand GOL D 301



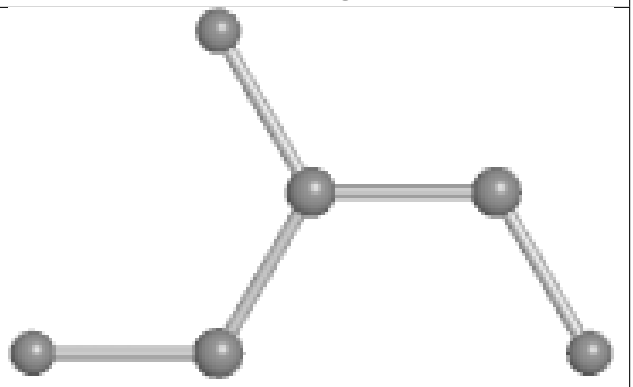
Bond lengths



Bond angles

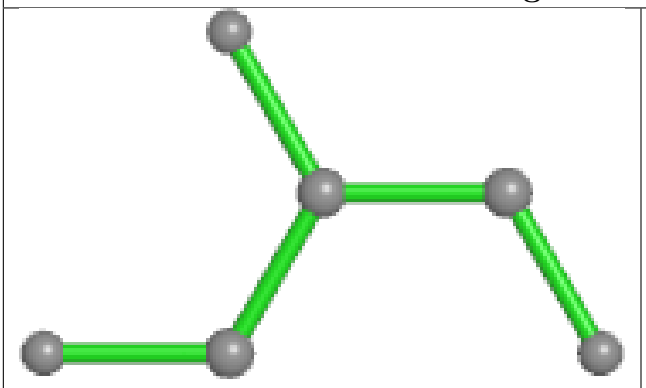


Torsions

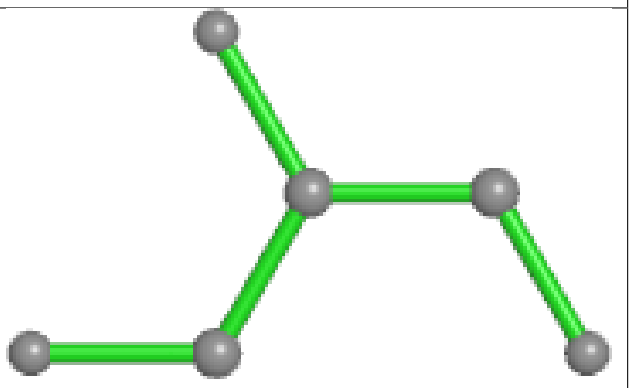


Rings

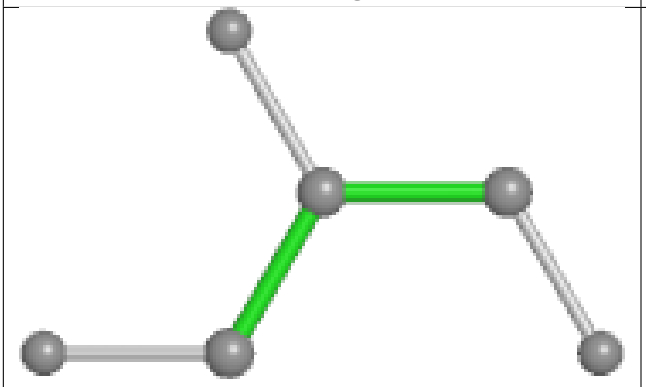
Ligand GOL C 301



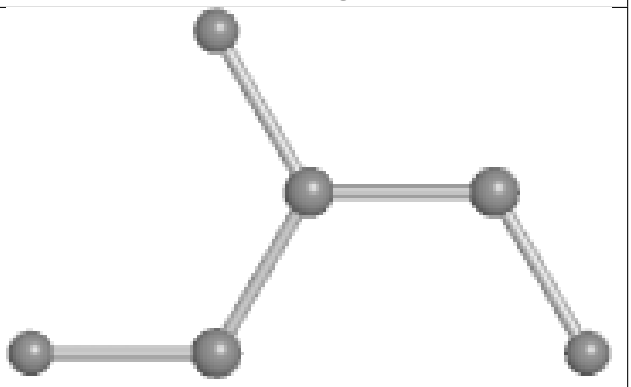
Bond lengths



Bond angles

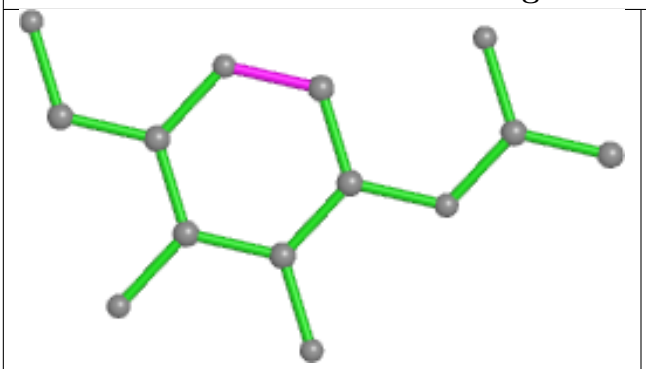


Torsions

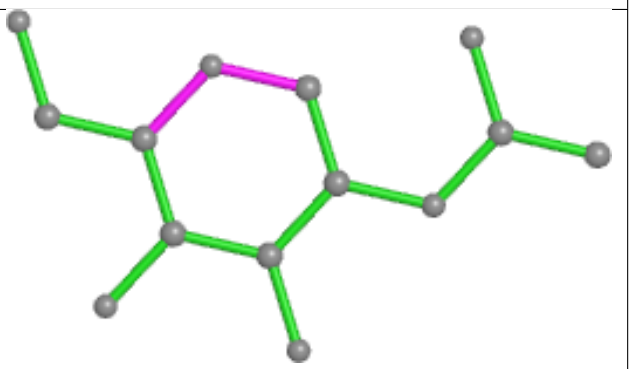


Rings

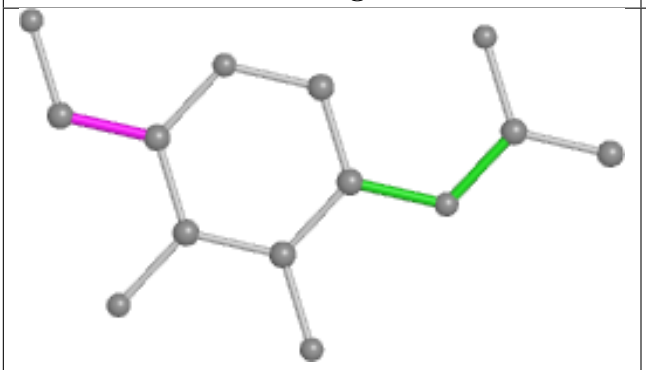
Ligand NAG F 201



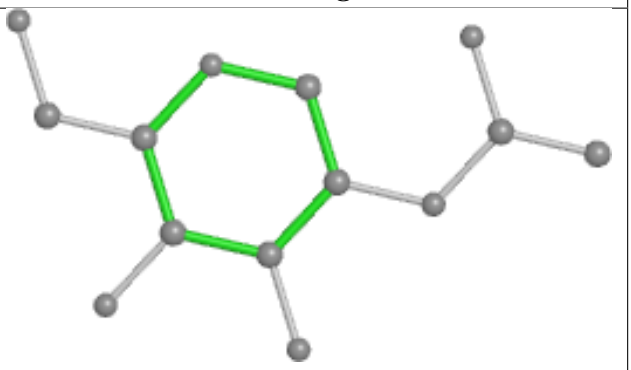
Bond lengths



Bond angles

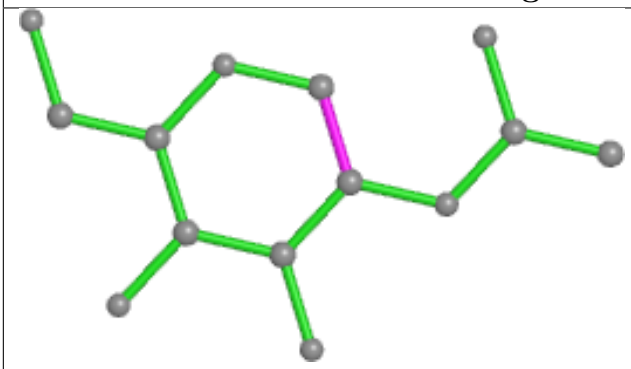


Torsions

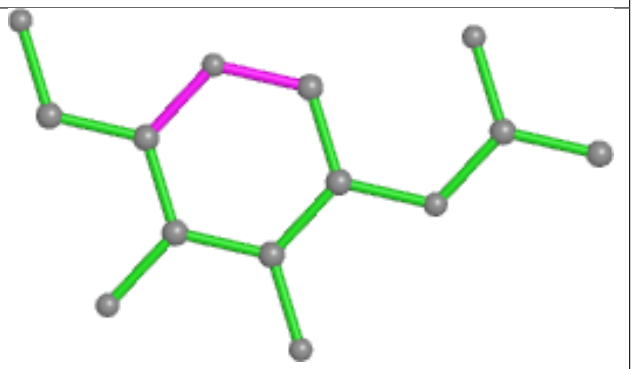


Rings

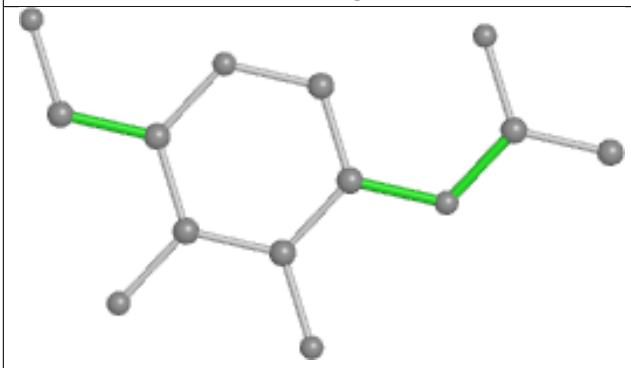
Ligand NAG F 202



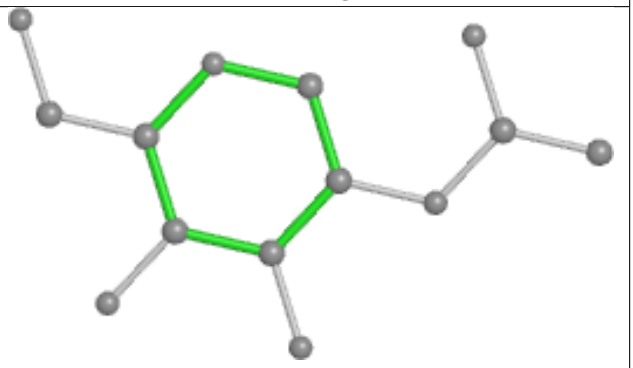
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	A	216/218 (99%)	0.13	2 (0%) 81 78	42, 48, 57, 73	0
1	B	215/218 (98%)	0.12	5 (2%) 61 58	39, 43, 47, 50	0
2	C	213/225 (94%)	0.09	1 (0%) 87 85	39, 43, 48, 57	0
2	D	214/225 (95%)	0.19	2 (0%) 81 78	41, 45, 49, 89	0
3	E	117/131 (89%)	0.02	0 100 100	36, 44, 51, 56	0
3	F	114/131 (87%)	0.09	1 (0%) 81 78	38, 48, 52, 53	0
All	All	1089/1148 (94%)	0.12	11 (1%) 79 76	36, 45, 52, 89	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	85	PHE	4.8
1	B	2	PRO	3.7
1	B	10	PHE	3.4
1	A	10	PHE	3.3
1	B	85	PHE	2.8
2	C	76	TYR	2.5
2	D	63	LYS	2.3
2	D	61	TRP	2.3
1	B	18	ARG	2.2
3	F	114	ARG	2.1
1	B	80	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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, 95^{th} 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
3	PCA	F	1	8/9	0.89	0.09	46,46,48,48	0
3	PCA	E	1	8/9	0.93	0.08	46,46,46,46	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

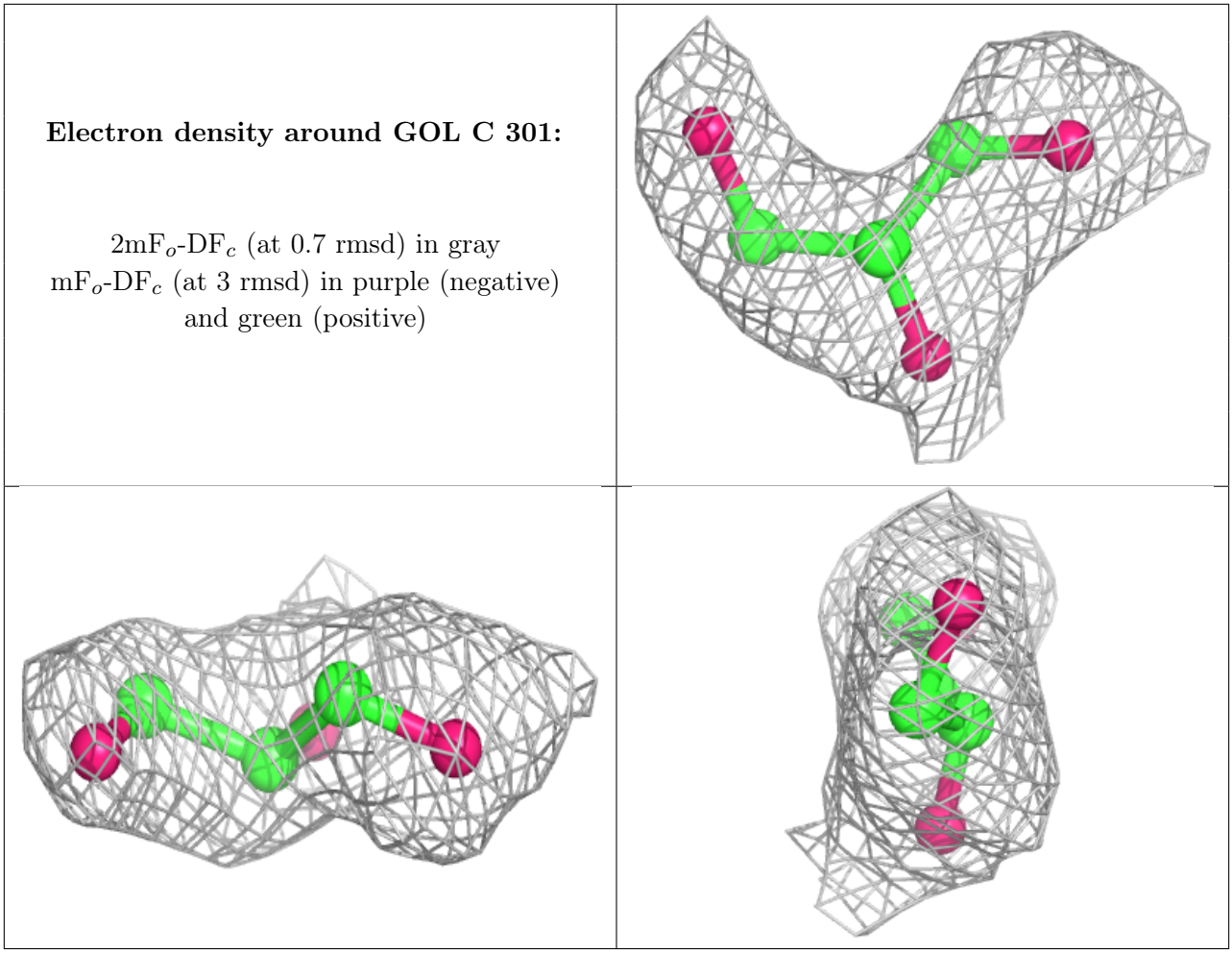
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	GOL	C	301	6/6	0.80	0.13	42,42,43,43	0
6	NAG	E	202	14/15	0.82	0.11	41,42,42,42	0
5	GOL	D	301	6/6	0.83	0.21	44,44,44,44	0
6	NAG	F	201	14/15	0.84	0.10	45,46,46,47	0
6	NAG	F	202	14/15	0.87	0.09	47,49,50,51	0
6	NAG	E	201	14/15	0.91	0.07	41,42,42,42	0
4	CA	A	301	1/1	0.99	0.02	45,45,45,45	0
4	CA	B	301	1/1	0.99	0.04	45,45,45,45	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.

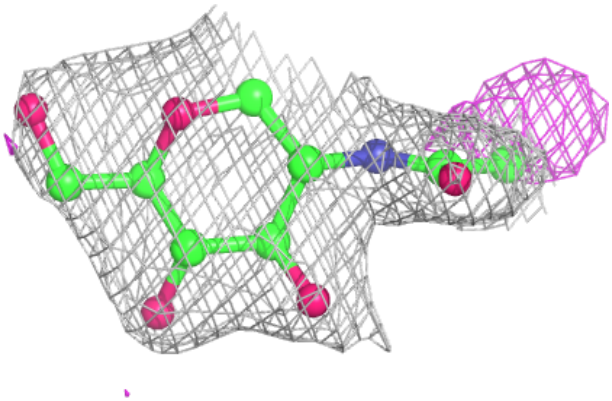
Electron density around GOL C 301:

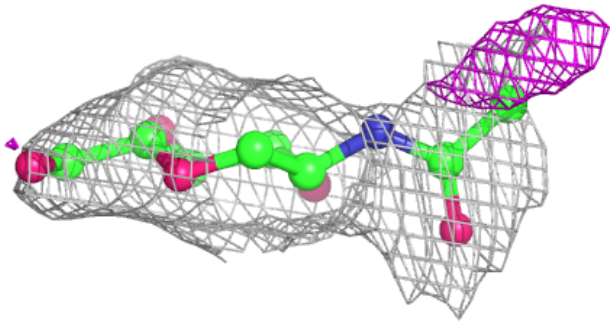
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

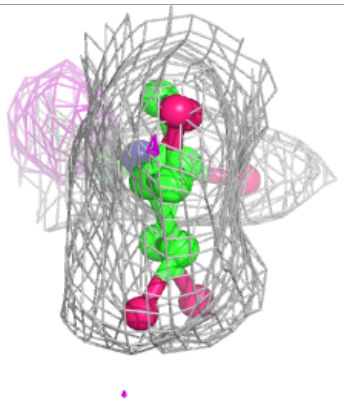


Electron density around NAG E 202:

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

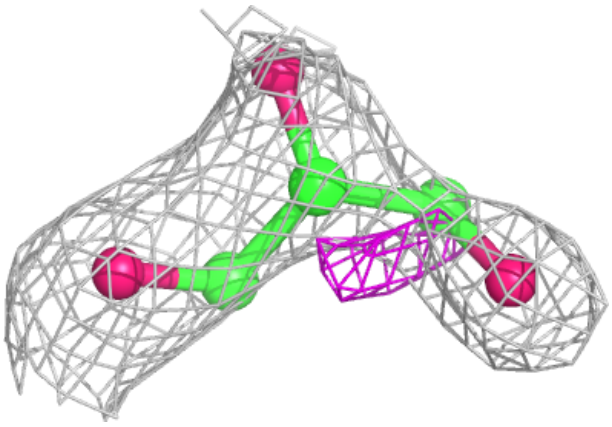


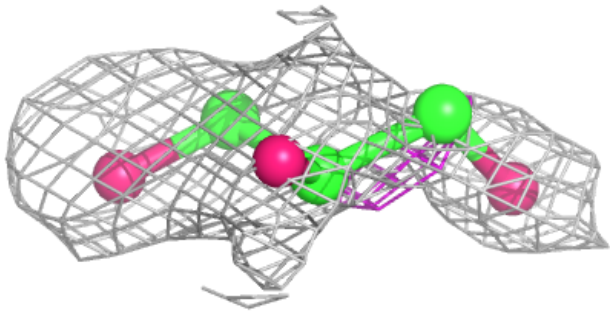


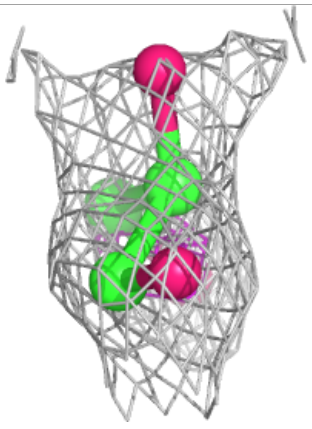


Electron density around GOL D 301:

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

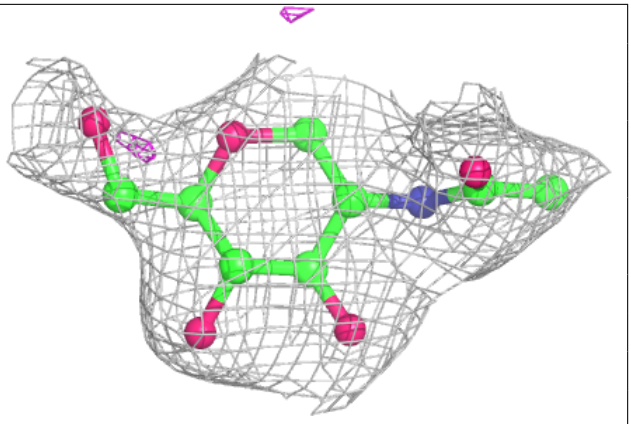


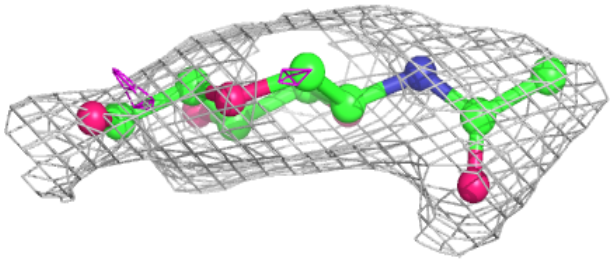


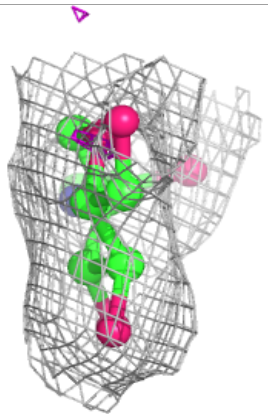


Electron density around NAG F 201:

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

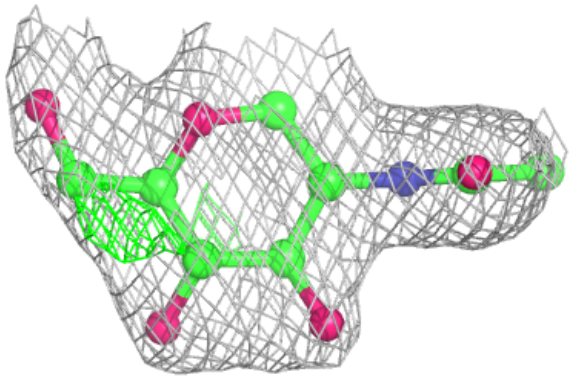


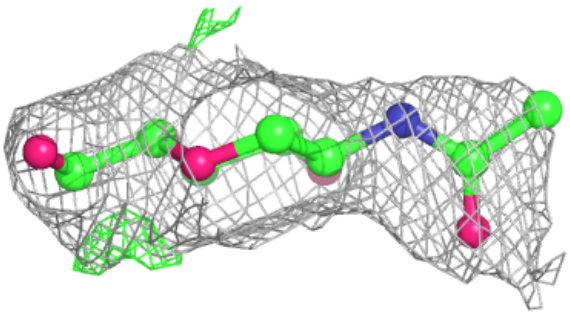


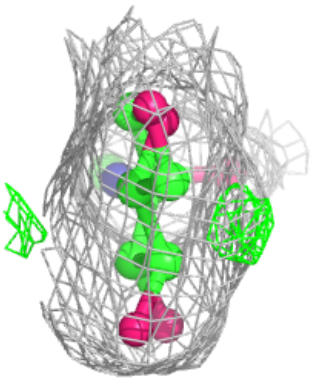


Electron density around NAG F 202:

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

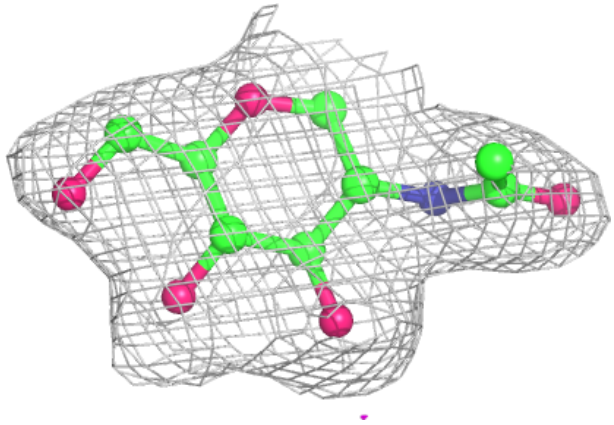


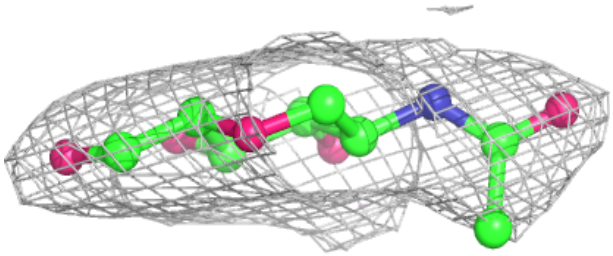


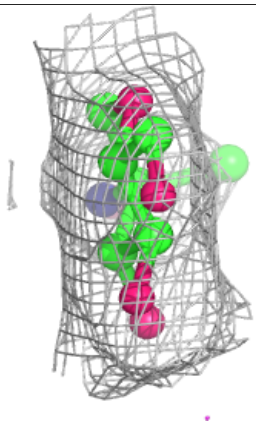


Electron density around NAG E 201:

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

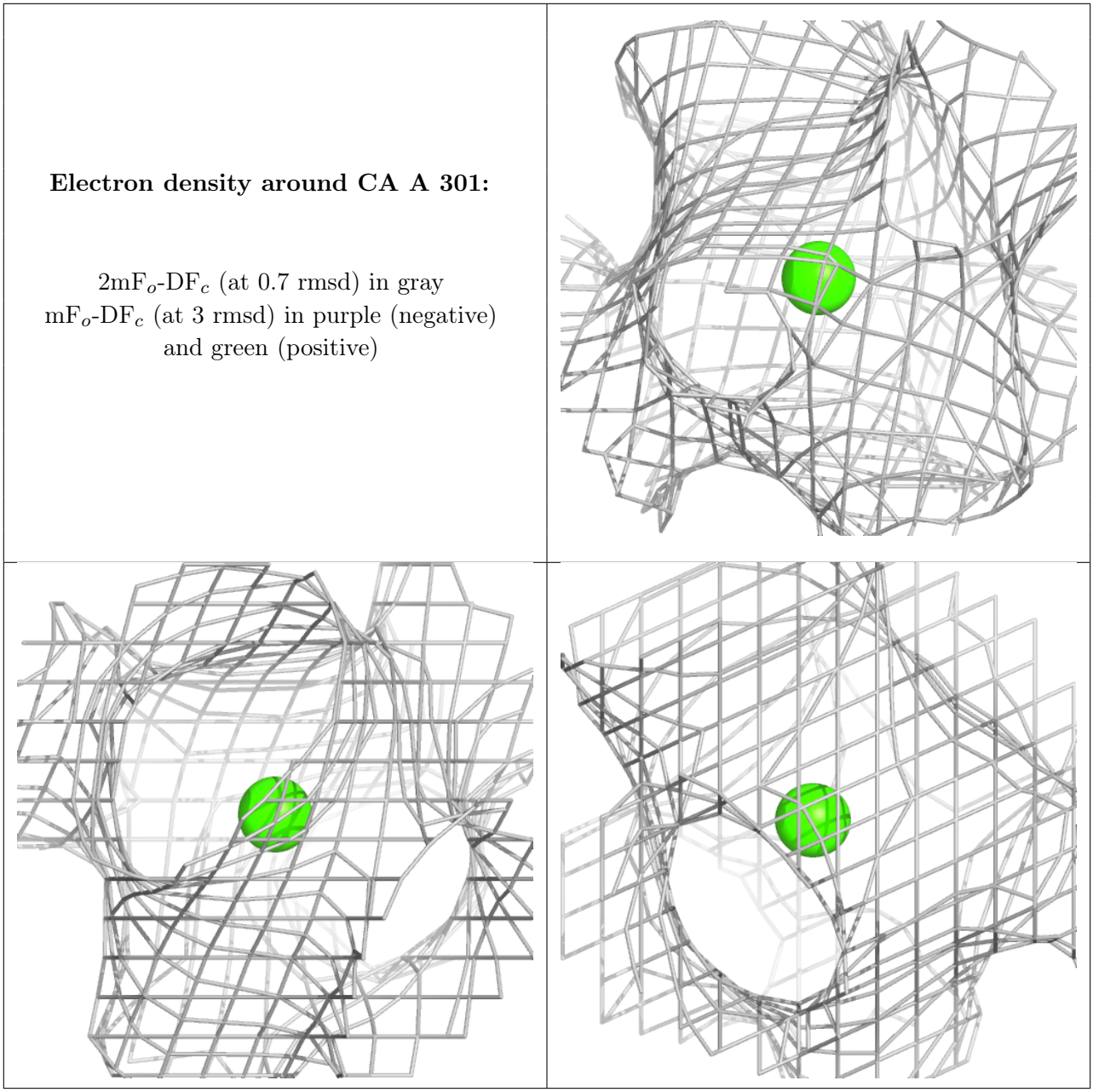






Electron density around CA A 301:

$2mF_o$-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 B 301:

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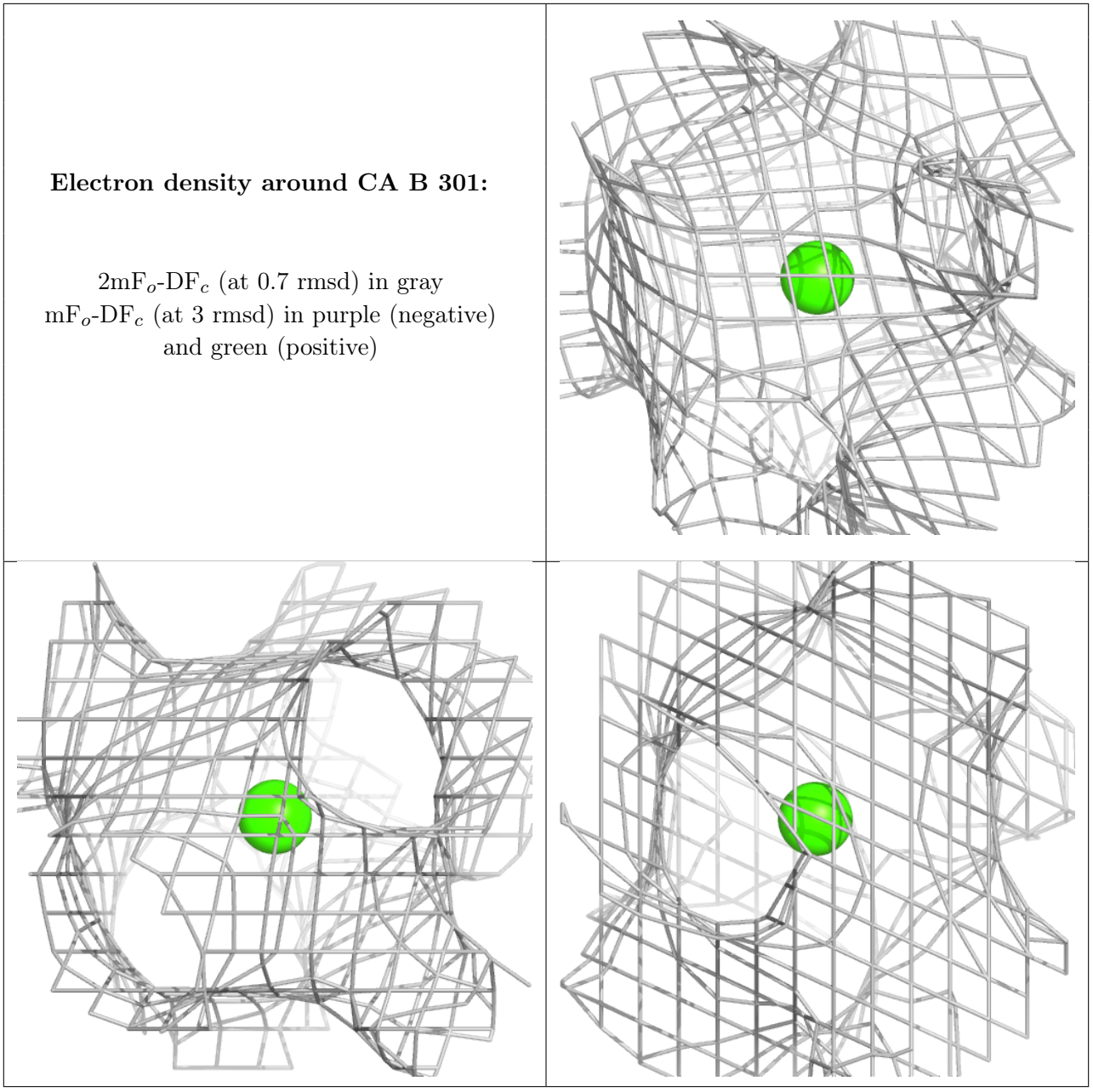
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.