wwPDB X-ray Structure Validation Summary Report (i)

May 26, 2020 – 02:48 am BST

PDB ID	:	6PUL
Title	:	Structure of human MAIT A-F7 TCR in complex with human MR1 3'D-5-OP-RU
Authors	:	Awad, W.; Keller, A.N.; Rossjohn, J.
Deposited on	:	2019-07-18
Resolution	:	1.84 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

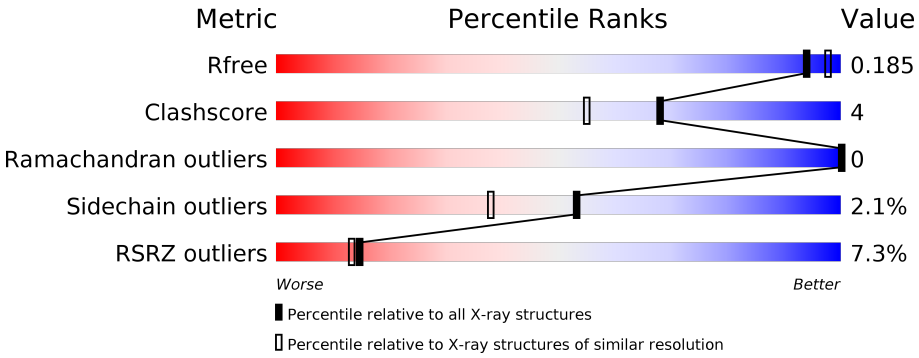
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.84 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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 on 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	271	6% 90% 7%
1	C	271	3% 89% 9%
2	B	204	89% 9%
2	D	204	21% 83% 12%
3	E	246	13% 89% 8%
3	G	246	% 87% 11%

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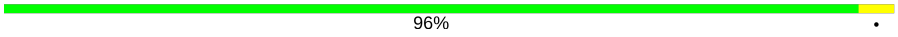
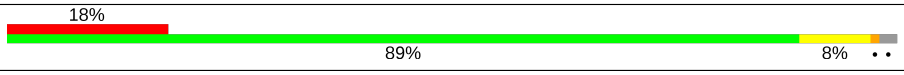
Mol	Chain	Length	Quality of chain
4	F	100	
4	H	100	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15099 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 Major histocompatibility complex class I-related gene protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	10	0
			2216	1419	378	407	12			
1	C	267	Total	C	N	O	S	0	12	0
			2247	1446	382	408	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q95460
A	261	SER	CYS	conflict	UNP Q95460
C	0	MET	-	initiating methionine	UNP Q95460
C	261	SER	CYS	conflict	UNP Q95460

- Molecule 2 is a protein called TRA@ protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	200	Total	C	N	O	S	0	22	0
			1676	1072	262	332	10			
2	D	195	Total	C	N	O	S	0	6	0
			1526	973	242	301	10			

- Molecule 3 is a protein called Human TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	241	Total	C	N	O	S	0	10	0
			1920	1220	326	363	11			
3	G	244	Total	C	N	O	S	0	17	0
			2000	1265	340	381	14			

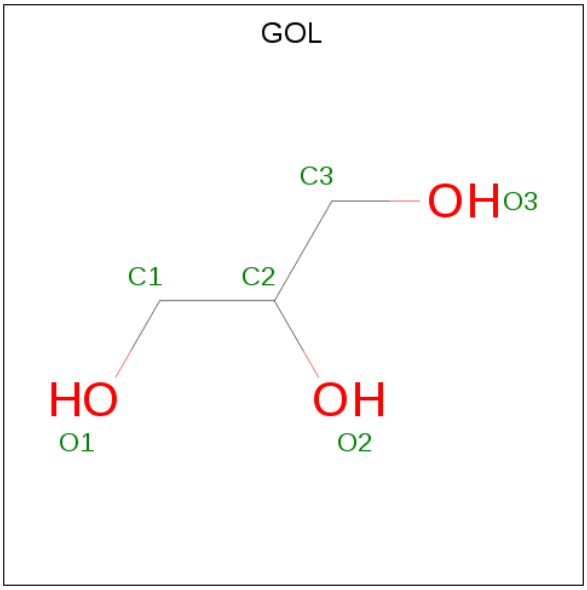
- Molecule 4 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	100	Total	C	N	O	S	0	1	0
			826	530	138	154	4			
4	H	98	Total	C	N	O	S	0	1	0
			801	515	135	148	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	0	MET	-	initiating methionine	UNP P61769
H	0	MET	-	initiating methionine	UNP P61769

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by author).



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

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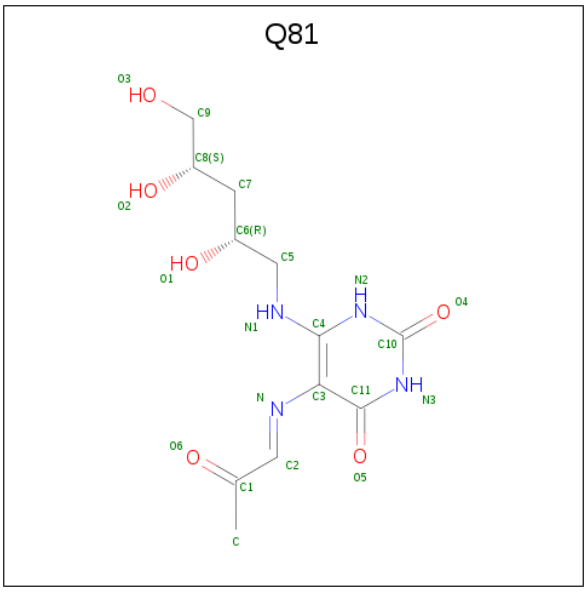
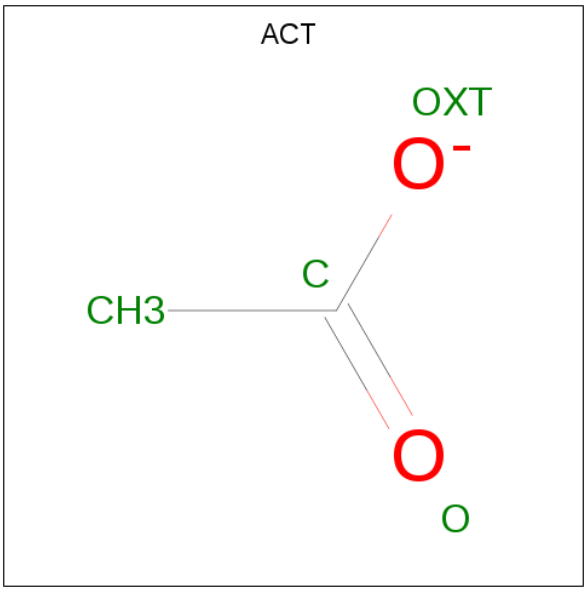
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 1,3-dideoxy-1-({2,6-dioxo-5-[(E)-(2-oxopropylidene)amino]-1,2,3,6-tetrahydropyrimidin-4-yl}amino)-D-erythro-pentitol (three-letter code: Q81) (formula: $C_{12}H_{18}N_4O_6$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			21	12	4	5		
6	C	1	Total	C	N	O	0	0
			21	12	4	5		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	1	Total C O 4 2 2	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total Na 1 1	0	0
8	G	1	Total Na 1 1	0	0
8	F	2	Total Na 2 2	0	0
8	E	1	Total Na 1 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	304	Total O 304 304	0	0
9	B	269	Total O 269 269	0	0
9	C	325	Total O 325 325	0	0
9	D	150	Total O 150 150	0	0

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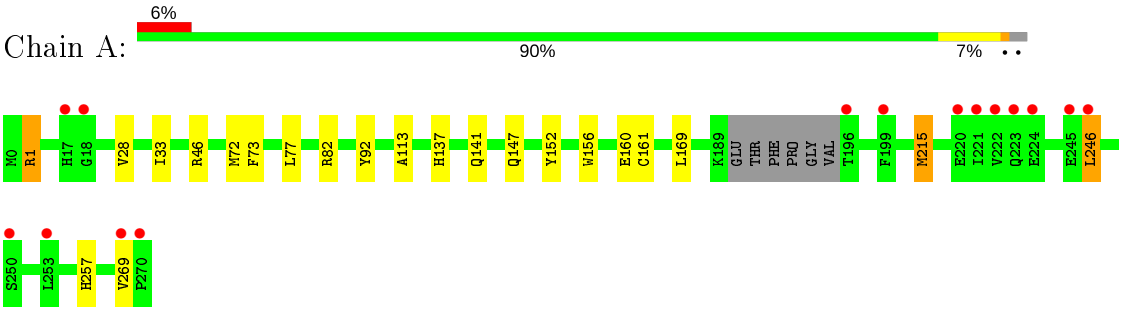
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	E	160	Total O 160 160	0	0
9	F	157	Total O 157 157	0	0
9	G	347	Total O 347 347	0	0
9	H	82	Total O 82 82	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

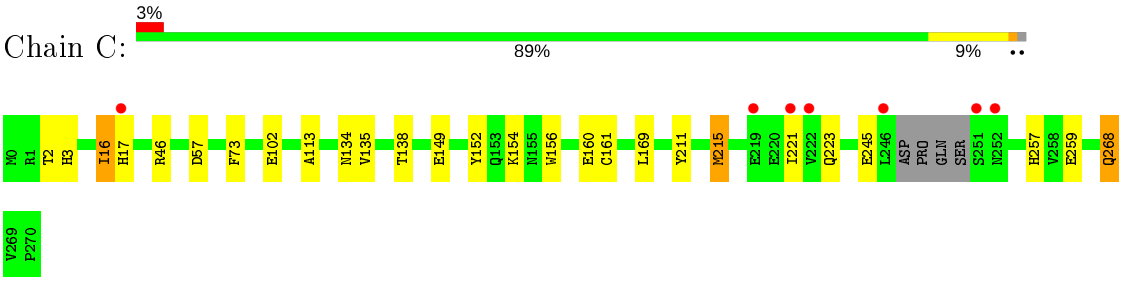
- Molecule 1: Major histocompatibility complex class I-related gene protein

Chain A:



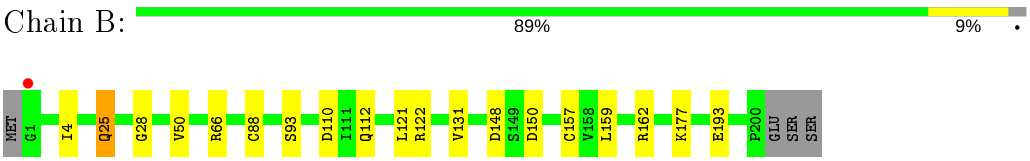
- Molecule 1: Major histocompatibility complex class I-related gene protein

Chain C:



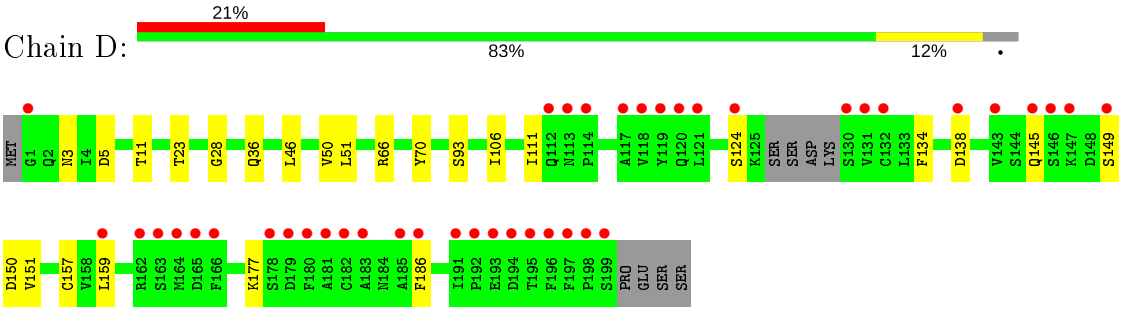
- Molecule 2: TRA@ protein

Chain B:



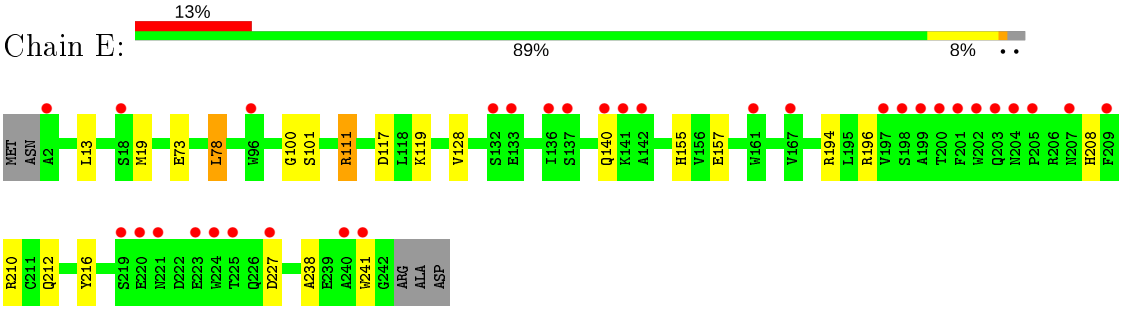
- Molecule 2: TRA@ protein

Chain D:



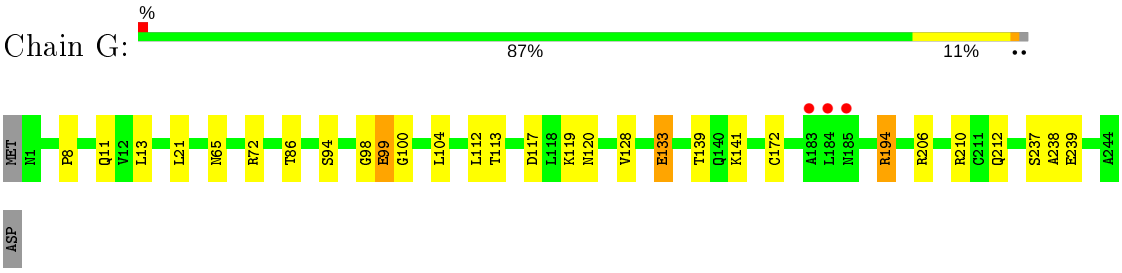
• Molecule 3: Human TCR beta chain

Chain E:



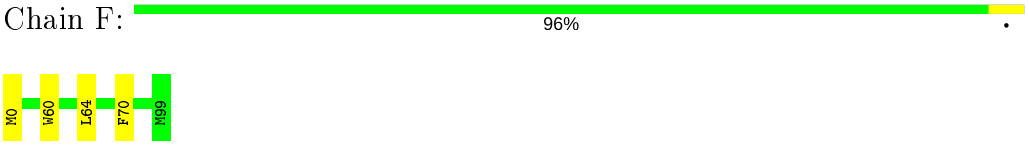
• Molecule 3: Human TCR beta chain

Chain G:



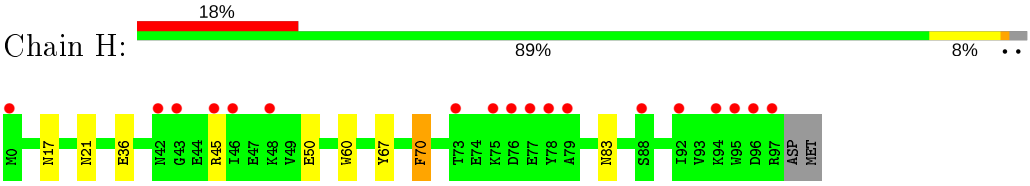
• Molecule 4: Beta-2-microglobulin

Chain F:



• Molecule 4: Beta-2-microglobulin

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	216.55Å 70.03Å 143.25Å 90.00° 104.30° 90.00°	Depositor
Resolution (Å)	49.49 – 1.84 49.98 – 1.84	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.49-1.84) 98.8 (49.98-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 1.84Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.155 , 0.184 0.157 , 0.185	Depositor DCC
R_{free} test set	8977 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	32.9	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15099	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: ACT, GOL, Q81, NA

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	0.46	0/2313	0.62	2/3145 (0.1%)
1	C	0.43	0/2351	0.60	0/3196
2	B	0.46	0/1775	0.64	0/2406
2	D	0.39	0/1578	0.57	0/2142
3	E	0.36	0/1994	0.56	1/2719 (0.0%)
3	G	0.45	0/2103	0.62	0/2856
4	F	0.43	0/852	0.57	0/1156
4	H	0.34	0/827	0.50	0/1123
All	All	0.42	0/13793	0.59	3/18743 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	ARG	NE-CZ-NH2	-7.64	116.48	120.30
3	E	78	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	1	ARG	NE-CZ-NH1	5.11	122.85	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2216	0	2101	13	0
1	C	2247	0	2158	20	0
2	B	1676	0	1661	16	0
2	D	1526	0	1438	14	0
3	E	1920	0	1800	14	0
3	G	2000	0	1935	23	0
4	F	826	0	783	2	0
4	H	801	0	756	5	0
5	A	12	0	16	0	0
5	B	6	0	8	1	0
5	D	6	0	8	0	0
5	F	12	0	16	0	0
5	G	6	0	8	1	0
6	A	21	0	0	0	0
6	C	21	0	0	0	0
7	E	4	0	3	0	0
8	E	1	0	0	0	0
8	F	2	0	0	0	0
8	G	1	0	0	0	0
8	H	1	0	0	0	0
9	A	304	0	0	4	1
9	B	269	0	0	3	0
9	C	325	0	0	2	0
9	D	150	0	0	2	0
9	E	160	0	0	2	0
9	F	157	0	0	1	1
9	G	347	0	0	10	0
9	H	82	0	0	1	0
All	All	15099	0	12691	99	1

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 4.

The worst 5 of 99 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)
1:A:72:MET:SD	9:G:679:HOH:O	2.30	0.88
3:G:98:GLY:O	9:G:401:HOH:O	1.99	0.80
2:D:3[A]:ASN:ND2	2:D:5:ASP:OD1	2.13	0.79
1:A:147:GLN:OE1	9:A:401:HOH:O	2.05	0.74
2:B:148:ASP:OD2	2:B:177:LYS:NZ	2.24	0.69

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:590:HOH:O	9:F:224:HOH:O[4_558]	2.11	0.09

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	271/271 (100%)	267 (98%)	4 (2%)	0	100	100
1	C	275/271 (102%)	269 (98%)	6 (2%)	0	100	100
2	B	220/204 (108%)	216 (98%)	4 (2%)	0	100	100
2	D	197/204 (97%)	192 (98%)	5 (2%)	0	100	100
3	E	249/246 (101%)	246 (99%)	3 (1%)	0	100	100
3	G	259/246 (105%)	256 (99%)	3 (1%)	0	100	100
4	F	99/100 (99%)	99 (100%)	0	0	100	100
4	H	97/100 (97%)	96 (99%)	1 (1%)	0	100	100
All	All	1667/1642 (102%)	1641 (98%)	26 (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 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	239/241 (99%)	231 (97%)	8 (3%)	38 20
1	C	243/241 (101%)	238 (98%)	5 (2%)	53 38
2	B	198/181 (109%)	195 (98%)	3 (2%)	65 52
2	D	167/181 (92%)	164 (98%)	3 (2%)	59 44
3	E	204/212 (96%)	199 (98%)	5 (2%)	47 31
3	G	224/212 (106%)	220 (98%)	4 (2%)	59 44
4	F	91/95 (96%)	88 (97%)	3 (3%)	38 20
4	H	87/95 (92%)	85 (98%)	2 (2%)	50 34
All	All	1453/1458 (100%)	1420 (98%)	33 (2%)	53 34

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	215	MET
2	D	157	CYS
3	G	194	ARG
1	C	268	GLN
2	D	124	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
5	GOL	G	301	-	5,5,5	0.43	0	5,5,5	1.55	1 (20%)
5	GOL	A	301	-	5,5,5	0.69	0	5,5,5	1.09	0
6	Q81	C	301	1	19,21,22	0.96	1 (5%)	18,27,29	4.56	6 (33%)
5	GOL	A	302	-	5,5,5	1.11	1 (20%)	5,5,5	1.16	0
5	GOL	B	401	-	5,5,5	0.89	0	5,5,5	1.04	0
7	ACT	E	301	-	1,3,3	5.64	1 (100%)	0,3,3	0.00	-
5	GOL	D	301	-	5,5,5	0.83	0	5,5,5	1.08	0
6	Q81	A	303	1	19,21,22	1.12	2 (10%)	18,27,29	4.64	5 (27%)
5	GOL	F	102	-	5,5,5	1.28	1 (20%)	5,5,5	0.92	0
5	GOL	F	101	-	5,5,5	1.12	1 (20%)	5,5,5	0.93	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
5	GOL	G	301	-	-	2/4/4/4	-
5	GOL	A	301	-	-	0/4/4/4	-
6	Q81	C	301	1	-	2/14/15/16	0/1/1/1
5	GOL	A	302	-	-	2/4/4/4	-
5	GOL	B	401	-	-	2/4/4/4	-
5	GOL	D	301	-	-	4/4/4/4	-
6	Q81	A	303	1	-	2/14/15/16	0/1/1/1
5	GOL	F	102	-	-	0/4/4/4	-
5	GOL	F	101	-	-	0/4/4/4	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	301	ACT	CH3-C	5.64	1.55	1.48
6	A	303	Q81	C11-N3	3.11	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	301	Q81	C11-N3	3.11	1.38	1.33
5	A	302	GOL	C3-C2	2.22	1.60	1.51
6	A	303	Q81	C4-N1	2.17	1.38	1.34

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	301	Q81	C11-N3-C10	14.38	127.29	115.14
6	A	303	Q81	C11-N3-C10	13.80	126.80	115.14
6	A	303	Q81	C11-C3-C4	10.50	121.40	114.53
6	C	301	Q81	C11-C3-C4	9.00	120.42	114.53
6	A	303	Q81	C3-C11-N3	-7.26	113.50	123.43

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	301	GOL	C1-C2-C3-O3
5	A	302	GOL	C1-C2-C3-O3
5	D	301	GOL	C1-C2-C3-O3
6	C	301	Q81	C4-C3-N-C2
6	A	303	Q81	C4-C3-N-C2

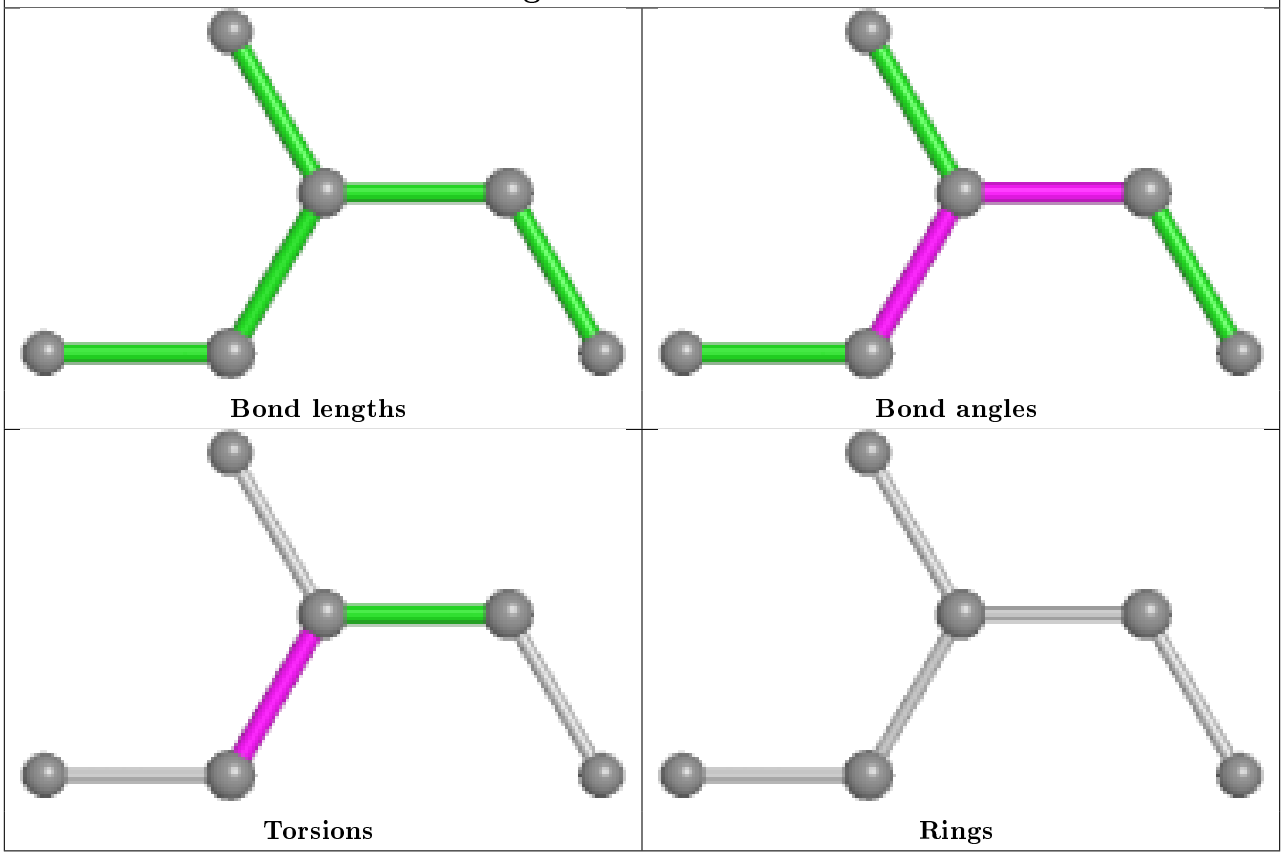
There are no ring outliers.

2 monomers are involved in 2 short contacts:

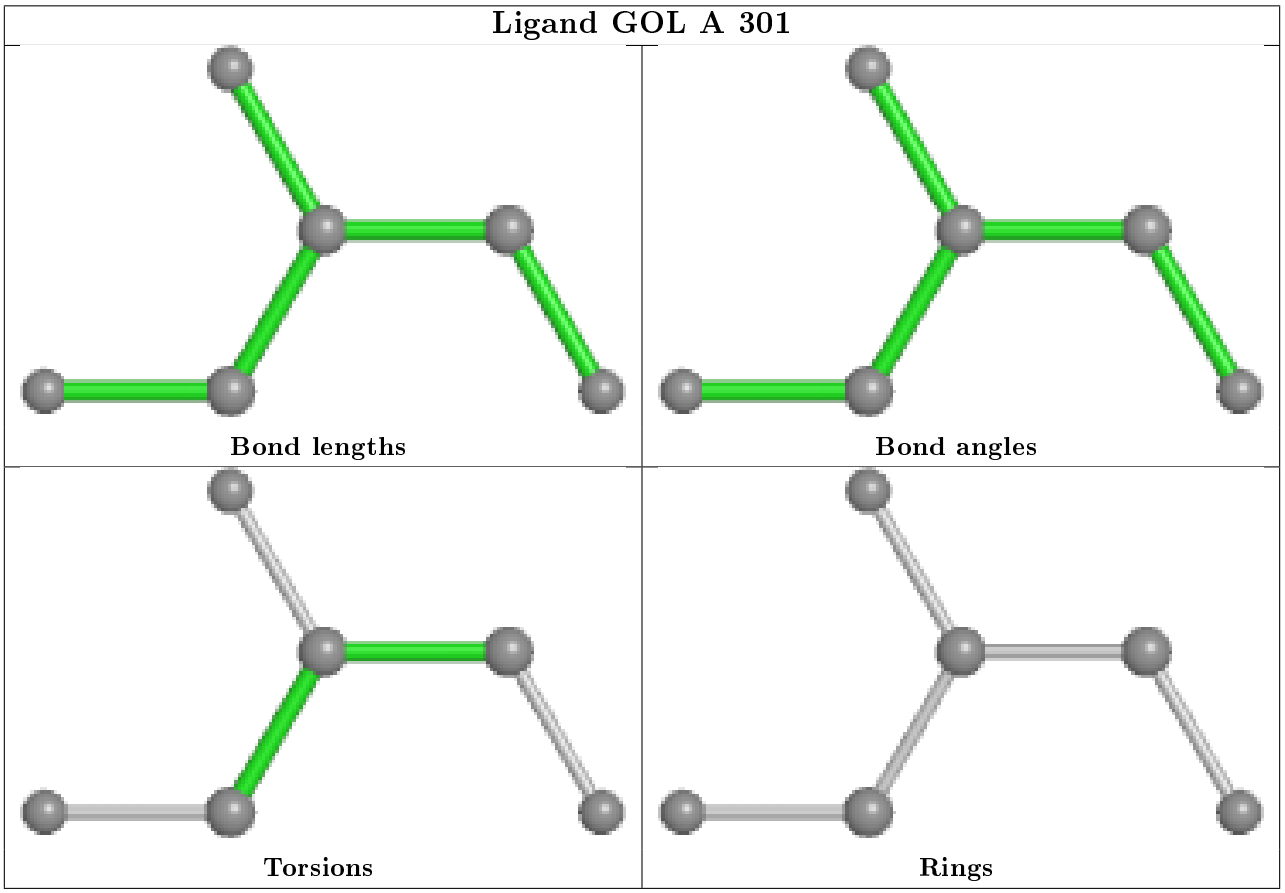
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	301	GOL	1	0
5	B	401	GOL	1	0

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.

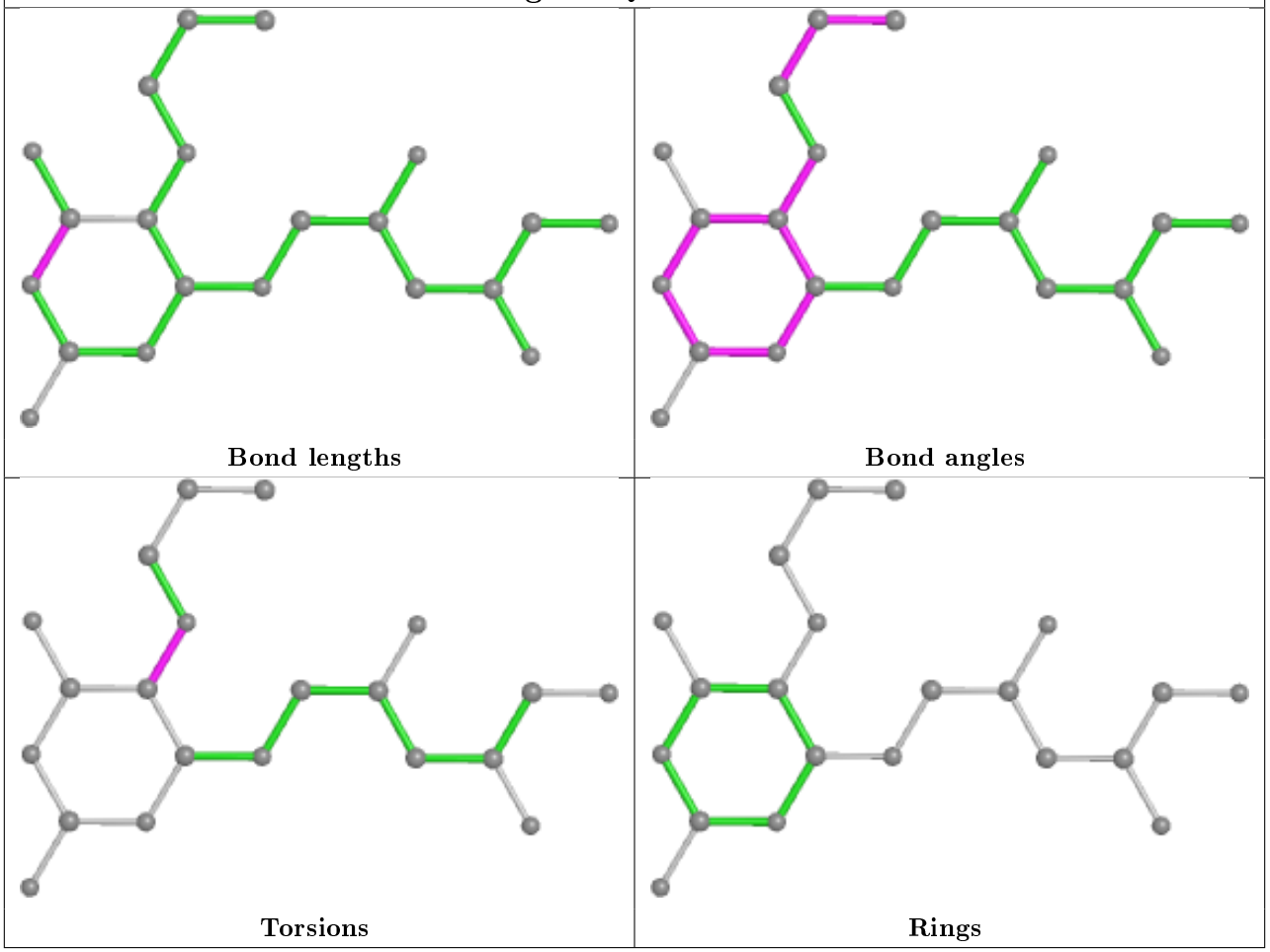
Ligand GOL G 301



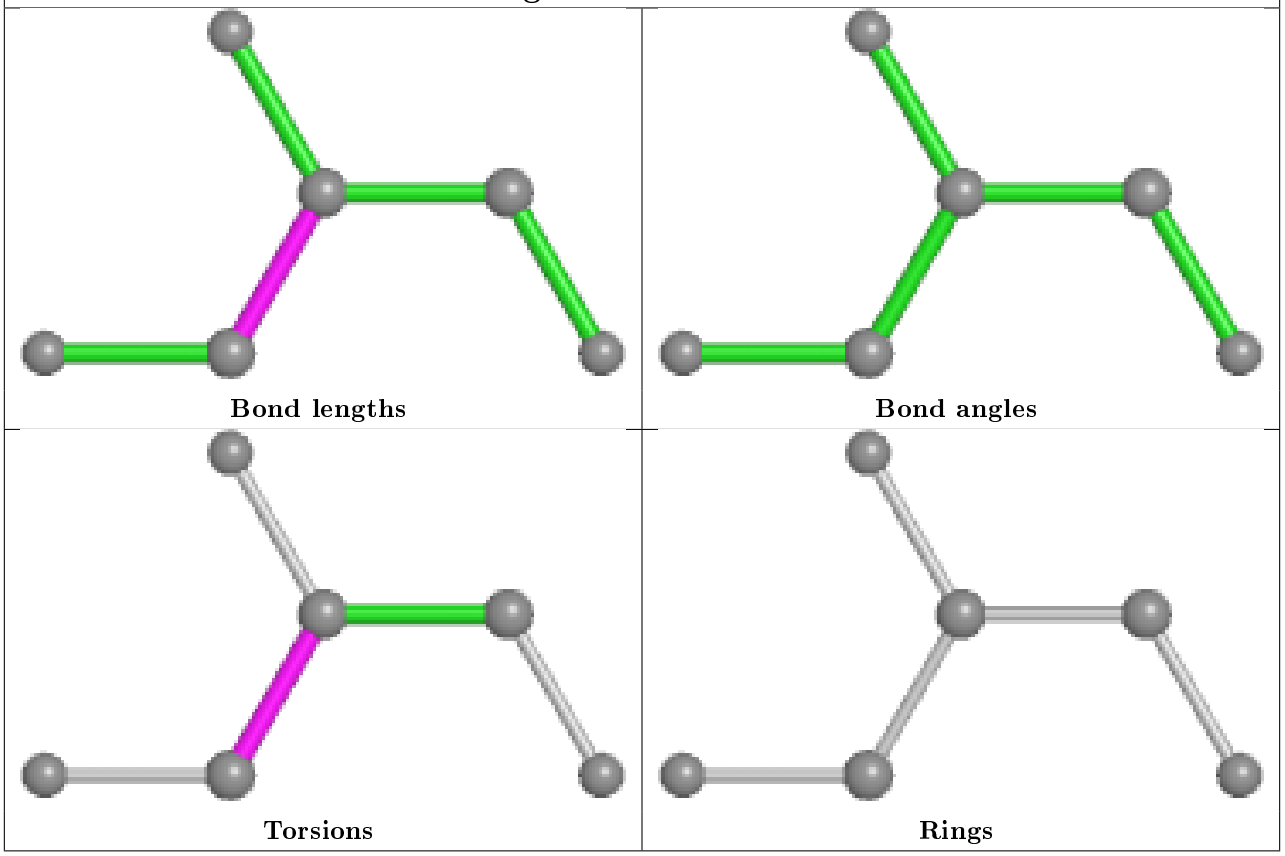
Ligand GOL A 301



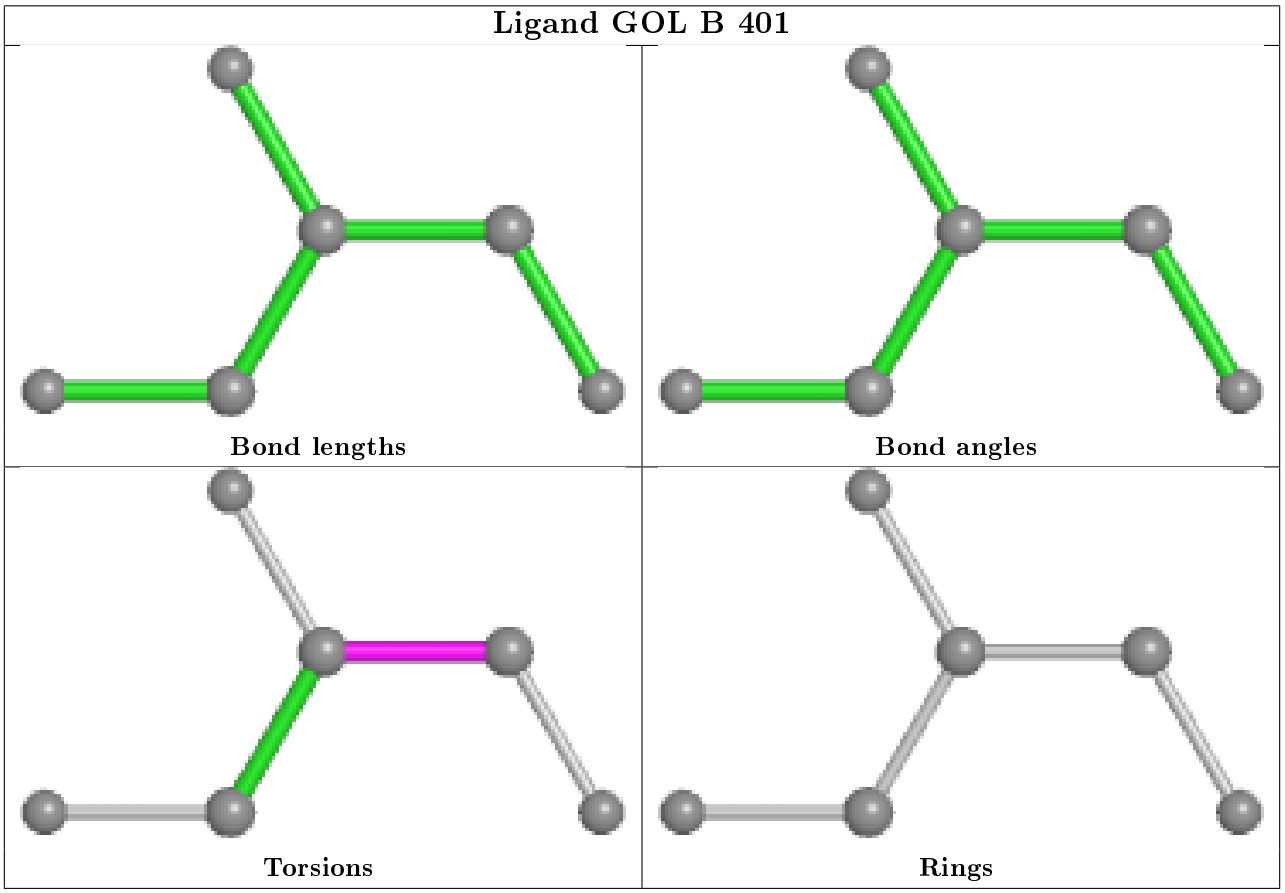
Ligand Q81 C 301



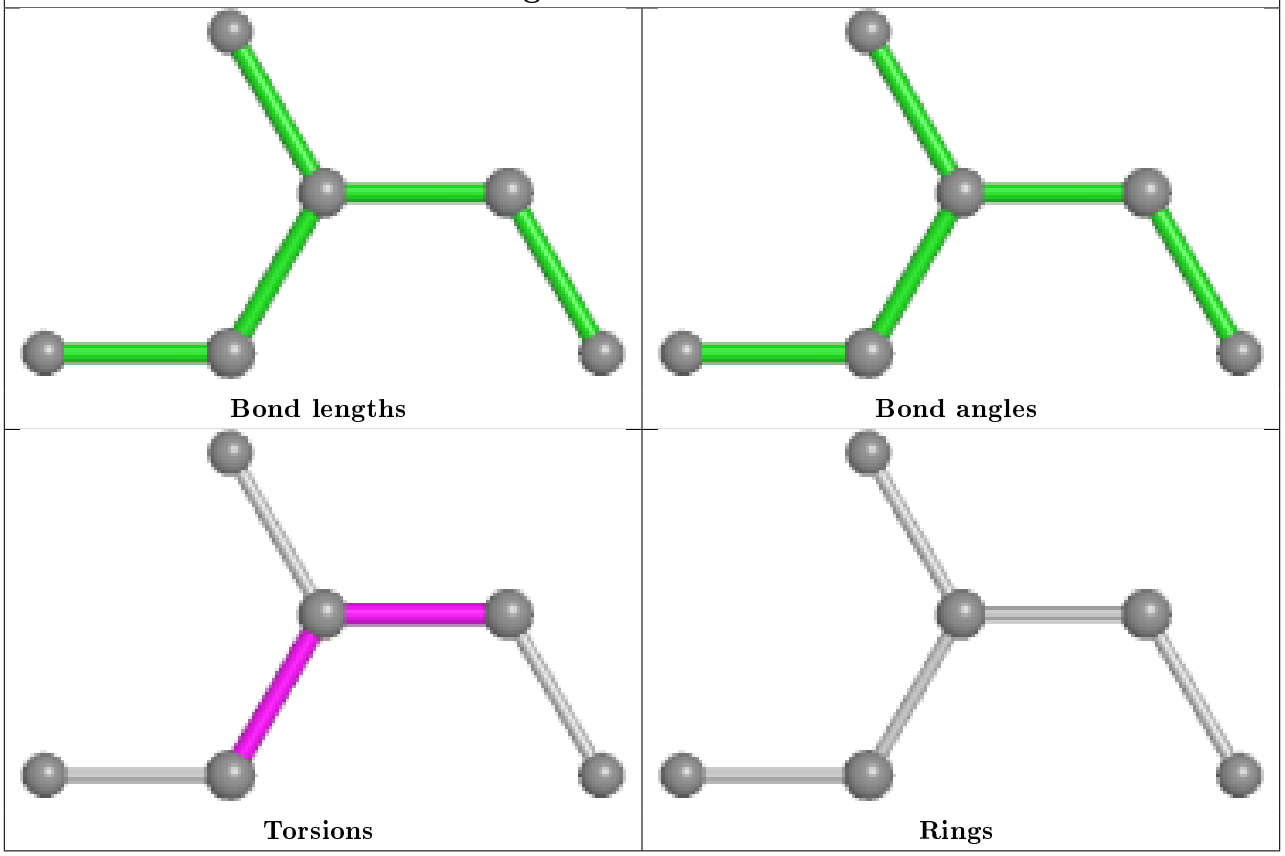
Ligand GOL A 302



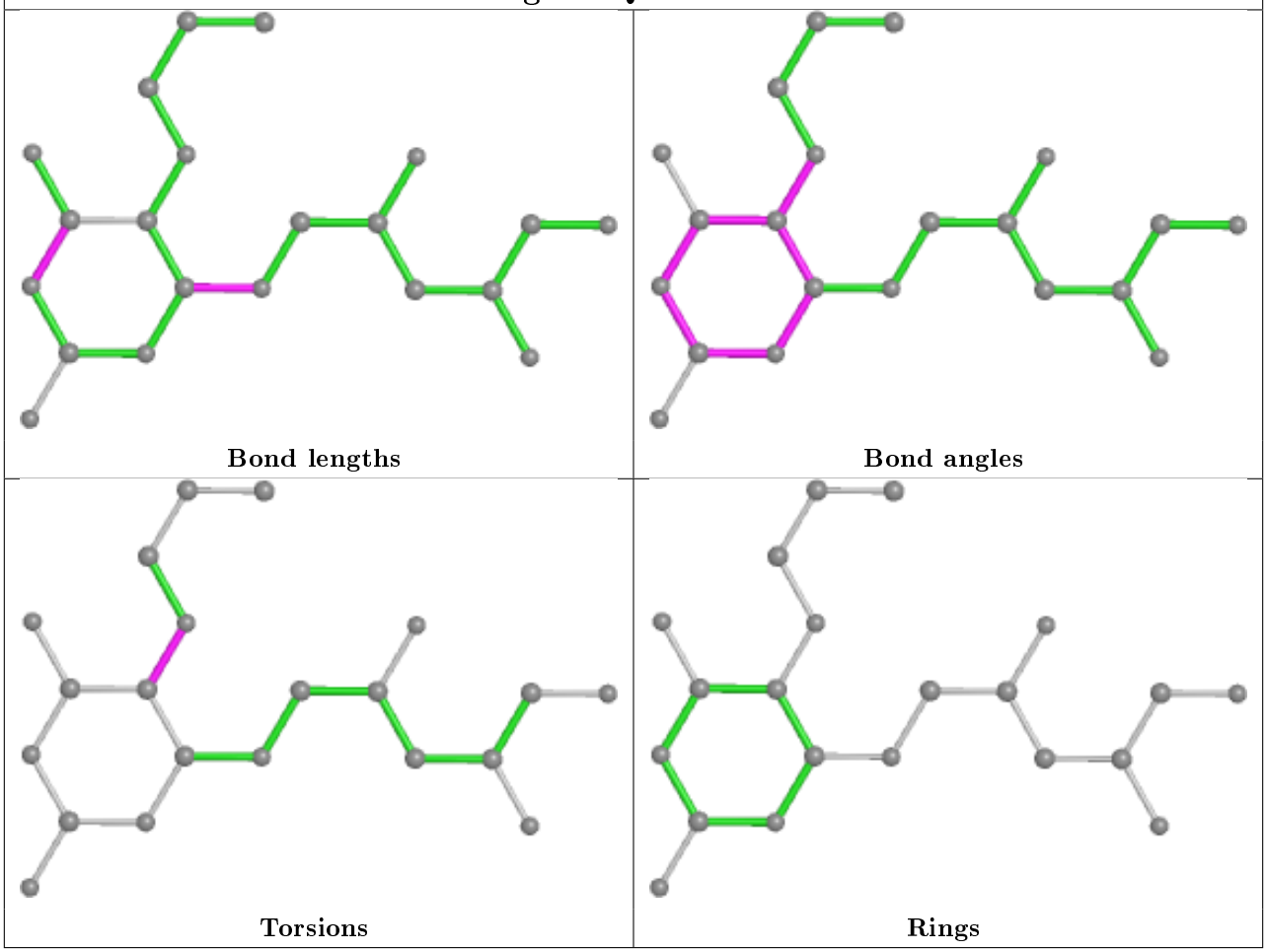
Ligand GOL B 401



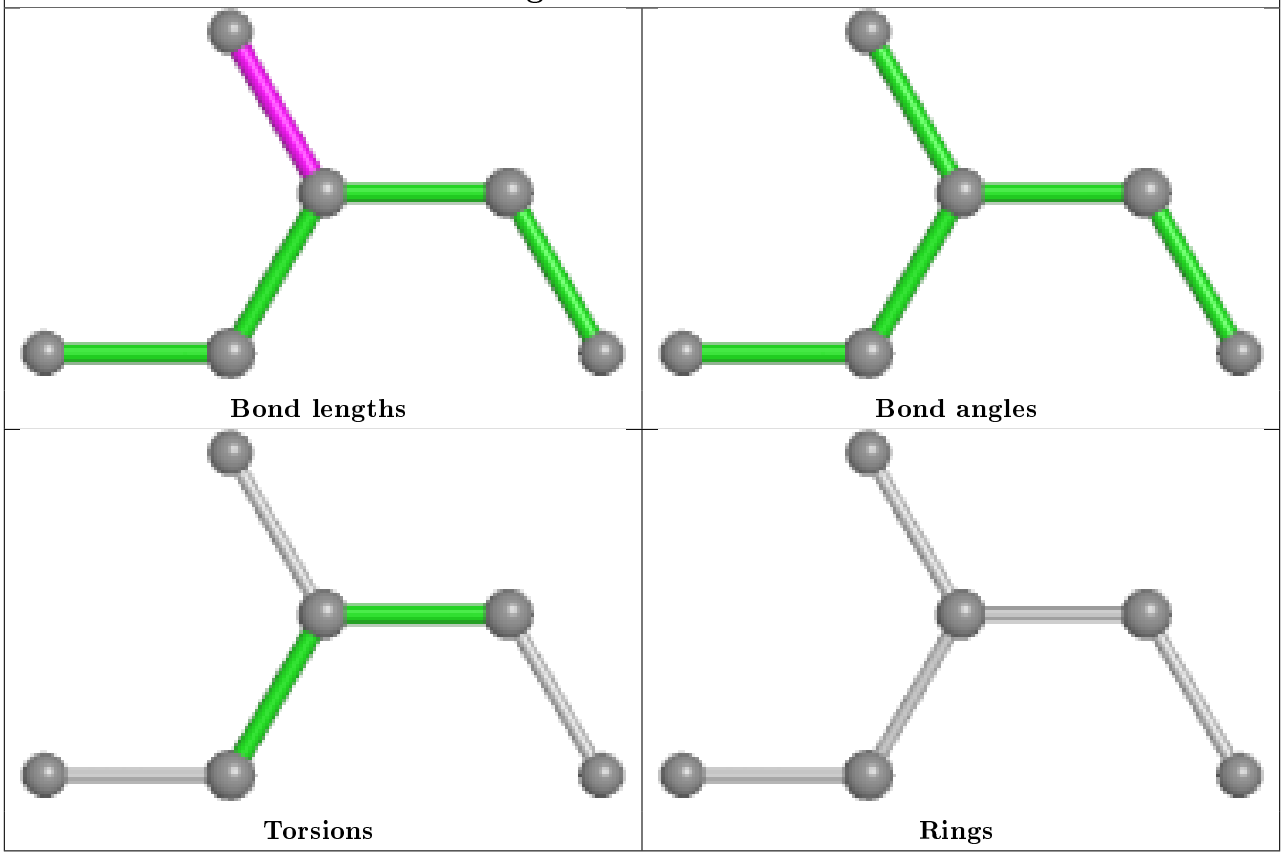
Ligand GOL D 301



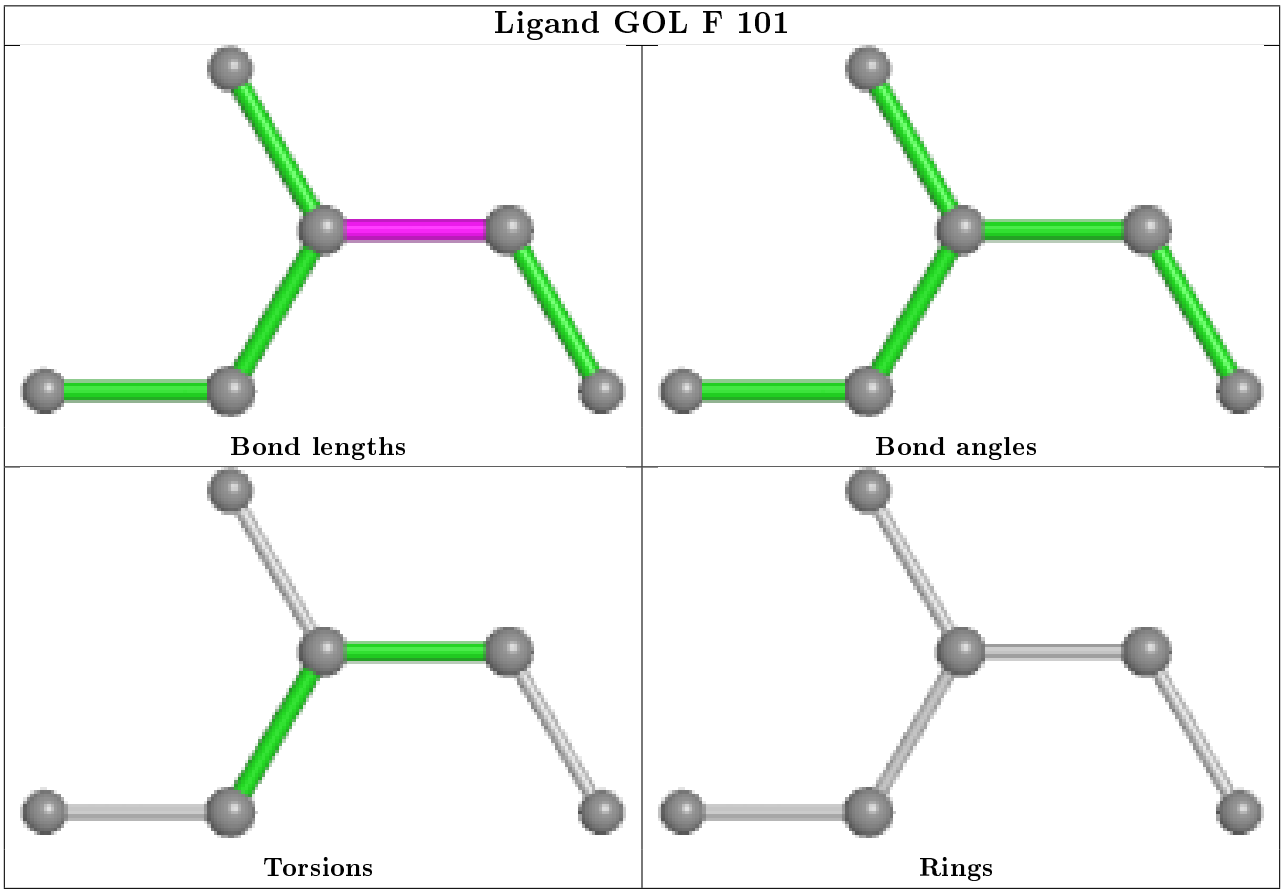
Ligand Q81 A 303



Ligand GOL F 102



Ligand GOL F 101



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	265/271 (97%)	-0.11	15 (5%) 23 21	25, 38, 73, 95	2 (0%)
1	C	267/271 (98%)	-0.14	7 (2%) 56 53	25, 34, 60, 97	4 (1%)
2	B	200/204 (98%)	-0.48	1 (0%) 91 91	23, 33, 57, 67	5 (2%)
2	D	195/204 (95%)	0.89	42 (21%) 0 0	29, 50, 94, 115	2 (1%)
3	E	241/246 (97%)	0.33	32 (13%) 3 2	32, 49, 84, 97	0
3	G	244/246 (99%)	-0.25	3 (1%) 79 79	26, 34, 50, 72	9 (3%)
4	F	100/100 (100%)	-0.29	0 100 100	28, 38, 57, 67	3 (3%)
4	H	98/100 (98%)	0.71	18 (18%) 1 1	30, 60, 86, 91	2 (2%)
All	All	1610/1642 (98%)	0.04	118 (7%) 15 13	23, 38, 80, 115	27 (1%)

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	VAL	9.1
1	A	221	ILE	6.5
2	D	197	PHE	6.5
1	C	252	ASN	5.5
1	A	223	GLN	5.4

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands (i)

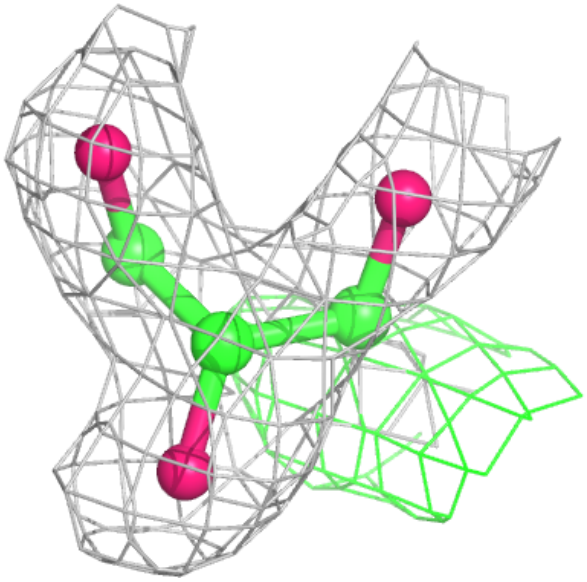
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

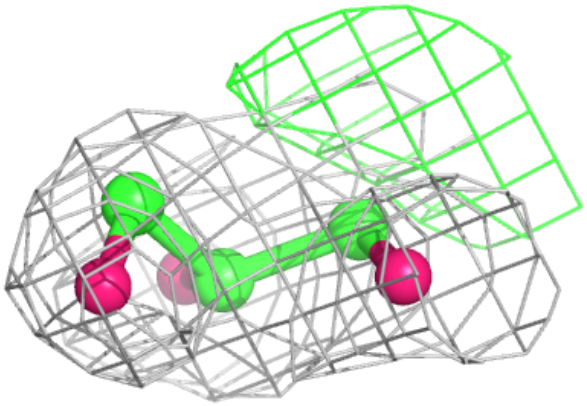
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	NA	H	501	1/1	0.80	0.22	70,70,70,70	0
5	GOL	B	401	6/6	0.82	0.15	41,52,59,63	0
5	GOL	D	301	6/6	0.84	0.13	49,57,59,64	0
8	NA	F	103	1/1	0.87	0.32	62,62,62,62	0
5	GOL	A	302	6/6	0.88	0.19	38,52,56,58	0
5	GOL	G	301	6/6	0.90	0.15	52,55,55,66	0
5	GOL	A	301	6/6	0.94	0.17	41,47,54,58	0
7	ACT	E	301	4/4	0.95	0.06	58,60,62,67	0
5	GOL	F	101	6/6	0.95	0.09	31,33,35,36	0
6	Q81	A	303	21/22	0.97	0.08	22,27,29,30	0
6	Q81	C	301	21/22	0.97	0.14	25,28,31,32	0
8	NA	F	104	1/1	0.97	0.18	46,46,46,46	0
8	NA	E	302	1/1	0.98	0.05	39,39,39,39	1
5	GOL	F	102	6/6	0.98	0.10	34,38,45,45	0
8	NA	G	302	1/1	0.99	0.08	38,38,38,38	0

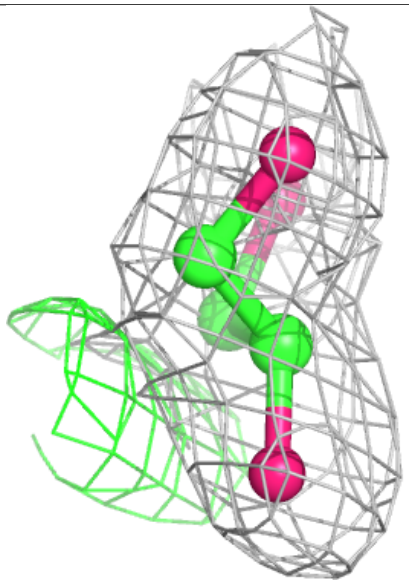
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GOL B 401:

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

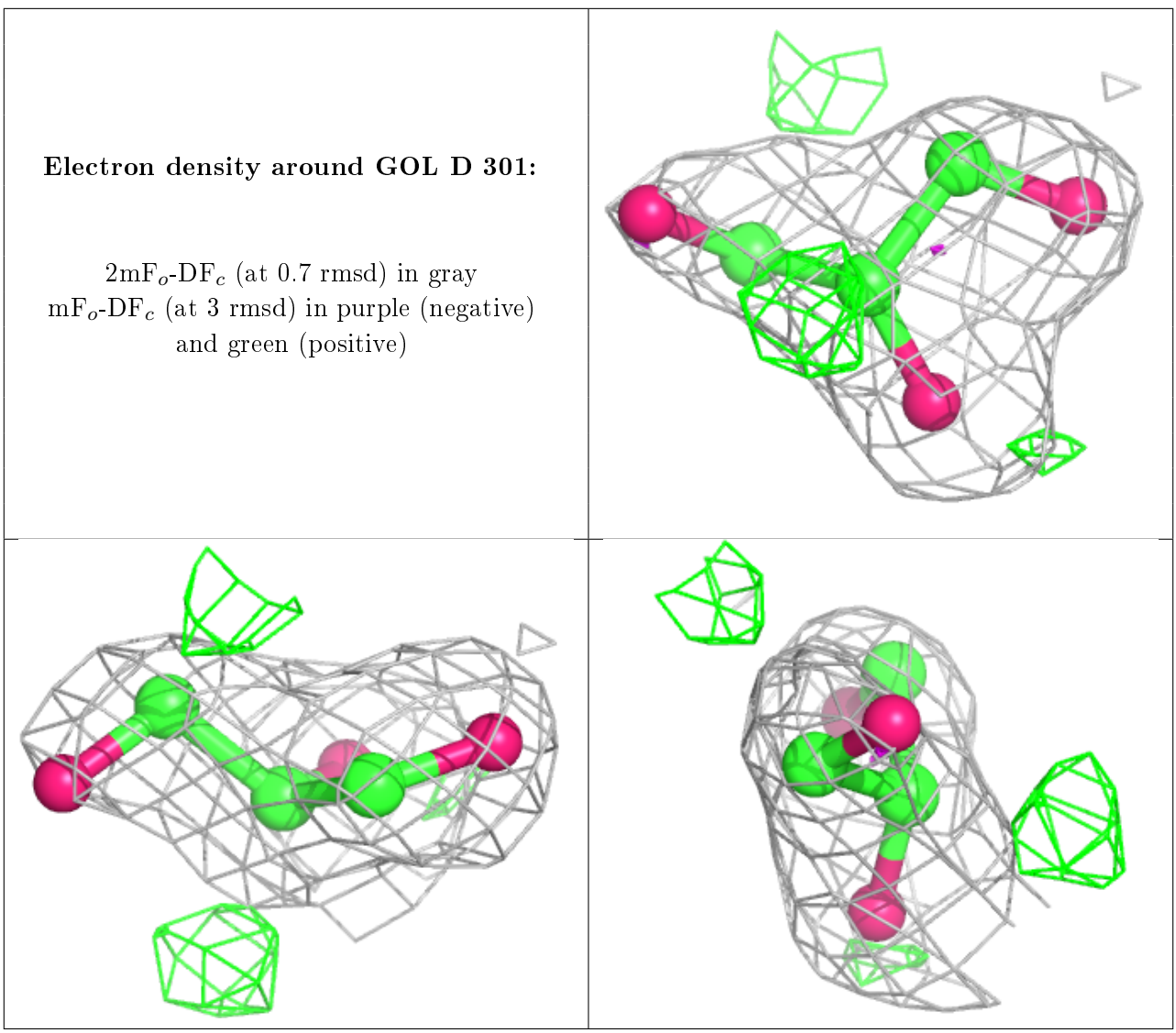






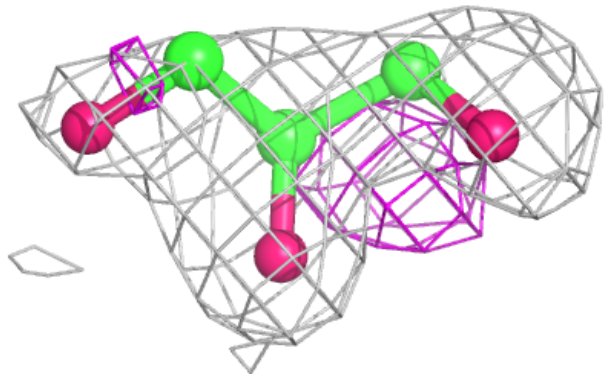
Electron density around GOL D 301:

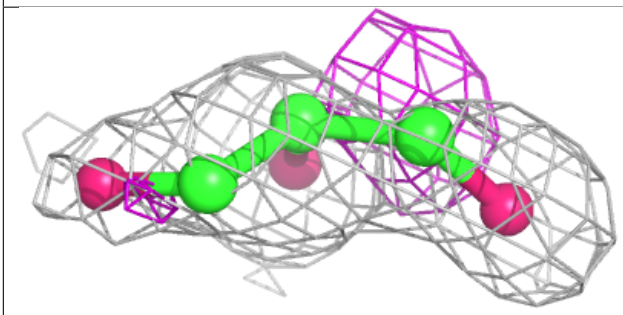
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

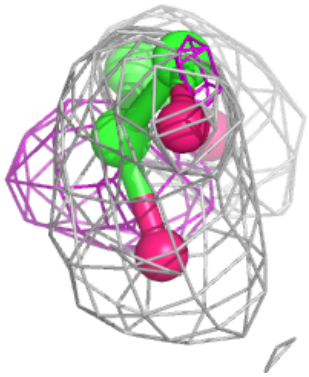


Electron density around GOL A 302:

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







Electron density around GOL G 301:

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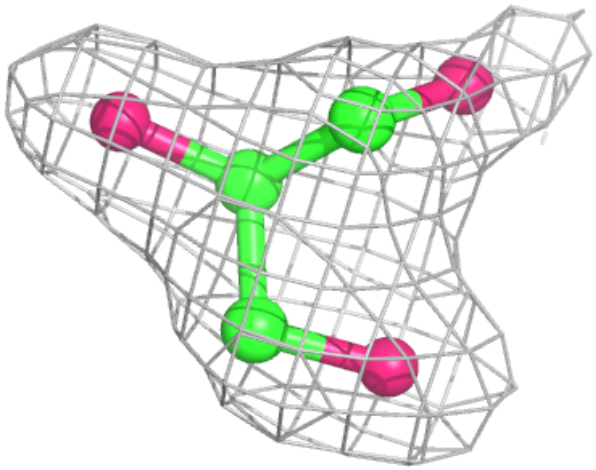
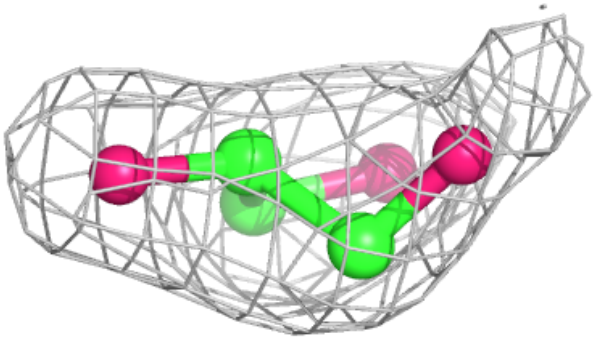
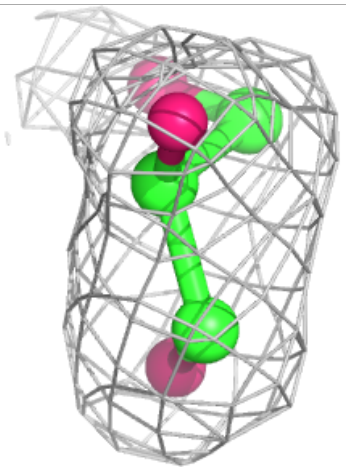
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







Electron density around GOL A 301:

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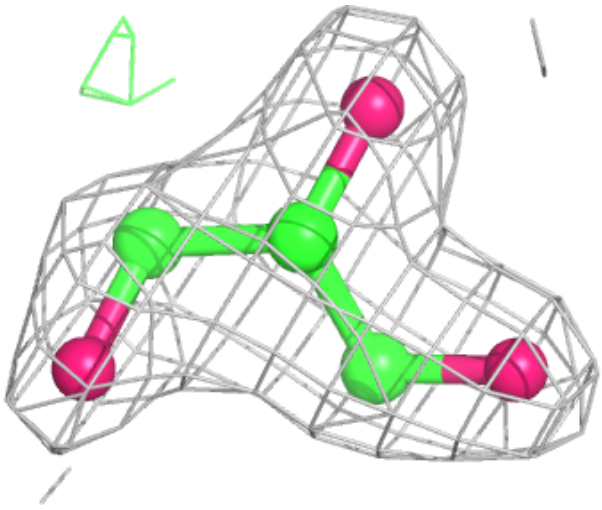
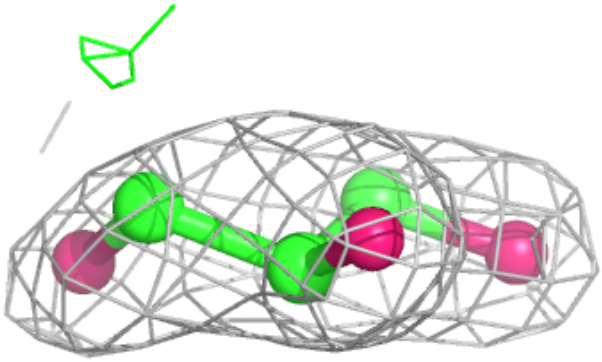
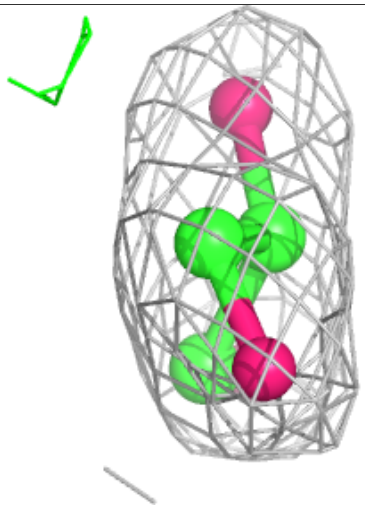
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

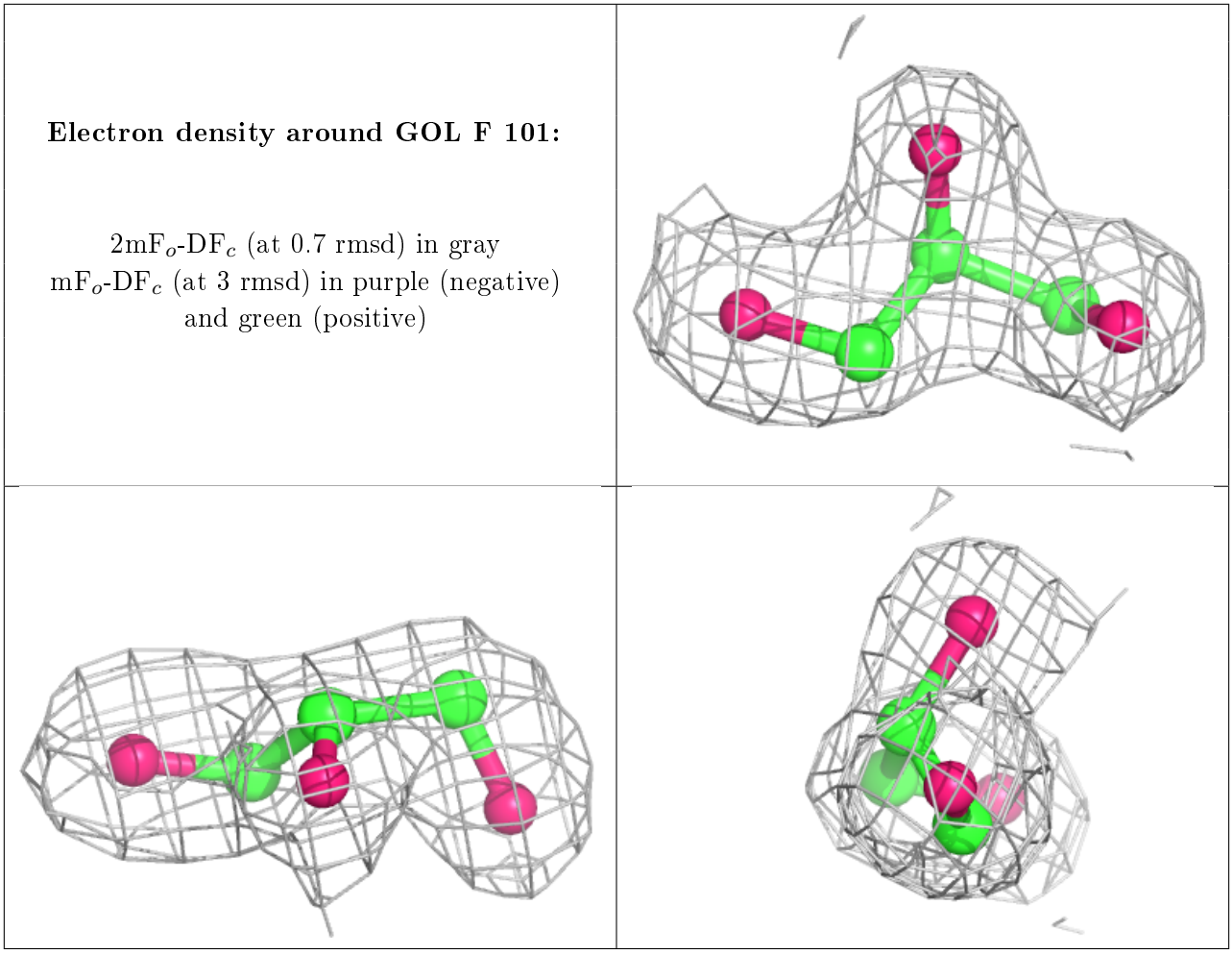






Electron density around GOL F 101:

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



Electron density around Q81 A 303:

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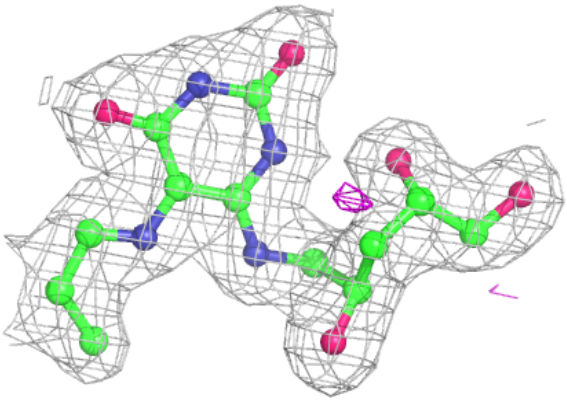
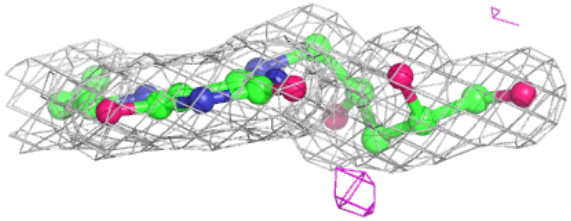
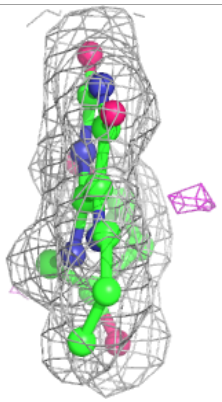
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

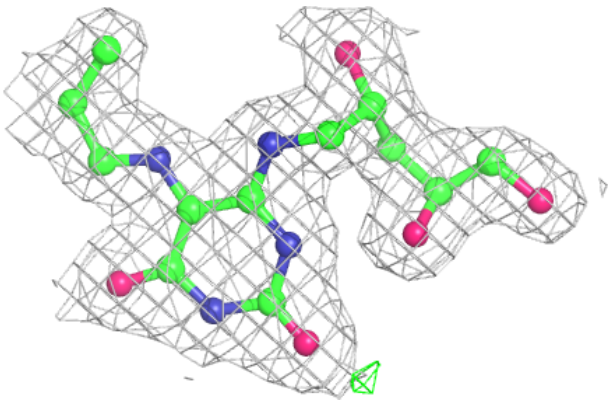


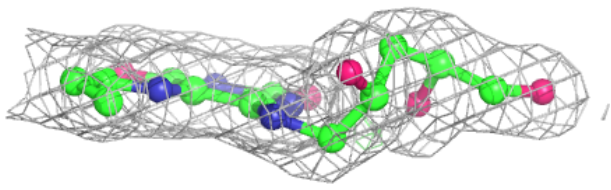


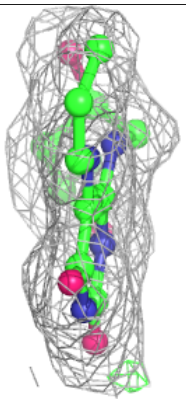


Electron density around Q81 C 301:

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







Electron density around GOL F 102:

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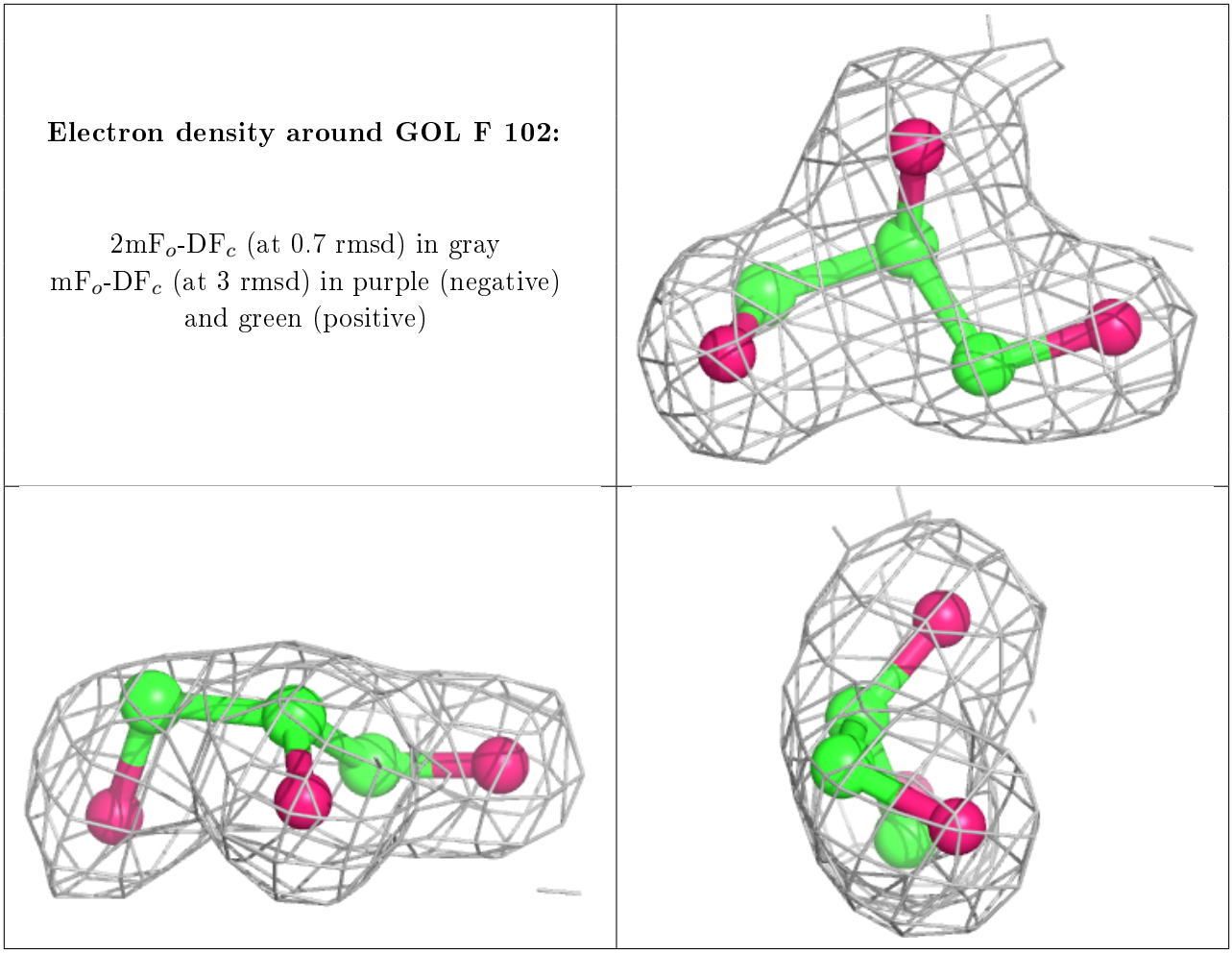
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.