Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 08:39 PM JST

PDB ID	:	7DFC
Title	:	Crystal of Arrestin2-V2Rpp-3-Fab30 complex
Authors	:	Sun, J.P.; Yu, X.; Xiao, P.; He, Q.T.; Lin, J.Y.; Zhu, Z.L.
Deposited on	:	2020-11-06
Resolution	:	2.49 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:

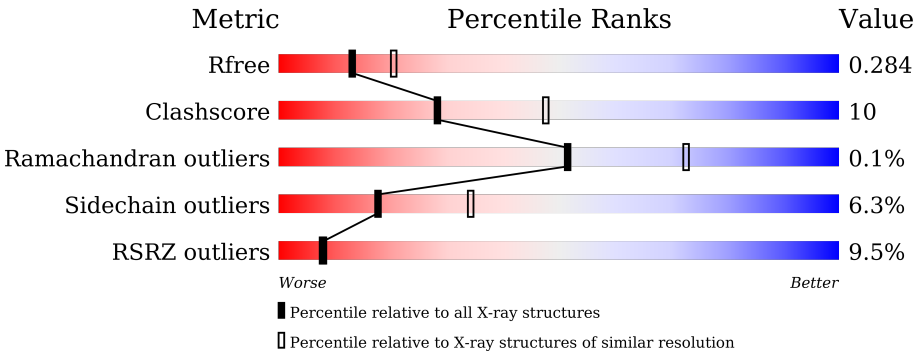
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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	426	2% 67% 16% 16%
2	V	22	5% 45% 36% 5% 14%
3	L	227	10% 69% 22% 7%
4	H	249	16% 60% 24% 16%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5978 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 Beta-arrestin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2729	1749	467	503	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	LEU	-	expression tag	UNP P17870
A	420	GLU	-	expression tag	UNP P17870
A	421	HIS	-	expression tag	UNP P17870
A	422	HIS	-	expression tag	UNP P17870
A	423	HIS	-	expression tag	UNP P17870
A	424	HIS	-	expression tag	UNP P17870
A	425	HIS	-	expression tag	UNP P17870
A	426	HIS	-	expression tag	UNP P17870

- Molecule 2 is a protein called V2Rpp-3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	V	19	Total	C	N	O	P	S	0	0	0
			146	71	19	48	7	1			

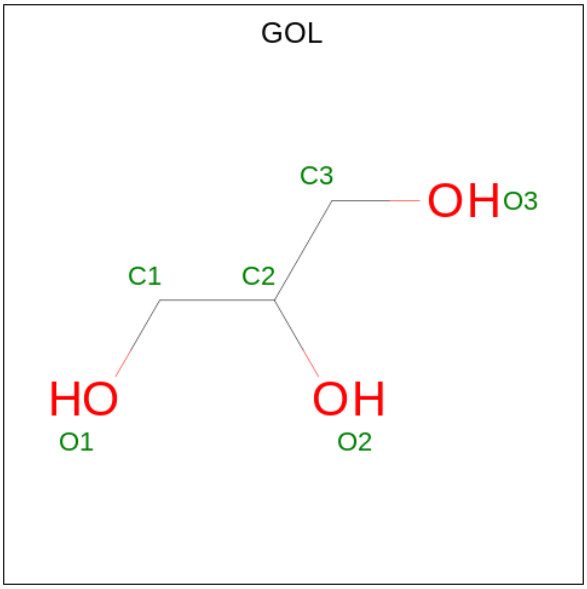
- Molecule 3 is a protein called FAB30 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1569	984	261	319	5			

- Molecule 4 is a protein called FAB30 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	210	Total	C	N	O	S	0	0	0
			1471	927	251	288	5			

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



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

- Molecule 6 is water.

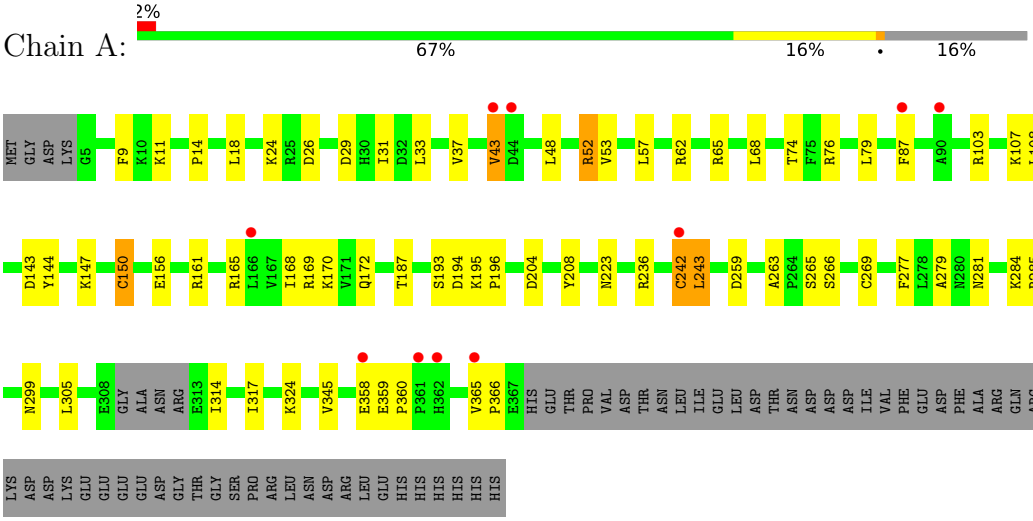
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	37	Total O 37 37	0	0
6	V	3	Total O 3 3	0	0
6	L	6	Total O 6 6	0	0
6	H	11	Total O 11 11	0	0

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.

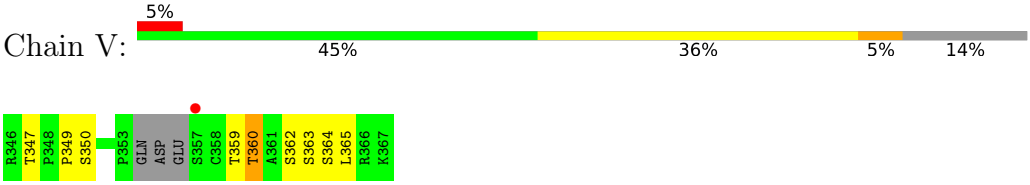
• Molecule 1: Beta-arrestin-1

Chain A:



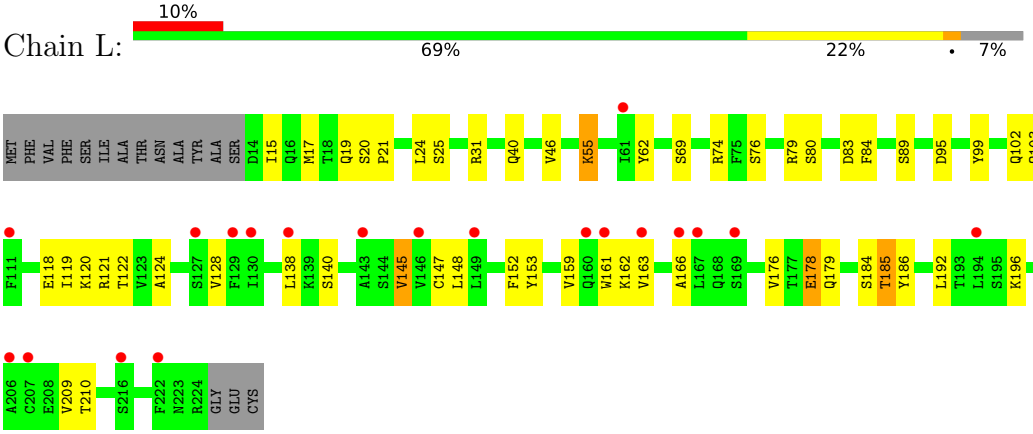
• Molecule 2: V2Rpp-3

Chain V:



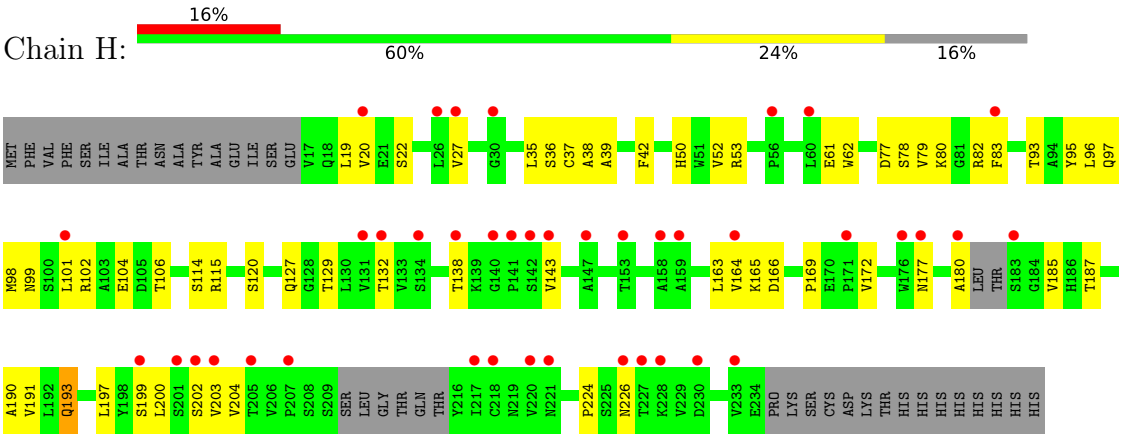
• Molecule 3: FAB30 LIGHT CHAIN

Chain L:



• Molecule 4: FAB30 HEAVY CHAIN

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	116.14Å 122.65Å 144.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.69 – 2.49 46.70 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.69-2.49) 99.6 (46.70-2.49)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.229 , 0.284 0.228 , 0.284	Depositor DCC
R_{free} test set	1892 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å^2)	60.5	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 64.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5978	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: SEP, TPO, GOL

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	0.51	0/2787	0.68	0/3795
2	V	0.35	0/70	0.58	0/88
3	L	0.45	0/1604	0.60	0/2189
4	H	0.45	0/1506	0.66	0/2062
All	All	0.48	0/5967	0.65	0/8134

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2729	0	2728	46	0
2	V	146	0	95	2	0
3	L	1569	0	1477	31	0
4	H	1471	0	1313	38	0
5	A	6	0	8	0	0
6	A	37	0	0	4	0
6	H	11	0	0	0	0
6	L	6	0	0	0	0
6	V	3	0	0	0	0
All	All	5978	0	5621	113	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 10.

All (113) 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)
4:H:79:VAL:HG11	4:H:83:PHE:CD2	2.06	0.90
1:A:242:CYS:SG	1:A:314:ILE:O	2.32	0.87
1:A:53:VAL:HG22	1:A:150:CYS:HB3	1.65	0.79
1:A:324:LYS:HG2	6:A:606:HOH:O	1.83	0.77
1:A:53:VAL:HB	1:A:87:PHE:HB3	1.66	0.77
1:A:281:ASN:OD1	1:A:284:LYS:HE2	1.86	0.76
4:H:79:VAL:HG11	4:H:83:PHE:CE2	2.21	0.74
1:A:285:ARG:HG2	6:A:620:HOH:O	1.88	0.73
3:L:128:VAL:HG21	3:L:209:VAL:HG21	1.74	0.68
4:H:190:ALA:HB2	4:H:200:LEU:HD23	1.77	0.67
4:H:169:PRO:HG2	4:H:224:PRO:HB2	1.77	0.67
4:H:97:GLN:NE2	4:H:99:ASN:OD1	2.28	0.67
4:H:98:MET:HB3	4:H:101:LEU:HD21	1.76	0.65
4:H:106:THR:HG23	4:H:132:THR:HA	1.78	0.65
1:A:76:ARG:NH2	1:A:143:ASP:OD1	2.23	0.65
4:H:187:THR:HG23	4:H:202:SER:HB2	1.77	0.64
4:H:20:VAL:HG13	4:H:38:ALA:HB3	1.82	0.62
4:H:50:HIS:HE2	4:H:114:SER:HB2	1.64	0.61
4:H:166:ASP:HA	4:H:197:LEU:HB3	1.81	0.60
3:L:19:GLN:NE2	3:L:99:TYR:O	2.26	0.60
1:A:365:VAL:HG12	1:A:366:PRO:HD3	1.85	0.59
4:H:79:VAL:CG1	4:H:83:PHE:CD2	2.83	0.59
3:L:148:LEU:HD21	4:H:203:VAL:HG21	1.85	0.58
3:L:162:LYS:HA	3:L:166:ALA:O	2.03	0.58
4:H:53:ARG:NE	4:H:61:GLU:OE2	2.23	0.58
4:H:79:VAL:HB	4:H:83:PHE:HB2	1.86	0.58
3:L:31:ARG:HG3	3:L:89:SER:HA	1.86	0.57
1:A:359:GLU:HG2	1:A:360:PRO:HD2	1.86	0.57
3:L:152:PHE:N	3:L:185:THR:OG1	2.37	0.57
4:H:185:VAL:HG22	4:H:204:VAL:HB	1.85	0.56
3:L:25:SER:HB3	3:L:120:LYS:HB2	1.88	0.56
1:A:196:PRO:O	1:A:223:ASN:HB2	2.07	0.55
1:A:193:SER:OG	1:A:195:LYS:HG2	2.07	0.55
4:H:50:HIS:HE2	4:H:114:SER:CB	2.20	0.55
4:H:193:GLN:OE1	4:H:199:SER:OG	2.25	0.54
1:A:11:LYS:NZ	2:V:360:TPO:O2P	2.24	0.54
1:A:14:PRO:HB2	1:A:161:ARG:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:159:VAL:HG22	3:L:209:VAL:HG12	1.90	0.53
4:H:143:VAL:HG12	4:H:164:VAL:HG22	1.90	0.53
3:L:105:LYS:HD3	3:L:106:TYR:CZ	2.44	0.52
4:H:36:SER:HB3	4:H:95:TYR:CE1	2.44	0.52
1:A:31:ILE:HD11	1:A:305:LEU:HB2	1.92	0.52
1:A:193:SER:OG	1:A:194:ASP:N	2.43	0.51
3:L:179:GLN:HB3	3:L:186:TYR:CE2	2.47	0.50
1:A:37:VAL:HB	1:A:117:PHE:HB2	1.93	0.49
1:A:9:PHE:HE2	1:A:24:LYS:HA	1.77	0.49
1:A:79:LEU:HD21	1:A:243:LEU:HD21	1.94	0.49
3:L:179:GLN:HB3	3:L:186:TYR:CZ	2.47	0.49
1:A:29:ASP:HB2	1:A:170:LYS:HE2	1.95	0.48
1:A:296:GLU:OE1	1:A:296:GLU:N	2.27	0.48
3:L:147:CYS:HB2	3:L:161:TRP:CZ2	2.49	0.48
1:A:195:LYS:HB2	1:A:223:ASN:HB3	1.95	0.48
1:A:204:ASP:OD1	1:A:208:TYR:OH	2.30	0.48
3:L:62:TYR:CD1	4:H:120:SER:HB3	2.49	0.47
1:A:269:CYS:SG	6:A:614:HOH:O	2.60	0.47
4:H:19:LEU:HD21	4:H:42:PHE:HZ	1.80	0.47
4:H:50:HIS:NE2	4:H:114:SER:HB2	2.28	0.47
1:A:107:LYS:HG2	1:A:108:LEU:HG	1.96	0.47
1:A:204:ASP:OD1	1:A:204:ASP:N	2.45	0.47
1:A:263:ALA:HB3	1:A:266:SER:OG	2.15	0.47
3:L:15:ILE:HG21	3:L:103:GLN:HG2	1.97	0.47
1:A:9:PHE:CE2	1:A:24:LYS:HA	2.49	0.47
4:H:165:LYS:NZ	4:H:193:GLN:OE1	2.48	0.47
1:A:144:TYR:HB2	1:A:168:ILE:O	2.15	0.46
1:A:147:LYS:HB2	6:A:617:HOH:O	2.15	0.46
1:A:26:ASP:OD2	1:A:169:ARG:NH1	2.48	0.46
3:L:138:LEU:HD23	3:L:138:LEU:HA	1.75	0.46
4:H:39:ALA:HB1	4:H:42:PHE:CZ	2.51	0.46
4:H:163:LEU:HD12	4:H:200:LEU:O	2.16	0.46
1:A:29:ASP:HB3	1:A:172:GLN:HG2	1.98	0.46
1:A:147:LYS:HG3	1:A:165:ARG:HG3	1.97	0.46
4:H:102:ARG:HB3	4:H:104:GLU:OE1	2.16	0.46
1:A:79:LEU:HD21	1:A:243:LEU:CD2	2.45	0.46
1:A:263:ALA:O	1:A:266:SER:HB2	2.16	0.46
4:H:177:ASN:CB	4:H:180:ALA:HB3	2.46	0.45
1:A:43:VAL:HG11	1:A:48:LEU:HD12	1.99	0.45
3:L:145:VAL:HG13	3:L:192:LEU:HB3	1.99	0.45
3:L:147:CYS:HB2	3:L:161:TRP:CH2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ARG:NH1	1:A:74:THR:OG1	2.51	0.44
1:A:65:ARG:HD2	1:A:68:LEU:HD11	2.00	0.44
3:L:178:GLU:H	3:L:178:GLU:CD	2.20	0.44
4:H:22:SER:O	4:H:35:LEU:HD22	2.17	0.44
1:A:129:LEU:HD21	1:A:317:ILE:HD13	1.99	0.44
3:L:121:ARG:NH2	3:L:124:ALA:HB2	2.33	0.44
3:L:121:ARG:HG3	3:L:122:THR:O	2.17	0.44
4:H:78:SER:O	4:H:82:ARG:NH1	2.48	0.43
3:L:17:MET:SD	3:L:103:GLN:HB3	2.58	0.43
1:A:187:THR:HG23	1:A:196:PRO:HB2	2.00	0.43
3:L:55:LYS:HA	3:L:55:LYS:HD2	1.64	0.43
4:H:82:ARG:HB2	4:H:99:ASN:O	2.18	0.42
1:A:169:ARG:HD3	1:A:291:GLY:O	2.20	0.42
3:L:46:VAL:HA	3:L:102:GLN:O	2.20	0.42
3:L:79:ARG:HG3	3:L:84:PHE:CE1	2.53	0.42
1:A:365:VAL:CG1	1:A:366:PRO:HD3	2.49	0.42
4:H:77:ASP:HA	4:H:80:LYS:HG3	2.00	0.42
3:L:119:ILE:HD12	3:L:184:SER:CB	2.50	0.42
3:L:119:ILE:HD12	3:L:184:SER:HA	2.02	0.42
1:A:52:ARG:HG3	1:A:87:PHE:O	2.19	0.42
4:H:52:VAL:HG22	4:H:62:TRP:HA	2.03	0.41
4:H:96:LEU:HD23	4:H:98:MET:HE2	2.01	0.41
4:H:39:ALA:HB1	4:H:42:PHE:CE1	2.55	0.41
4:H:96:LEU:HD12	4:H:96:LEU:HA	1.91	0.41
3:L:120:LYS:HA	3:L:153:TYR:OH	2.21	0.41
4:H:190:ALA:HA	4:H:200:LEU:HB3	2.03	0.41
1:A:103:ARG:HB2	2:V:365:LEU:HD21	2.02	0.41
3:L:20:SER:OG	3:L:21:PRO:HD3	2.21	0.41
3:L:74:ARG:NE	3:L:95:ASP:OD2	2.48	0.41
3:L:138:LEU:O	3:L:196:LYS:HD3	2.21	0.41
1:A:144:TYR:HB2	1:A:168:ILE:HG13	2.02	0.40
3:L:21:PRO:HB2	3:L:24:LEU:HD23	2.02	0.40
1:A:277:PHE:CE1	1:A:279:ALA:HB3	2.56	0.40
4:H:79:VAL:CG1	4:H:83:PHE:CE2	3.01	0.40
1:A:57:LEU:CD1	1:A:168:ILE:HD11	2.51	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	355/426 (83%)	332 (94%)	23 (6%)	0	100 100
2	V	8/22 (36%)	7 (88%)	0	1 (12%)	0 0
3	L	209/227 (92%)	194 (93%)	15 (7%)	0	100 100
4	H	204/249 (82%)	192 (94%)	12 (6%)	0	100 100
All	All	776/924 (84%)	725 (93%)	50 (6%)	1 (0%)	51 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	349	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	A	294/380 (77%)	280 (95%)	14 (5%)	25 48
2	V	7/13 (54%)	7 (100%)	0	100 100
3	L	173/199 (87%)	159 (92%)	14 (8%)	11 23
4	H	141/209 (68%)	130 (92%)	11 (8%)	12 24
All	All	615/801 (77%)	576 (94%)	39 (6%)	18 34

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	33	LEU
1	A	43	VAL
1	A	52	ARG
1	A	150	CYS
1	A	156	GLU
1	A	236	ARG
1	A	242	CYS
1	A	243	LEU
1	A	259	ASP
1	A	265	SER
1	A	299	ASN
1	A	345	VAL
1	A	358	GLU
3	L	40	GLN
3	L	55	LYS
3	L	69	SER
3	L	76	SER
3	L	80	SER
3	L	83	ASP
3	L	118	GLU
3	L	140	SER
3	L	145	VAL
3	L	163	VAL
3	L	176	VAL
3	L	178	GLU
3	L	185	THR
3	L	210	THR
4	H	27	VAL
4	H	37	CYS
4	H	93	THR
4	H	115	ARG
4	H	127	GLN
4	H	129	THR
4	H	138	THR
4	H	172	VAL
4	H	191	VAL
4	H	193	GLN
4	H	226	ASN

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

7 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	$\#\|Z\| > 2$
2	SEP	V	363	2	8,9,10	1.58	1 (12%)	8,12,14	1.86	2 (25%)
2	SEP	V	364	2	8,9,10	1.56	1 (12%)	8,12,14	1.02	0
2	TPO	V	347	2	8,10,11	1.08	0	10,14,16	1.67	1 (10%)
2	TPO	V	360	2	8,10,11	1.58	1 (12%)	10,14,16	1.30	1 (10%)
2	TPO	V	359	2	8,10,11	1.63	1 (12%)	10,14,16	2.22	1 (10%)
2	SEP	V	350	2	8,9,10	1.60	1 (12%)	8,12,14	1.80	2 (25%)
2	SEP	V	362	2	8,9,10	1.64	1 (12%)	8,12,14	1.13	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	V	363	2	-	2/5/8/10	-
2	SEP	V	364	2	-	0/5/8/10	-
2	TPO	V	347	2	-	4/9/11/13	-
2	TPO	V	360	2	-	1/9/11/13	-
2	TPO	V	359	2	-	4/9/11/13	-
2	SEP	V	350	2	-	5/5/8/10	-
2	SEP	V	362	2	-	0/5/8/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	362	SEP	P-O1P	3.67	1.62	1.50
2	V	359	TPO	P-O1P	3.49	1.61	1.50
2	V	364	SEP	P-O1P	3.40	1.61	1.50
2	V	363	SEP	P-O1P	3.39	1.61	1.50
2	V	360	TPO	P-O1P	3.30	1.61	1.50
2	V	350	SEP	P-O1P	3.29	1.61	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V	359	TPO	P-OG1-CB	-6.66	103.08	123.21
2	V	347	TPO	P-OG1-CB	-4.42	109.85	123.21
2	V	363	SEP	OG-CB-CA	3.88	111.92	108.14
2	V	350	SEP	OG-CB-CA	3.77	111.81	108.14
2	V	360	TPO	P-OG1-CB	-3.13	113.77	123.21
2	V	350	SEP	P-OG-CB	-3.08	109.81	118.30
2	V	363	SEP	P-OG-CB	-2.97	110.11	118.30
2	V	362	SEP	OG-CB-CA	-2.10	106.11	108.14

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	V	347	TPO	N-CA-CB-CG2
2	V	347	TPO	N-CA-CB-OG1
2	V	347	TPO	C-CA-CB-CG2
2	V	347	TPO	O-C-CA-CB
2	V	350	SEP	CB-OG-P-O2P
2	V	350	SEP	CB-OG-P-O3P
2	V	359	TPO	N-CA-CB-CG2
2	V	359	TPO	N-CA-CB-OG1
2	V	359	TPO	C-CA-CB-CG2
2	V	359	TPO	O-C-CA-CB
2	V	360	TPO	O-C-CA-CB
2	V	363	SEP	N-CA-CB-OG
2	V	350	SEP	CB-OG-P-O1P
2	V	363	SEP	CA-CB-OG-P
2	V	350	SEP	N-CA-CB-OG
2	V	350	SEP	CA-CB-OG-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	V	360	TPO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
5	GOL	A	501	-	5,5,5	1.04	0	5,5,5	0.84	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	A	501	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

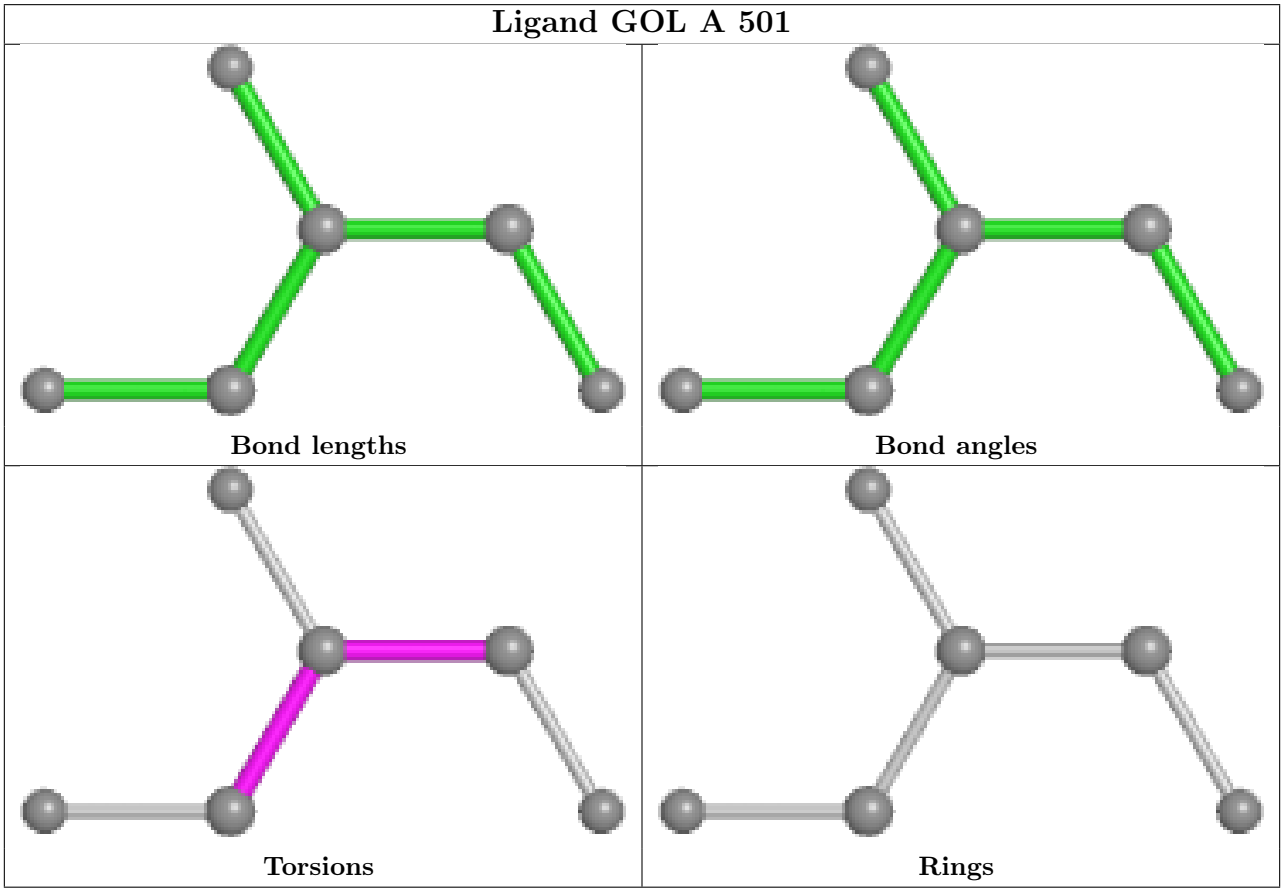
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GOL	O1-C1-C2-C3
5	A	501	GOL	C1-C2-C3-O3
5	A	501	GOL	O1-C1-C2-O2
5	A	501	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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.



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, 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	359/426 (84%)	0.42	10 (2%) 53 56	36, 72, 122, 152	0
2	V	12/22 (54%)	0.74	1 (8%) 11 11	76, 92, 129, 142	0
3	L	211/227 (92%)	0.77	23 (10%) 5 5	60, 94, 131, 142	0
4	H	210/249 (84%)	1.16	41 (19%) 1 1	53, 108, 146, 175	0
All	All	792/924 (85%)	0.71	75 (9%) 8 8	36, 88, 135, 175	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	143	VAL	5.9
4	H	230	ASP	5.6
4	H	101	LEU	5.1
4	H	176	TRP	4.9
3	L	163	VAL	4.9
4	H	217	ILE	4.3
1	A	365	VAL	4.3
4	H	177	ASN	4.2
3	L	222	PHE	4.2
4	H	153	THR	4.2
4	H	202	SER	4.1
4	H	218	CYS	4.1
1	A	90	ALA	4.0
4	H	205	THR	3.9
4	H	141	PRO	3.8
4	H	26	LEU	3.8
4	H	221	ASN	3.8
3	L	199	TYR	3.7
4	H	207	PRO	3.7
1	A	87	PHE	3.7
3	L	205	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
3	L	166	ALA	3.5
4	H	142	SER	3.5
3	L	130	ILE	3.5
4	H	83	PHE	3.5
4	H	164	VAL	3.3
1	A	43	VAL	3.2
3	L	161	TRP	3.2
4	H	203	VAL	3.2
3	L	129	PHE	3.1
3	L	146	VAL	3.1
4	H	131	VAL	3.1
4	H	158	ALA	3.1
3	L	149	LEU	3.1
3	L	143	ALA	3.0
1	A	361	PRO	2.9
4	H	147	ALA	2.9
3	L	167	LEU	2.9
1	A	44	ASP	2.9
4	H	226	ASN	2.8
4	H	27	VAL	2.8
4	H	228	LYS	2.8
4	H	159	ALA	2.7
3	L	138	LEU	2.7
3	L	204	VAL	2.7
3	L	206	ALA	2.7
4	H	30	GLY	2.6
4	H	183	SER	2.6
4	H	227	THR	2.6
4	H	199	SER	2.5
3	L	169	SER	2.5
4	H	134	SER	2.4
4	H	220	VAL	2.4
4	H	180	ALA	2.4
4	H	132	THR	2.3
1	A	242	CYS	2.3
4	H	56	PRO	2.3
3	L	160	GLN	2.3
1	A	166	LEU	2.3
4	H	138	THR	2.3
2	V	357	SER	2.3
3	L	194	LEU	2.2
1	A	358	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
3	L	207	CYS	2.2
3	L	127	SER	2.2
4	H	60	LEU	2.2
3	L	216	SER	2.1
4	H	201	SER	2.1
4	H	20	VAL	2.1
4	H	140	GLY	2.1
4	H	233	VAL	2.0
4	H	171	PRO	2.0
1	A	362	HIS	2.0
3	L	61	ILE	2.0
3	L	111	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
2	TPO	V	347	11/12	0.84	0.14	85,116,130,131	0
2	TPO	V	359	11/12	0.89	0.18	88,110,149,150	0
2	SEP	V	350	10/11	0.92	0.25	75,90,104,107	0
2	SEP	V	363	10/11	0.92	0.21	71,77,98,106	0
2	SEP	V	364	10/11	0.94	0.17	77,85,99,110	0
2	TPO	V	360	11/12	0.97	0.21	66,73,81,83	0
2	SEP	V	362	10/11	0.98	0.17	71,74,78,78	0

6.3 Carbohydrates (i)

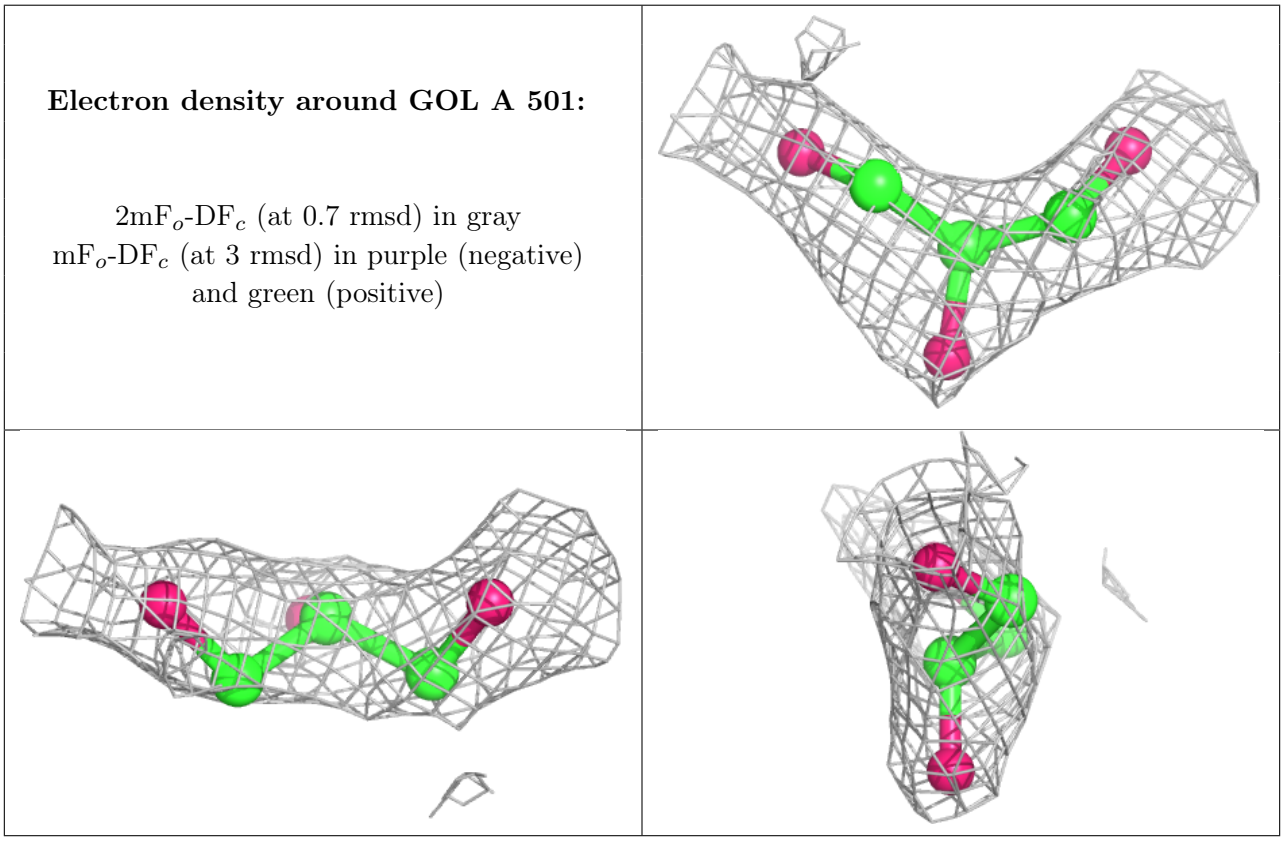
There are no monosaccharides in this entry.

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	A	501	6/6	0.76	0.36	88,90,93,93	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.



6.5 Other polymers

There are no such residues in this entry.