Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:26 PM UTC

PDB ID	:	3IVG / pdb_00003ivg
Title	:	Crystal structure of pantothenate synthetase in complex with 2-(2-((benzofuran-2-sulfonamido)methyl)-5-methoxy-1H-indol-1-yl)acetic acid
Authors	:	Silvestre, H.L.; Hung, A.W.; Wen, S.; Ciulli, A.; Blundell, T.L.; Abell, C.
Deposited on	:	2009-09-01
Resolution	:	1.95 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:

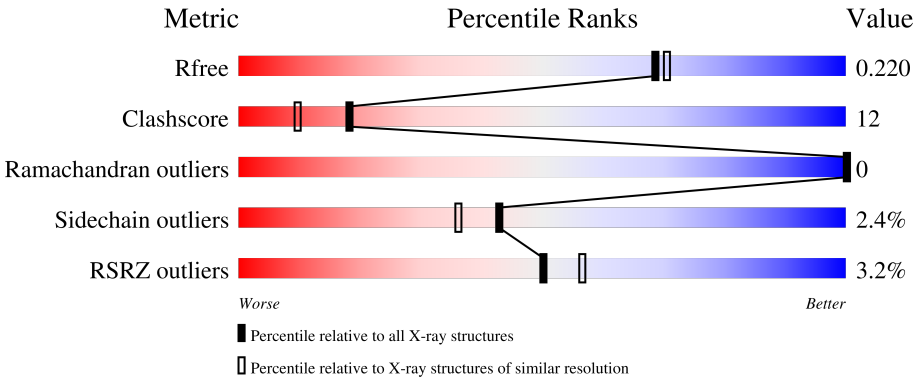
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	301	3% 77% 16% • 5%
1	B	301	3% 83% 8% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	309	-	-	X	-
2	GOL	A	310	-	-	X	-
2	GOL	B	302	-	-	X	-
3	EOH	A	304	-	-	X	-
3	EOH	B	303	-	-	X	-
3	EOH	B	304	-	-	X	-
3	EOH	B	422	-	-	X	-
5	FG5	B	305	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4705 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.

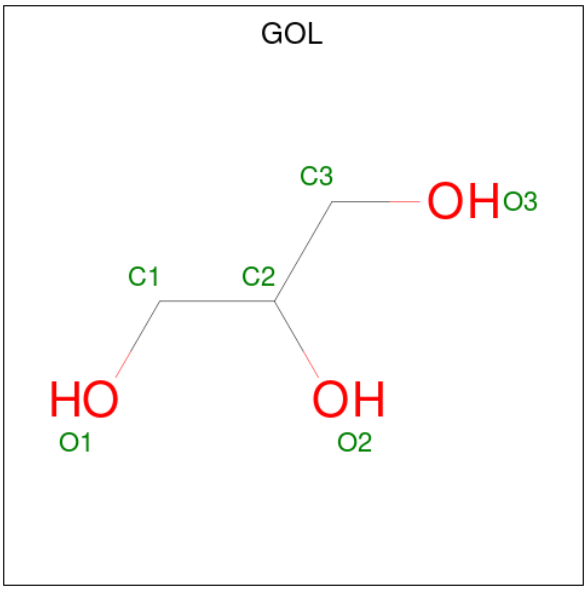
- Molecule 1 is a protein called Pantothenate synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	5	0
			2128	1348	379	395	6			
1	B	275	Total	C	N	O	S	0	6	0
			2060	1308	371	375	6			

There are 4 discrepancies between the modelled and reference sequences:

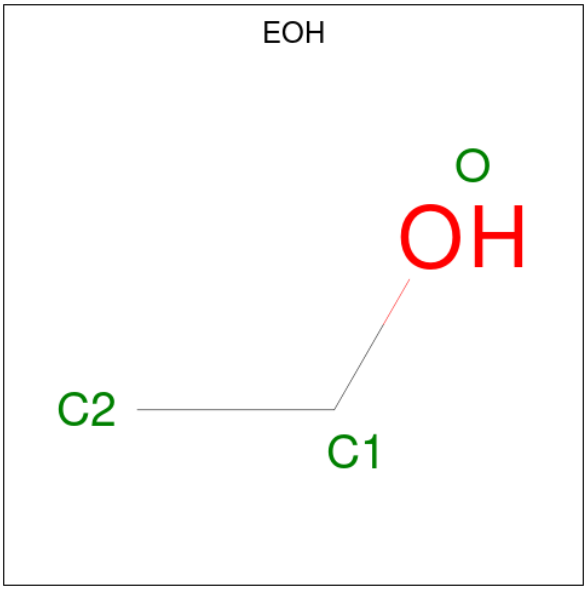
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	THR	engineered mutation	UNP P0A5R0
A	77	GLY	GLU	engineered mutation	UNP P0A5R0
B	2	ALA	THR	engineered mutation	UNP P0A5R0
B	77	GLY	GLU	engineered mutation	UNP P0A5R0

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



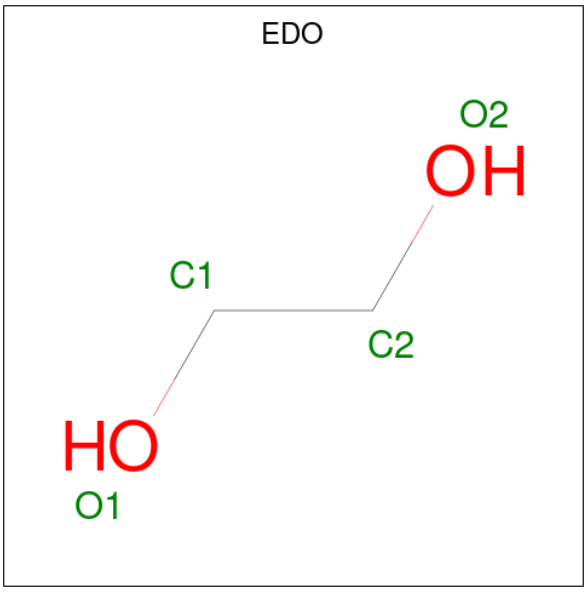
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0

- Molecule 3 is ETHANOL (CCD ID: EOH) (formula: C_2H_6O).



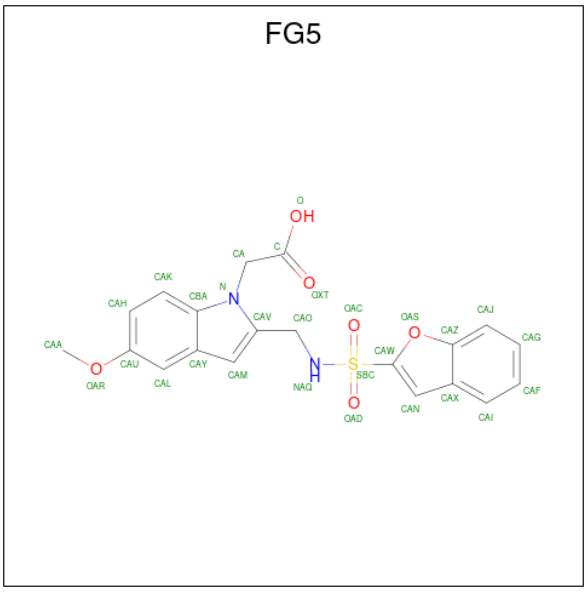
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 3 2 1	0	0
3	A	1	Total C O 3 2 1	0	0
3	A	1	Total C O 3 2 1	0	0
3	B	1	Total C O 3 2 1	0	0
3	B	1	Total C O 3 2 1	0	0
3	B	1	Total C O 3 2 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is (2-{[(1-benzofuran-2-ylsulfonyl)amino]methyl}-5-methoxy-1H-indol-1-yl)aceti c acid (CCD ID: FG5) (formula: $C_{20}H_{18}N_2O_6S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O S 29 20 2 6 1	0	0

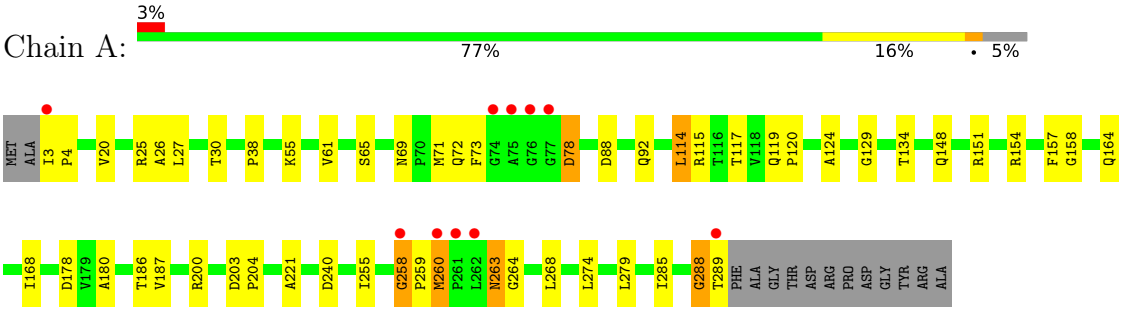
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	230	Total O 230 230	0	0
6	B	202	Total O 202 202	0	0

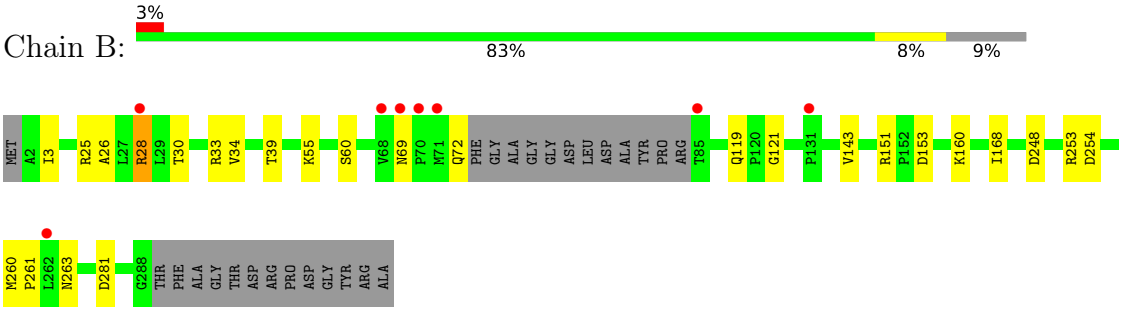
3 Residue-property plots

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: Pantothenate synthetase



• Molecule 1: Pantothenate synthetase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.33Å 70.71Å 81.85Å 90.00° 99.60° 90.00°	Depositor
Resolution (Å)	44.40 – 1.95 44.40 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.40-1.95) 99.4 (44.40-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.172 , 0.221 0.172 , 0.220	Depositor DCC
R_{free} test set	1982 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	24.4	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4705	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.21% 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: EOH, EDO, FG5, 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	1.04	1/2172 (0.0%)	1.01	3/2967 (0.1%)
1	B	0.97	0/2106	0.97	2/2875 (0.1%)
All	All	1.01	1/4278 (0.0%)	0.99	5/5842 (0.1%)

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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	GLY	N-CA	5.35	1.52	1.44

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	121	GLY	CA-C-N	8.52	128.25	119.56
1	B	121	GLY	C-N-CA	8.52	128.25	119.56
1	A	240	ASP	N-CA-C	6.37	119.03	111.71
1	A	288	GLY	CA-C-N	5.83	132.19	121.70
1	A	288	GLY	C-N-CA	5.83	132.19	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	288	GLY	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	2128	0	2168	55	0
1	B	2060	0	2134	45	0
2	A	24	0	32	15	0
2	B	6	0	8	9	0
3	A	9	0	18	3	0
3	B	9	0	18	15	0
4	A	8	0	12	0	0
5	B	29	0	17	8	0
6	A	230	0	0	4	0
6	B	202	0	0	7	0
All	All	4705	0	4407	105	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 12.

All (105) 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:B:160:LYS:HD2	3:B:303:EOH:H12	1.15	1.15
1:A:289:THR:O	1:A:289:THR:HG23	1.55	1.07
1:A:151:ARG:HH21	2:B:302:GOL:H31	1.16	1.05
1:A:186:THR:HA	2:A:309:GOL:H12	1.39	1.05
1:B:160:LYS:HD2	3:B:303:EOH:C1	1.87	1.05
1:A:263:ASN:CG	1:A:264:GLY:H	1.72	0.97
1:B:281:ASP:HA	3:B:303:EOH:H22	1.49	0.94
1:A:158:GLY:HA3	2:A:309:GOL:H32	1.52	0.91
1:B:160:LYS:CD	3:B:303:EOH:H12	2.00	0.89
1:B:28:ARG:HH21	1:B:28:ARG:HB2	1.37	0.87
1:B:248:ASP:HB3	6:B:513:HOH:O	1.75	0.87
1:A:151:ARG:HH21	2:B:302:GOL:C3	1.87	0.86
1:A:258:GLY:HA3	1:A:260:MET:HE2	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ARG:HB2	1:B:28:ARG:NH2	1.92	0.85
3:B:304:EOH:C2	6:B:336:HOH:O	2.26	0.83
1:B:260:MET:SD	1:B:261:PRO:HD2	2.19	0.82
1:A:151:ARG:NH2	2:B:302:GOL:H31	1.96	0.81
3:B:304:EOH:H22	6:B:336:HOH:O	1.82	0.79
1:B:160:LYS:O	3:B:303:EOH:H23	1.83	0.78
5:B:305:FG5:OXT	6:B:433:HOH:O	2.00	0.78
1:A:263:ASN:CG	1:A:264:GLY:N	2.42	0.76
1:A:289:THR:O	1:A:289:THR:CG2	2.30	0.75
1:B:143:VAL:HG11	1:B:168[A]:ILE:HD12	1.67	0.75
1:A:69:ASN:HD22	1:A:72:GLN:HE21	1.35	0.75
1:A:26:ALA:O	1:A:30:THR:HG23	1.87	0.74
1:B:39:THR:CA	5:B:305:FG5:HAN	2.16	0.74
1:B:281:ASP:HA	3:B:303:EOH:C2	2.18	0.73
1:B:28:ARG:HH22	1:B:34:VAL:CG2	2.02	0.72
1:B:28:ARG:HH21	1:B:28:ARG:CB	2.04	0.71
1:B:254:ASP:HB3	1:B:261:PRO:HD3	1.72	0.71
1:B:69:ASN:HB3	1:B:72:GLN:HG2	1.73	0.70
1:A:158:GLY:HA3	2:A:309:GOL:C3	2.19	0.70
1:B:39:THR:HA	5:B:305:FG5:HAN	1.73	0.68
1:A:71:MET:SD	1:A:114:LEU:HD21	2.36	0.66
1:A:158:GLY:CA	2:A:309:GOL:C3	2.73	0.66
1:B:28:ARG:NH2	1:B:34:VAL:HG23	2.11	0.66
1:A:148:GLN:HE22	2:B:302:GOL:C3	2.10	0.65
1:B:160:LYS:HD2	3:B:303:EOH:C2	2.25	0.64
1:A:158:GLY:CA	2:A:309:GOL:H32	2.28	0.64
1:B:39:THR:C	5:B:305:FG5:HAN	2.23	0.64
1:A:114:LEU:HD11	2:A:310:GOL:H11	1.80	0.64
3:B:304:EOH:H11	6:B:328:HOH:O	1.98	0.63
5:B:305:FG5:HAAC	6:B:387:HOH:O	2.00	0.61
1:B:281:ASP:CA	3:B:303:EOH:H22	2.25	0.61
1:A:27:LEU:HD13	1:A:61:VAL:HG11	1.82	0.60
1:A:186:THR:HA	2:A:309:GOL:C1	2.24	0.59
1:B:28:ARG:NH1	1:B:153:ASP:OD2	2.36	0.59
1:B:253:ARG:NE	3:B:304:EOH:O	2.36	0.59
1:A:73:PHE:HD2	1:A:78:ASP:HB3	1.70	0.57
1:B:28:ARG:NH2	1:B:34:VAL:CG2	2.66	0.57
1:A:221:ALA:HA	1:A:285:ILE:HD13	1.87	0.56
1:B:28:ARG:HG2	3:B:422:EOH:H23	1.88	0.56
1:B:160:LYS:HG2	5:B:305:FG5:HA	1.87	0.56
1:B:253:ARG:HE	3:B:304:EOH:HO	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ARG:HG2	2:B:302:GOL:O2	2.06	0.55
1:B:69:ASN:ND2	1:B:72:GLN:HB3	2.22	0.54
1:B:3:ILE:HD13	1:B:26:ALA:HB2	1.90	0.53
1:B:160:LYS:HG2	5:B:305:FG5:CA	2.39	0.52
1:A:268:LEU:HB2	1:A:285:ILE:HG13	1.92	0.52
1:A:187:VAL:H	2:A:309:GOL:C1	2.23	0.51
1:A:187:VAL:H	2:A:309:GOL:H12	1.73	0.51
1:A:151:ARG:HH21	2:B:302:GOL:C2	2.24	0.51
1:B:28:ARG:HH22	1:B:34:VAL:HG21	1.73	0.51
1:A:158:GLY:HA2	2:A:309:GOL:C3	2.41	0.50
1:A:259:PRO:HD2	1:A:260:MET:HE2	1.94	0.49
1:A:200:ARG:NH2	6:A:441:HOH:O	2.35	0.49
1:B:25:ARG:HA	3:B:422:EOH:H12	1.95	0.49
1:A:134:THR:HB	2:A:310:GOL:H2	1.94	0.49
1:A:258:GLY:HA3	1:A:260:MET:CE	2.37	0.49
1:B:69:ASN:HB3	1:B:72:GLN:CG	2.42	0.49
1:A:115:ARG:O	3:A:304:EOH:H22	2.13	0.48
1:A:3:ILE:HG22	1:A:4:PRO:O	2.14	0.48
1:A:157:PHE:CE2	1:A:168:ILE:HD13	2.50	0.47
1:A:117:THR:OG1	3:A:304:EOH:H21	2.15	0.47
1:B:28:ARG:CZ	1:B:153:ASP:OD2	2.63	0.47
1:A:3:ILE:HD11	6:A:346:HOH:O	2.15	0.47
1:B:26:ALA:O	1:B:30:THR:HG23	2.16	0.46
1:B:151:ARG:CZ	6:B:396:HOH:O	2.63	0.46
1:A:71:MET:HE3	2:A:310:GOL:O1	2.16	0.46
1:A:157:PHE:CZ	1:A:168:ILE:HD13	2.51	0.46
1:A:38:PRO:HA	1:A:65:SER:OG	2.16	0.45
1:A:148:GLN:HE22	2:B:302:GOL:H32	1.80	0.45
1:A:158:GLY:HA2	2:A:309:GOL:H31	1.97	0.45
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.76	0.45
5:B:305:FG5:HAK	5:B:305:FG5:HAA	1.83	0.45
1:A:164:GLN:OE1	2:A:302:GOL:H12	2.17	0.44
1:A:25:ARG:HD3	6:A:346:HOH:O	2.17	0.44
1:A:148:GLN:NE2	2:B:302:GOL:C3	2.80	0.44
1:B:151:ARG:HG2	2:B:302:GOL:HO2	1.82	0.44
1:A:124:ALA:O	1:A:129:GLY:HA3	2.18	0.43
1:B:151:ARG:HH11	1:B:151:ARG:HG3	1.83	0.43
1:A:274:LEU:HD13	1:A:279:LEU:HD12	2.00	0.43
1:A:178[A]:ASP:OD2	1:B:25:ARG:NH2	2.52	0.43
1:A:71:MET:CE	2:A:310:GOL:O1	2.67	0.42
1:B:33:ARG:O	1:B:60:SER:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:PRO:HB2	1:A:124:ALA:HB2	2.02	0.42
1:B:254:ASP:OD1	1:B:254:ASP:C	2.62	0.42
1:A:203:ASP:HB2	1:A:204:PRO:CD	2.50	0.42
1:A:55:LYS:HD2	6:A:477:HOH:O	2.20	0.41
1:A:73:PHE:CD2	1:A:78:ASP:HB3	2.53	0.41
1:B:28:ARG:HH12	1:B:34:VAL:HB	1.85	0.41
1:A:154:ARG:HG2	1:A:180:ALA:HB3	2.01	0.41
3:A:304:EOH:H21	1:B:119:GLN:HG2	2.03	0.41
1:B:143:VAL:HG21	1:B:168[A]:ILE:HD11	2.02	0.41
1:A:88:ASP:O	1:A:92:GLN:HG3	2.21	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	288/301 (96%)	278 (96%)	10 (4%)	0	100	100
1	B	277/301 (92%)	273 (99%)	4 (1%)	0	100	100
All	All	565/602 (94%)	551 (98%)	14 (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	215/223 (96%)	208 (97%)	7 (3%)	33	24
1	B	210/223 (94%)	207 (99%)	3 (1%)	59	56
All	All	425/446 (95%)	415 (98%)	10 (2%)	43	36

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	78	ASP
1	A	114	LEU
1	A	119	GLN
1	A	255	ILE
1	A	260	MET
1	A	263	ASN
1	B	28	ARG
1	B	55	LYS
1	B	263	ASN

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	72	GLN
1	A	119	GLN
1	A	148	GLN
1	A	170	GLN
1	A	222	HIS
1	B	119	GLN
1	B	148	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

14 ligands 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	EOH	B	304	-	2,2,2	0.48	0	1,1,1	0.23	0
2	GOL	A	310	-	5,5,5	0.34	0	5,5,5	0.95	0
5	FG5	B	305	-	29,32,32	4.14	15 (51%)	40,47,47	2.47	15 (37%)
3	EOH	B	422	-	2,2,2	0.57	0	1,1,1	0.14	0
2	GOL	A	302	-	5,5,5	0.49	0	5,5,5	0.68	0
3	EOH	A	305	-	2,2,2	0.53	0	1,1,1	0.22	0
4	EDO	A	307	-	3,3,3	0.27	0	2,2,2	0.79	0
4	EDO	A	308	-	3,3,3	0.21	0	2,2,2	0.99	0
2	GOL	B	302	-	5,5,5	0.46	0	5,5,5	0.96	0
2	GOL	A	303	-	5,5,5	0.47	0	5,5,5	0.47	0
2	GOL	A	309	-	5,5,5	0.91	0	5,5,5	1.40	1 (20%)
3	EOH	A	306	-	2,2,2	0.49	0	1,1,1	0.37	0
3	EOH	B	303	-	2,2,2	0.59	0	1,1,1	0.15	0
3	EOH	A	304	-	2,2,2	0.48	0	1,1,1	0.13	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
2	GOL	A	310	-	-	1/4/4/4	-
5	FG5	B	305	-	-	12/17/18/18	0/4/4/4
4	EDO	A	307	-	-	1/1/1/1	-
2	GOL	A	302	-	-	2/4/4/4	-
4	EDO	A	308	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	302	-	-	4/4/4/4	-
2	GOL	A	303	-	-	3/4/4/4	-
2	GOL	A	309	-	-	2/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	305	FG5	SBC-NAQ	13.02	1.81	1.61
5	B	305	FG5	CAO-CAV	9.37	1.55	1.49
5	B	305	FG5	OAD-SBC	7.55	1.54	1.43
5	B	305	FG5	OAC-SBC	7.30	1.54	1.43
5	B	305	FG5	CAI-CAX	-3.98	1.34	1.41
5	B	305	FG5	CBA-N	-3.85	1.32	1.39
5	B	305	FG5	CAY-CBA	-3.84	1.35	1.41
5	B	305	FG5	CAX-CAN	-3.55	1.33	1.44
5	B	305	FG5	CAL-CAY	-3.38	1.35	1.40
5	B	305	FG5	CAX-CAZ	-3.15	1.34	1.39
5	B	305	FG5	CAY-CAM	-3.12	1.34	1.44
5	B	305	FG5	CAJ-CAZ	-3.00	1.33	1.39
5	B	305	FG5	CAK-CBA	-2.89	1.35	1.39
5	B	305	FG5	CA-N	2.70	1.51	1.46
5	B	305	FG5	CAV-N	-2.15	1.34	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	305	FG5	OAD-SBC-NAQ	8.09	114.97	107.41
5	B	305	FG5	CA-N-CBA	-5.22	117.20	125.18
5	B	305	FG5	OAD-SBC-OAC	-4.70	111.20	119.82
5	B	305	FG5	CAO-NAQ-SBC	-4.33	110.70	119.78
5	B	305	FG5	CBA-N-CAV	-4.01	106.62	111.11
5	B	305	FG5	CAM-CAV-N	3.27	110.95	108.87
5	B	305	FG5	CAI-CAX-CAZ	3.26	122.80	118.59
5	B	305	FG5	CAK-CAH-CAU	-3.24	116.03	119.73
5	B	305	FG5	CAY-CAM-CAV	-2.88	105.03	108.41
5	B	305	FG5	OAS-CAZ-CAJ	2.52	131.80	126.49
5	B	305	FG5	C-CA-N	2.51	119.58	113.08
5	B	305	FG5	CAG-CAF-CAI	-2.48	117.18	120.24
2	A	309	GOL	C3-C2-C1	-2.31	103.32	111.80
5	B	305	FG5	CAJ-CAZ-CAX	-2.27	120.41	123.81
5	B	305	FG5	CAO-CAV-N	-2.16	120.65	122.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	305	FG5	CBA-CAY-CAM	2.09	109.12	107.05

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	309	GOL	C1-C2-C3-O3
5	B	305	FG5	C-CA-N-CBA
5	B	305	FG5	CAN-CAW-SBC-NAQ
5	B	305	FG5	OAS-CAW-SBC-OAC
5	B	305	FG5	OAS-CAW-SBC-OAD
5	B	305	FG5	CAO-NAQ-SBC-OAC
5	B	305	FG5	CAO-NAQ-SBC-CAW
2	B	302	GOL	O1-C1-C2-O2
2	A	302	GOL	O1-C1-C2-C3
2	A	303	GOL	O1-C1-C2-C3
2	A	303	GOL	C1-C2-C3-O3
2	B	302	GOL	O1-C1-C2-C3
2	B	302	GOL	C1-C2-C3-O3
2	A	309	GOL	O2-C2-C3-O3
4	A	307	EDO	O1-C1-C2-O2
2	A	302	GOL	O1-C1-C2-O2
5	B	305	FG5	C-CA-N-CAV
2	A	310	GOL	O2-C2-C3-O3
2	A	303	GOL	O2-C2-C3-O3
2	B	302	GOL	O2-C2-C3-O3
5	B	305	FG5	CAV-CAO-NAQ-SBC
5	B	305	FG5	NAQ-CAO-CAV-N
5	B	305	FG5	CAN-CAW-SBC-OAD
4	A	308	EDO	O1-C1-C2-O2
5	B	305	FG5	CAO-NAQ-SBC-OAD
5	B	305	FG5	CAN-CAW-SBC-OAC

There are no ring outliers.

9 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	304	EOH	5	0
2	A	310	GOL	4	0
5	B	305	FG5	8	0
3	B	422	EOH	2	0

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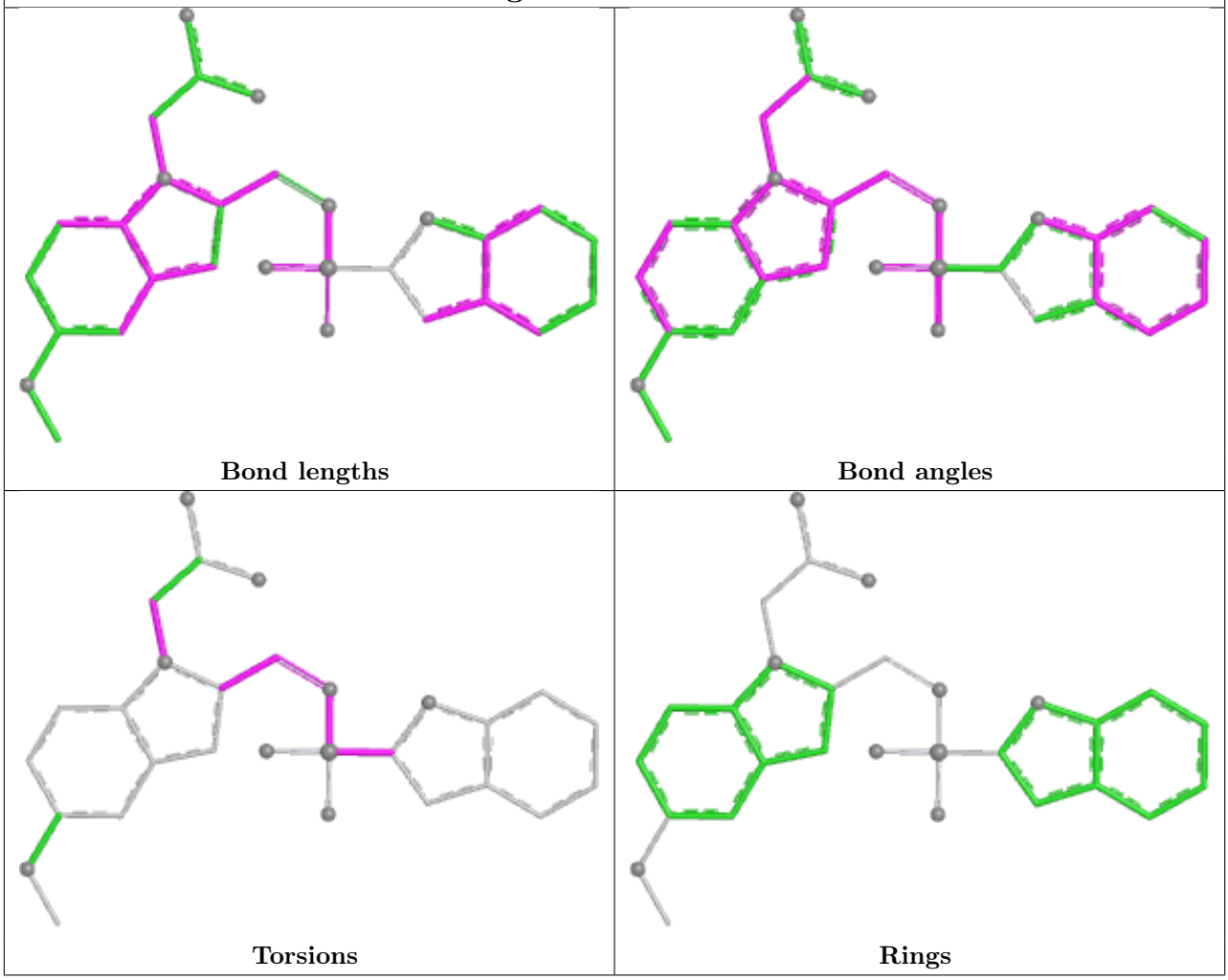
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	GOL	1	0
2	B	302	GOL	9	0
2	A	309	GOL	10	0
3	B	303	EOH	8	0
3	A	304	EOH	3	0

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 FG5 B 305



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	287/301 (95%)	-0.11	10 (3%) 47 53	13, 22, 41, 49	7 (2%)
1	B	275/301 (91%)	-0.00	8 (2%) 53 60	8, 25, 49, 73	7 (2%)
All	All	562/602 (93%)	-0.06	18 (3%) 50 56	8, 24, 45, 73	14 (2%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	69	ASN	4.6
1	A	258	GLY	4.1
1	A	75	ALA	3.9
1	A	76	GLY	3.8
1	B	131	PRO	3.8
1	A	289	THR	3.8
1	B	71	MET	3.7
1	B	70	PRO	3.7
1	A	74	GLY	3.3
1	A	260	MET	2.7
1	B	85	THR	2.7
1	B	68	VAL	2.6
1	B	262	LEU	2.5
1	A	262	LEU	2.5
1	A	77	GLY	2.3
1	A	261	PRO	2.2
1	B	28	ARG	2.2
1	A	3	ILE	2.0

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 (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

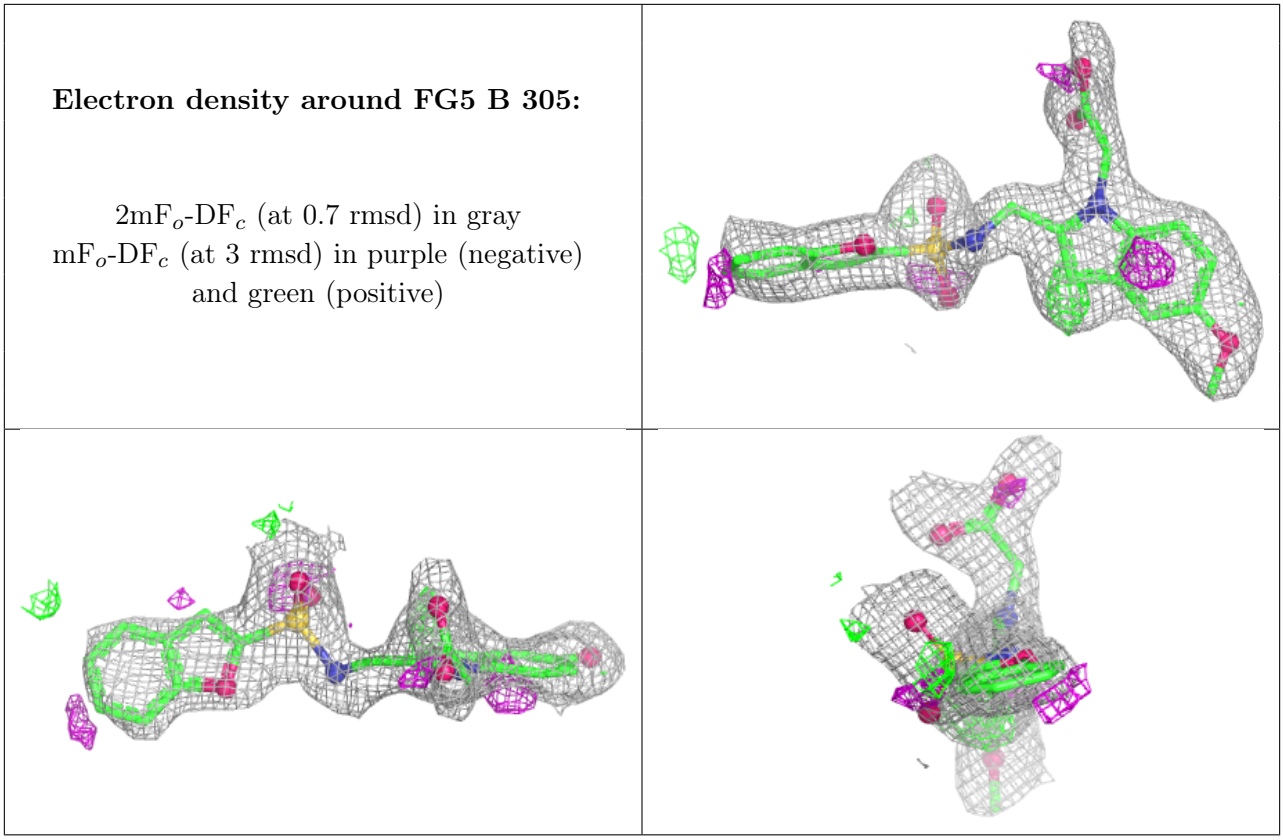
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	EOH	B	422	3/3	0.59	0.30	44,44,45,45	0
3	EOH	B	303	3/3	0.79	0.34	38,38,39,39	0
3	EOH	B	304	3/3	0.81	0.19	58,58,58,59	0
5	FG5	B	305	29/29	0.82	0.13	42,46,56,57	0
2	GOL	A	310	6/6	0.83	0.12	43,47,48,51	0
2	GOL	A	309	6/6	0.85	0.22	35,36,39,39	0
3	EOH	A	305	3/3	0.85	0.14	32,32,33,35	0
3	EOH	A	304	3/3	0.86	0.14	31,31,38,38	0
2	GOL	B	302	6/6	0.86	0.15	56,57,58,58	0
2	GOL	A	303	6/6	0.89	0.12	32,36,40,49	0
4	EDO	A	307	4/4	0.90	0.12	44,44,45,48	0
3	EOH	A	306	3/3	0.90	0.12	42,42,42,43	0
2	GOL	A	302	6/6	0.94	0.08	33,38,40,42	0
4	EDO	A	308	4/4	0.96	0.09	21,24,25,27	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 FG5 B 305:

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



6.5 Other polymers (i)

There are no such residues in this entry.