Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 03:17 AM EDT

PDB ID	:	6BPO
Title	:	The crystal structure of the Ferric-Catecholate import receptor Fiu from K12 E. coli: Closed form (P1)
Authors	:	Grinter, R.
Deposited on	:	2017-11-23
Resolution	:	2.90 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:

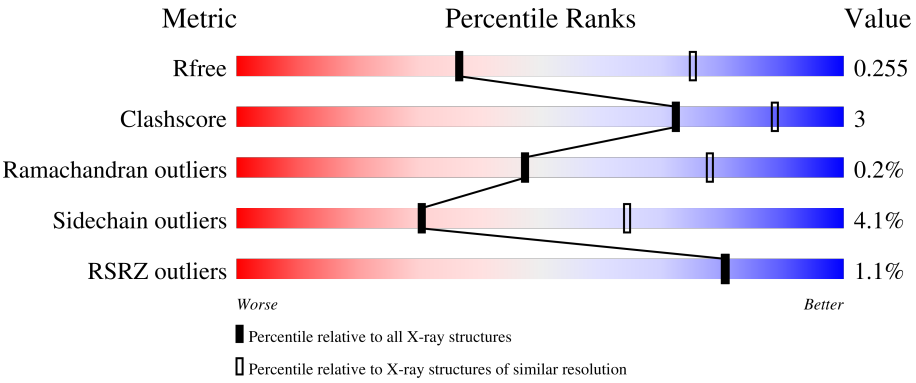
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	727	86% 11%
1	B	727	85% 12%
1	C	727	86% 11%
1	D	727	87% 10%

2 Entry composition

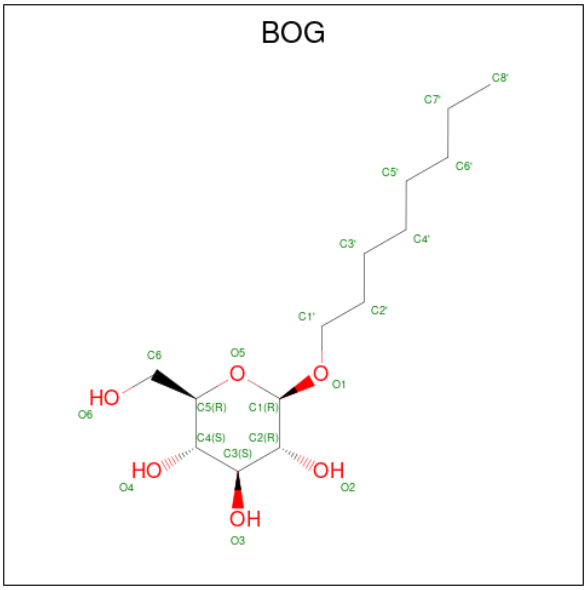
There are 3 unique types of molecules in this entry. The entry contains 22034 atoms, of which 56 are hydrogens and 0 are deuteriums.

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 Catecholate siderophore receptor Fiu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	711	Total	C	N	O	S	0	1	0
			5417	3348	955	1102	12			
1	B	711	Total	C	N	O	S	0	1	0
			5421	3351	957	1101	12			
1	C	711	Total	C	N	O	S	0	2	0
			5427	3354	958	1103	12			
1	D	711	Total	C	N	O	S	0	1	0
			5417	3348	955	1102	12			

- Molecule 2 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			48	14	28	6		
2	B	1	Total	C	H	O	0	0
			48	14	28	6		

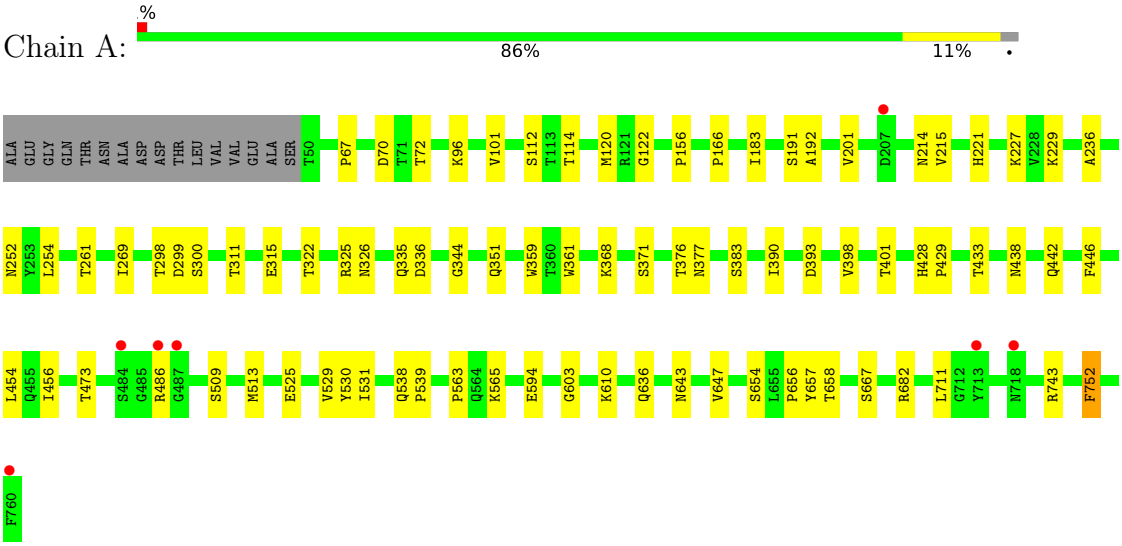
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	73	Total O 73 73	0	0
3	B	58	Total O 58 58	0	0
3	C	58	Total O 58 58	0	0
3	D	67	Total O 67 67	0	0

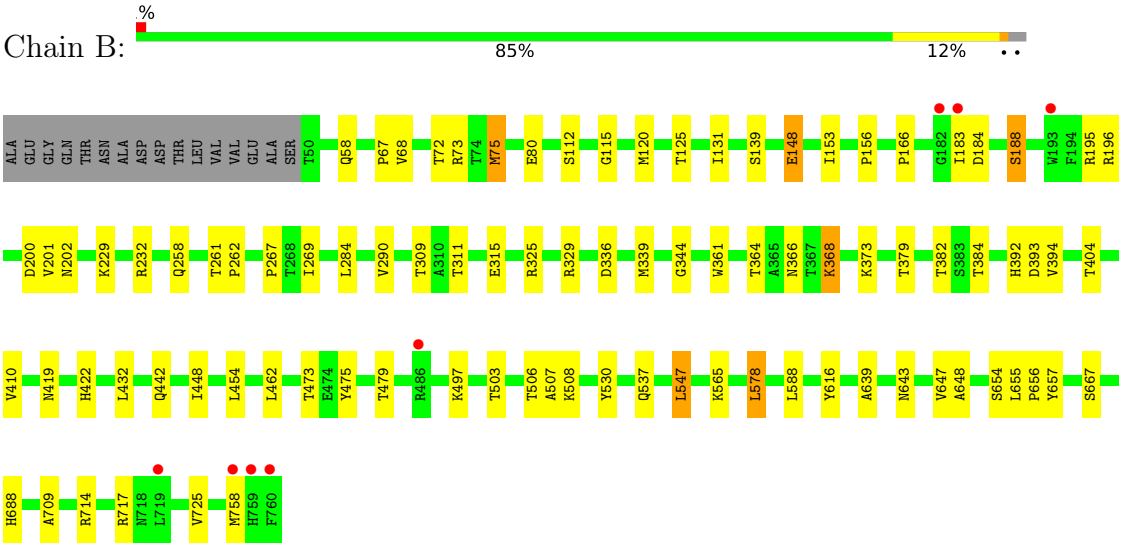
3 Residue-property plots (i)

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.

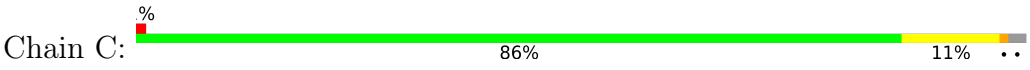
• Molecule 1: Catecholate siderophore receptor Fiu

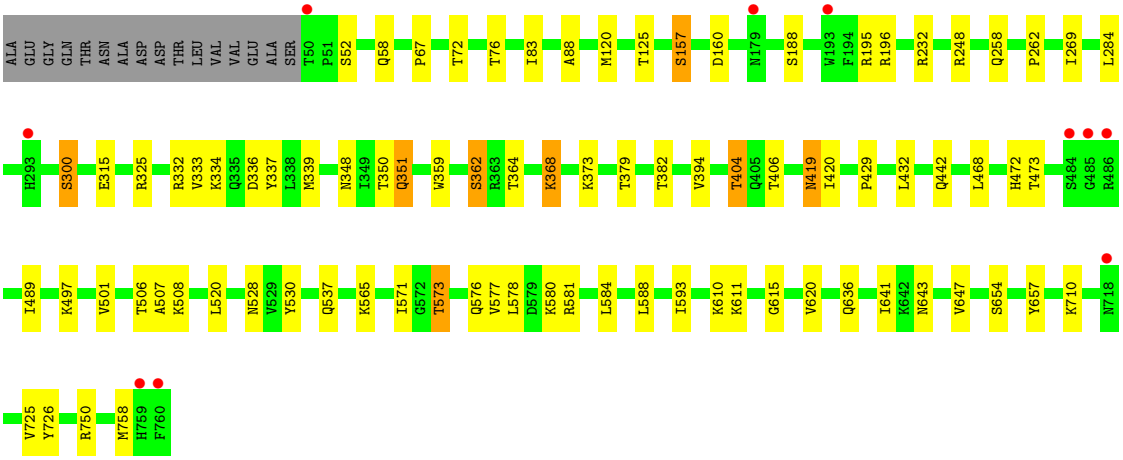


• Molecule 1: Catecholate siderophore receptor Fiu



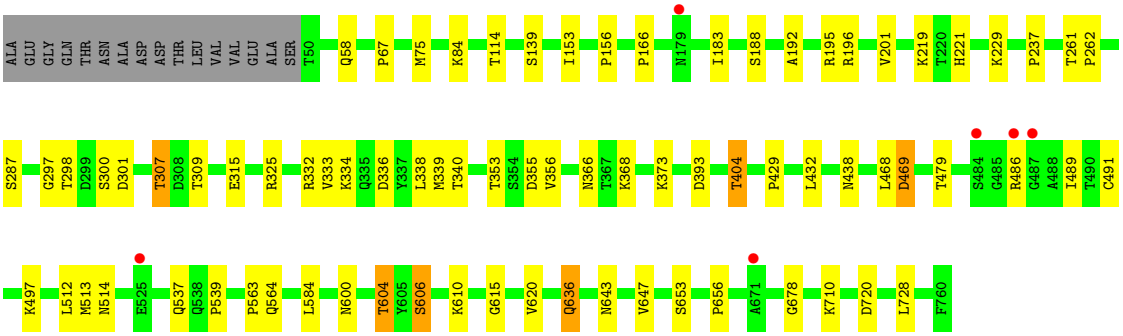
• Molecule 1: Catecholate siderophore receptor Fiu





• Molecule 1: Catecholate siderophore receptor Fiu

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	81.67Å 133.16Å 135.10Å 101.50° 107.42° 92.88°	Depositor
Resolution (Å)	29.23 – 2.90 29.21 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.23-2.90) 99.0 (29.21-2.90)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 2.90Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.197 , 0.238 0.215 , 0.255	Depositor DCC
R_{free} test set	5866 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	47.9	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 43.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	22034	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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: BOG

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	0.41	0/5533	0.66	0/7536
1	B	0.42	0/5538	0.67	0/7543
1	C	0.42	0/5544	0.67	0/7551
1	D	0.41	0/5533	0.68	0/7536
All	All	0.42	0/22148	0.67	0/30166

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	5417	0	5147	33	0
1	B	5421	0	5149	40	0
1	C	5427	0	5153	37	0
1	D	5417	0	5147	33	0
2	A	20	28	28	0	0
2	B	20	28	28	0	0
3	A	73	0	0	1	0
3	B	58	0	0	2	0
3	C	58	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	67	0	0	0	0
All	All	21978	56	20652	143	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 3.

All (143) 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:D:300:SER:HB2	1:D:429:PRO:HD2	1.71	0.71
1:A:298:THR:HG22	1:A:300:SER:H	1.56	0.70
1:D:307:THR:HB	1:D:333:VAL:HG22	1.79	0.64
1:C:332:ARG:HD3	1:C:334:LYS:HG3	1.80	0.63
1:D:336:ASP:HA	1:D:368:LYS:O	1.99	0.62
1:D:353:THR:HG22	1:D:355:ASP:H	1.67	0.60
1:C:188:SER:HB2	1:C:196:ARG:HB3	1.82	0.60
1:C:373:LYS:HB2	1:C:404:THR:HG23	1.83	0.60
1:B:184:ASP:HB2	1:B:200:ASP:HB3	1.84	0.59
1:A:183:ILE:HG23	1:A:201:VAL:HG22	1.85	0.58
1:A:326:ASN:HD21	1:A:377:ASN:HD21	1.50	0.58
1:A:390:ILE:HD12	1:A:456:ILE:HA	1.87	0.57
1:D:156:PRO:HG3	1:D:166:PRO:HA	1.87	0.57
1:B:112:SER:HB2	1:B:366:ASN:HD22	1.71	0.56
1:C:157:SER:HB3	1:C:160:ASP:HB2	1.87	0.56
1:C:52:SER:HA	1:C:581:ARG:HH21	1.71	0.56
1:A:122:GLY:HA2	1:A:658:THR:OG1	2.06	0.56
1:A:96:LYS:HB3	1:A:682:ARG:HD3	1.87	0.55
1:A:191:SER:HG	1:A:752:PHE:HD1	1.54	0.55
1:B:336:ASP:HA	1:B:368:LYS:O	2.08	0.54
1:B:229:LYS:H	1:B:261:THR:HB	1.72	0.54
1:D:262:PRO:HB2	1:D:339:MET:HG2	1.88	0.54
1:A:538:GLN:HE21	1:A:539:PRO:HD2	1.72	0.53
1:D:584:LEU:HD23	1:D:620:VAL:HG12	1.91	0.53
1:D:229:LYS:H	1:D:261:THR:HB	1.73	0.53
1:C:576:GLN:HB3	1:C:580:LYS:HG3	1.90	0.53
1:C:610:LYS:HB2	1:C:643:ASN:HB2	1.90	0.53
1:A:67:PRO:HD2	1:A:70:ASP:HB2	1.91	0.52
1:D:615:GLY:HA3	1:D:636:GLN:O	2.10	0.52
1:D:315:GLU:HG2	1:D:325:ARG:HG2	1.92	0.52
1:D:339:MET:HB2	1:D:366:ASN:HB2	1.91	0.52
1:B:183:ILE:HG12	1:B:201:VAL:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:THR:HG21	1:A:429:PRO:CD	2.40	0.51
1:B:639:ALA:HB1	1:B:655:LEU:HD12	1.93	0.50
1:A:315:GLU:HG2	1:A:325:ARG:HG2	1.92	0.50
1:D:373:LYS:HB2	1:D:404:THR:HG23	1.93	0.50
1:C:584:LEU:HD23	1:C:620:VAL:HG12	1.93	0.50
1:A:112:SER:HB3	1:A:743:ARG:HH22	1.77	0.50
1:D:75:MET:HE2	1:D:153:ILE:HG12	1.93	0.50
1:C:419:ASN:HD22	1:C:420:ILE:N	2.10	0.49
1:A:156:PRO:HG3	1:A:166:PRO:HA	1.92	0.49
1:A:336:ASP:HA	1:A:368:LYS:O	2.11	0.49
1:A:398:VAL:HG13	1:A:446:PHE:HE1	1.77	0.49
1:B:262:PRO:HB2	1:B:339:MET:HG3	1.94	0.49
1:B:714:ARG:HH21	1:B:717:ARG:HA	1.77	0.49
1:A:335:GLN:HG3	3:A:902:HOH:O	2.12	0.49
1:B:410:VAL:HG21	1:B:432:LEU:HD22	1.94	0.49
1:C:348:ASN:HB3	1:C:362:SER:HB3	1.94	0.49
1:D:600:ASN:HD21	1:D:606:SER:HB2	1.77	0.49
1:B:131:ILE:HB	1:B:329:ARG:HH12	1.78	0.49
1:B:339:MET:HB3	1:B:366:ASN:HB2	1.93	0.48
1:C:269:ILE:HD13	1:C:284:LEU:HD22	1.94	0.48
1:A:376:THR:HB	1:A:401:THR:HG23	1.96	0.48
1:B:647:VAL:HG23	1:B:656:PRO:HD3	1.96	0.48
1:C:654:SER:HB2	3:C:840:HOH:O	2.14	0.48
1:C:262:PRO:HB2	1:C:339:MET:HG3	1.96	0.48
1:D:192:ALA:O	1:D:221:HIS:HB2	2.13	0.48
1:D:647:VAL:HG23	1:D:656:PRO:HD3	1.96	0.48
1:B:58:GLN:HG3	1:B:67:PRO:HA	1.97	0.47
1:C:577:VAL:HG12	1:C:578:LEU:N	2.30	0.47
1:A:647:VAL:HG23	1:A:656:PRO:HD3	1.96	0.47
1:D:183:ILE:HG12	1:D:201:VAL:HG12	1.97	0.47
1:A:322:THR:HG23	1:A:383:SER:HB2	1.97	0.47
1:A:344:GLY:HA3	1:A:361:TRP:CE2	2.50	0.47
1:B:68:VAL:HG13	1:B:75:MET:HB3	1.97	0.47
1:C:577:VAL:HG12	1:C:578:LEU:H	1.80	0.47
1:A:214:ASN:HB2	1:A:236:ALA:HB3	1.96	0.46
1:C:641:ILE:HD11	1:C:647:VAL:HG22	1.97	0.46
1:B:120:MET:HB3	1:B:125:THR:HG21	1.97	0.46
1:C:571:ILE:HG23	1:C:588:LEU:HB2	1.97	0.46
1:B:382:THR:HA	1:B:394:VAL:O	2.15	0.46
1:A:539:PRO:HA	1:A:563:PRO:HB3	1.97	0.46
1:C:232:ARG:HB3	1:C:258:GLN:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:GLN:HG3	1:D:67:PRO:HA	1.97	0.46
1:A:192:ALA:O	1:A:221:HIS:HB2	2.16	0.46
1:B:588:LEU:HD23	1:B:616:TYR:HB3	1.97	0.46
1:B:75:MET:HG3	1:B:153:ILE:HG12	1.97	0.45
1:B:419:ASN:HB3	1:B:422:HIS:O	2.16	0.45
1:C:315:GLU:HG2	1:C:325:ARG:HG2	1.98	0.45
1:D:298:THR:HG22	1:D:301:ASP:OD1	2.17	0.45
1:A:298:THR:CG2	1:A:429:PRO:CD	2.95	0.45
1:C:120:MET:HB3	1:C:125:THR:HG21	1.99	0.45
1:C:336:ASP:HA	1:C:368:LYS:O	2.17	0.45
1:B:479:THR:HG23	3:B:908:HOH:O	2.16	0.45
1:C:489:ILE:HD11	1:C:501:VAL:HB	1.98	0.45
1:B:373:LYS:HB2	1:B:404:THR:HG22	1.99	0.45
1:C:472[B]:HIS:HE1	1:C:507:ALA:HB1	1.80	0.45
1:B:112:SER:HB2	1:B:366:ASN:ND2	2.32	0.44
1:A:101:VAL:HG22	1:A:120:MET:HG3	2.00	0.44
1:C:726:TYR:O	1:C:750:ARG:HA	2.17	0.44
1:C:442:GLN:O	1:C:473:THR:HA	2.18	0.44
1:D:514:ASN:ND2	1:D:537:GLN:HE21	2.16	0.44
1:D:491:CYS:SG	1:D:497:LYS:HA	2.57	0.44
1:B:475:TYR:HB3	1:B:547:LEU:HB2	1.99	0.44
1:B:503:THR:HB	3:B:908:HOH:O	2.17	0.44
1:B:648:ALA:HB1	1:B:688:HIS:CD2	2.53	0.44
1:D:195:ARG:HH21	1:D:219:LYS:HG2	1.83	0.44
1:B:344:GLY:HA3	1:B:361:TRP:CE2	2.52	0.44
1:B:442:GLN:O	1:B:473:THR:HA	2.17	0.44
1:C:72:THR:HG22	1:C:530:TYR:HB2	2.00	0.44
1:D:469:ASP:HB2	1:D:512:LEU:HB2	1.99	0.44
1:B:73:ARG:HE	1:B:153:ILE:HG21	1.81	0.44
1:B:232:ARG:HB3	1:B:258:GLN:HG2	2.00	0.44
1:D:539:PRO:HA	1:D:563:PRO:HB3	1.99	0.44
1:B:269:ILE:HD13	1:B:284:LEU:HD22	1.99	0.43
1:C:577:VAL:HG12	1:C:578:LEU:HG	2.00	0.43
1:A:442:GLN:O	1:A:473:THR:HA	2.18	0.43
1:D:300:SER:CB	1:D:429:PRO:HD2	2.43	0.43
1:A:229:LYS:H	1:A:261:THR:HB	1.83	0.43
1:A:610:LYS:HB2	1:A:643:ASN:HB2	1.99	0.43
1:C:615:GLY:HA3	1:C:636:GLN:O	2.18	0.43
1:A:299:ASP:HB3	1:A:428:HIS:CE1	2.53	0.43
1:C:528:ASN:O	1:C:573:THR:HG22	2.18	0.43
1:D:338:LEU:HB2	1:D:432:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:SER:HB2	1:D:196:ARG:HB3	2.01	0.43
1:A:72:THR:HG22	1:A:530:TYR:HB2	2.01	0.43
1:C:58:GLN:HG3	1:C:67:PRO:HA	2.00	0.43
1:B:267:PRO:HD2	1:B:290:VAL:HG21	2.01	0.42
1:B:315:GLU:HG2	1:B:325:ARG:HG2	2.01	0.42
1:B:537:GLN:HG2	1:B:565:LYS:HG2	2.00	0.42
1:C:382:THR:HA	1:C:394:VAL:O	2.19	0.42
1:D:298:THR:HG23	1:D:300:SER:H	1.83	0.42
1:B:72:THR:HG22	1:B:530:TYR:HB2	2.01	0.42
1:D:610:LYS:HB2	1:D:643:ASN:HB2	2.01	0.42
1:B:384:THR:HA	1:B:392:HIS:O	2.19	0.42
1:B:473:THR:O	1:B:507:ALA:HA	2.20	0.42
1:D:332:ARG:HG2	1:D:373:LYS:HG2	2.01	0.42
1:B:709:ALA:HB3	1:B:725:VAL:HG22	2.02	0.42
1:A:565:LYS:HB2	1:A:594:GLU:HG3	2.01	0.42
1:C:593:ILE:HB	1:C:611:LYS:HB2	2.01	0.42
1:D:678:GLY:HA3	1:D:710:LYS:HB3	2.01	0.42
1:B:156:PRO:HG3	1:B:166:PRO:HA	2.02	0.41
1:C:351:GLN:HB3	1:C:359:TRP:NE1	2.36	0.41
1:C:537:GLN:HG2	1:C:565:LYS:HG2	2.01	0.41
1:B:80:GLU:HB2	1:B:148:GLU:O	2.20	0.41
1:A:269:ILE:H	1:A:269:ILE:HG13	1.77	0.41
1:D:332:ARG:HD3	1:D:334:LYS:HG3	2.03	0.41
1:A:351:GLN:HG2	1:A:359:TRP:CE2	2.56	0.40
1:C:337:TYR:CE1	1:C:368:LYS:HD2	2.56	0.40
1:B:188:SER:HB2	1:B:196:ARG:HB3	2.02	0.40
1:C:83:ILE:HG23	1:C:88:ALA:O	2.22	0.40
1:C:300:SER:HB2	1:C:429:PRO:HD2	2.03	0.40
1:D:297:GLY:HA2	1:D:340:THR:HB	2.04	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	710/727 (98%)	680 (96%)	28 (4%)	2 (0%)	41	71
1	B	710/727 (98%)	680 (96%)	28 (4%)	2 (0%)	41	71
1	C	711/727 (98%)	683 (96%)	27 (4%)	1 (0%)	51	82
1	D	710/727 (98%)	679 (96%)	30 (4%)	1 (0%)	51	82
All	All	2841/2908 (98%)	2722 (96%)	113 (4%)	6 (0%)	47	78

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	115	GLY
1	D	604	THR
1	C	157	SER
1	A	227	LYS
1	A	603	GLY
1	B	578	LEU

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	580/591 (98%)	558 (96%)	22 (4%)	33	67
1	B	580/591 (98%)	555 (96%)	25 (4%)	29	62
1	C	581/591 (98%)	556 (96%)	25 (4%)	29	62
1	D	580/591 (98%)	556 (96%)	24 (4%)	30	64
All	All	2321/2364 (98%)	2225 (96%)	96 (4%)	30	64

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	THR
1	A	215	VAL
1	A	252	ASN
1	A	254	LEU
1	A	311	THR

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Mol	Chain	Res	Type
1	A	371	SER
1	A	393	ASP
1	A	433	THR
1	A	438	ASN
1	A	454	LEU
1	A	486	ARG
1	A	509	SER
1	A	513	MET
1	A	525	GLU
1	A	529	VAL
1	A	531	ILE
1	A	636	GLN
1	A	654	SER
1	A	657	TYR
1	A	667	SER
1	A	711	LEU
1	A	752	PHE
1	B	75	MET
1	B	139	SER
1	B	148	GLU
1	B	188	SER
1	B	195	ARG
1	B	202	ASN
1	B	309	THR
1	B	311	THR
1	B	364	THR
1	B	368	LYS
1	B	379	THR
1	B	393	ASP
1	B	448	ILE
1	B	454	LEU
1	B	462	LEU
1	B	497	LYS
1	B	506	THR
1	B	508	LYS
1	B	547	LEU
1	B	578	LEU
1	B	643	ASN
1	B	654	SER
1	B	657	TYR
1	B	667	SER
1	B	758	MET

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Mol	Chain	Res	Type
1	C	76	THR
1	C	195	ARG
1	C	248	ARG
1	C	300	SER
1	C	333	VAL
1	C	350	THR
1	C	351	GLN
1	C	362	SER
1	C	364	THR
1	C	368	LYS
1	C	379	THR
1	C	404	THR
1	C	406	THR
1	C	419	ASN
1	C	432	LEU
1	C	468	LEU
1	C	497	LYS
1	C	506	THR
1	C	508	LYS
1	C	520	LEU
1	C	573	THR
1	C	657	TYR
1	C	710	LYS
1	C	725	VAL
1	C	758	MET
1	D	84	LYS
1	D	114	THR
1	D	139	SER
1	D	237	PRO
1	D	287	SER
1	D	307	THR
1	D	309	THR
1	D	356	VAL
1	D	393	ASP
1	D	404	THR
1	D	438	ASN
1	D	468	LEU
1	D	469	ASP
1	D	479	THR
1	D	486	ARG
1	D	489	ILE
1	D	513	MET

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Mol	Chain	Res	Type
1	D	564	GLN
1	D	604	THR
1	D	606	SER
1	D	636	GLN
1	D	653	SER
1	D	720	ASP
1	D	728	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	326	ASN
1	A	428	HIS
1	A	463	ASN
1	A	532	ASN
1	A	538	GLN
1	A	564	GLN
1	A	599	GLN
1	B	214	ASN
1	B	326	ASN
1	B	366	ASN
1	B	377	ASN
1	B	564	GLN
1	B	599	GLN
1	B	600	ASN
1	B	722	GLN
1	B	724	ASN
1	C	357	ASN
1	C	366	ASN
1	C	419	ASN
1	C	511	ASN
1	D	214	ASN
1	D	357	ASN
1	D	366	ASN
1	D	514	ASN
1	D	649	GLN
1	D	722	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
2	BOG	A	801	-	20,20,20	0.17	0	25,25,25	0.19	0
2	BOG	B	801	-	20,20,20	0.21	0	25,25,25	0.22	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	BOG	A	801	-	-	4/11/31/31	0/1/1/1
2	BOG	B	801	-	-	4/11/31/31	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	BOG	O1-C1'-C2'-C3'
2	B	801	BOG	C2'-C3'-C4'-C5'

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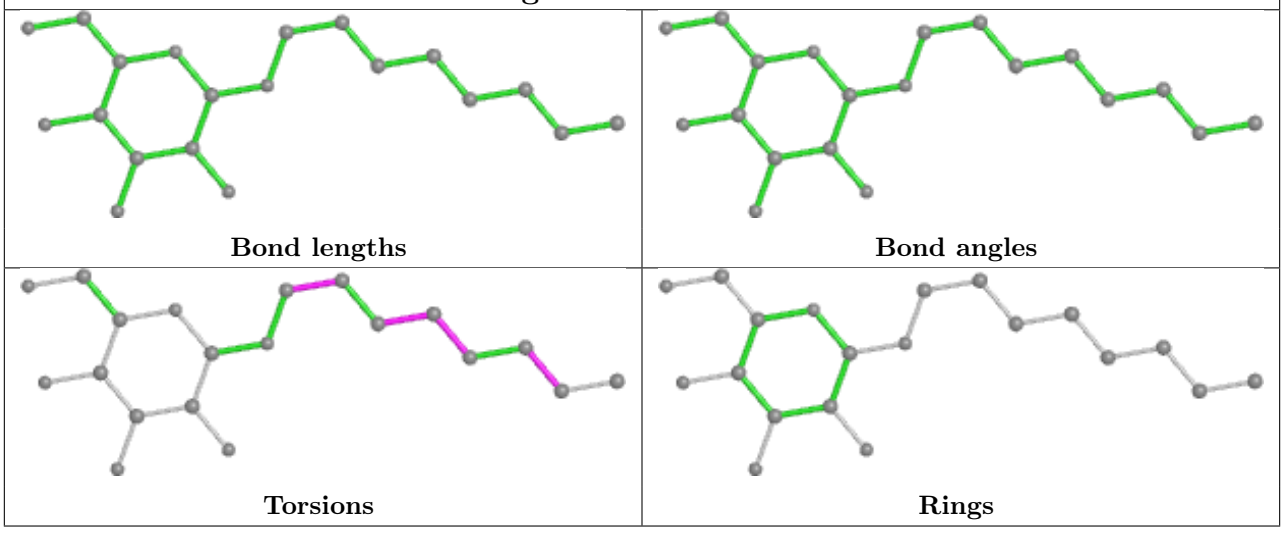
Mol	Chain	Res	Type	Atoms
2	B	801	BOG	C1'-C2'-C3'-C4'
2	A	801	BOG	O1-C1'-C2'-C3'
2	A	801	BOG	C5'-C6'-C7'-C8'
2	A	801	BOG	C3'-C4'-C5'-C6'
2	B	801	BOG	C4'-C5'-C6'-C7'
2	A	801	BOG	C2'-C3'-C4'-C5'

There are no ring outliers.

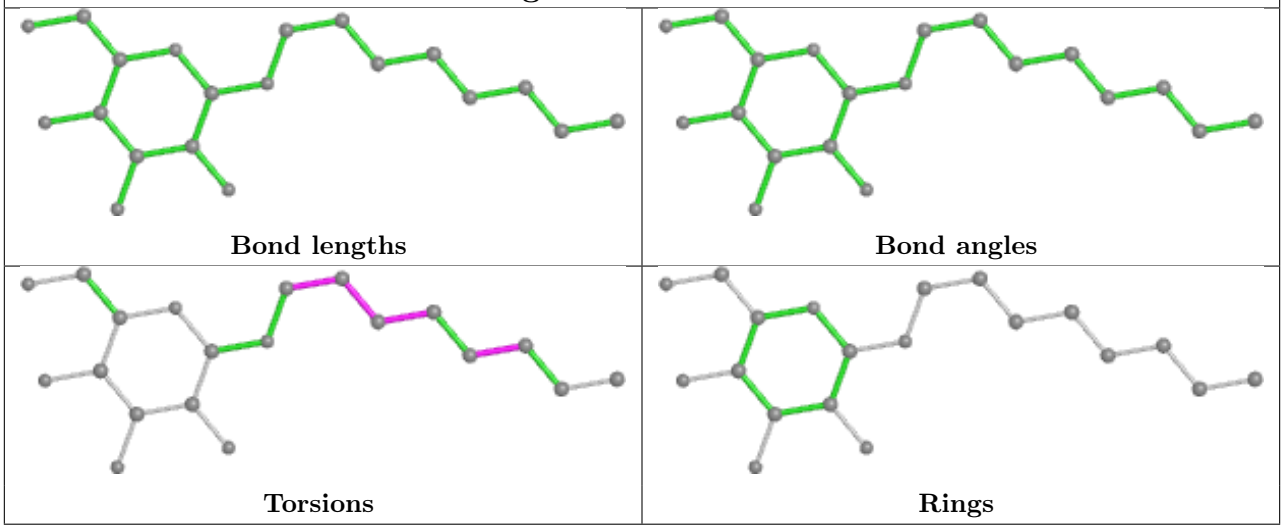
No monomer is involved in short contacts.

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.

Ligand BOG A 801



Ligand BOG B 801



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	711/727 (97%)	-0.44	7 (0%)	82	82	36, 54, 82, 125	0
1	B	711/727 (97%)	-0.49	8 (1%)	80	80	31, 52, 77, 122	0
1	C	711/727 (97%)	-0.48	10 (1%)	75	75	32, 52, 78, 117	0
1	D	711/727 (97%)	-0.44	6 (0%)	86	86	32, 53, 80, 113	0
All	All	2844/2908 (97%)	-0.46	31 (1%)	80	80	31, 53, 79, 125	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	487	GLY	5.8
1	D	484	SER	5.1
1	A	760	PHE	5.0
1	C	484	SER	4.8
1	C	760	PHE	4.4
1	B	760	PHE	4.1
1	B	758	MET	3.6
1	D	486	ARG	3.3
1	D	525	GLU	3.2
1	A	486	ARG	3.1
1	B	759	HIS	3.0
1	D	179	ASN	3.0
1	A	207	ASP	2.8
1	C	486	ARG	2.8
1	A	487	GLY	2.7
1	A	484	SER	2.7
1	A	713	TYR	2.6
1	C	485	GLY	2.4
1	A	718	ASN	2.4
1	C	50	THR	2.4
1	B	183	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	719	LEU	2.3
1	B	486	ARG	2.3
1	C	718	ASN	2.3
1	B	182	GLY	2.2
1	C	179	ASN	2.1
1	C	759	HIS	2.1
1	C	193	TRP	2.1
1	C	293	HIS	2.0
1	D	671	ALA	2.0
1	B	193	TRP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

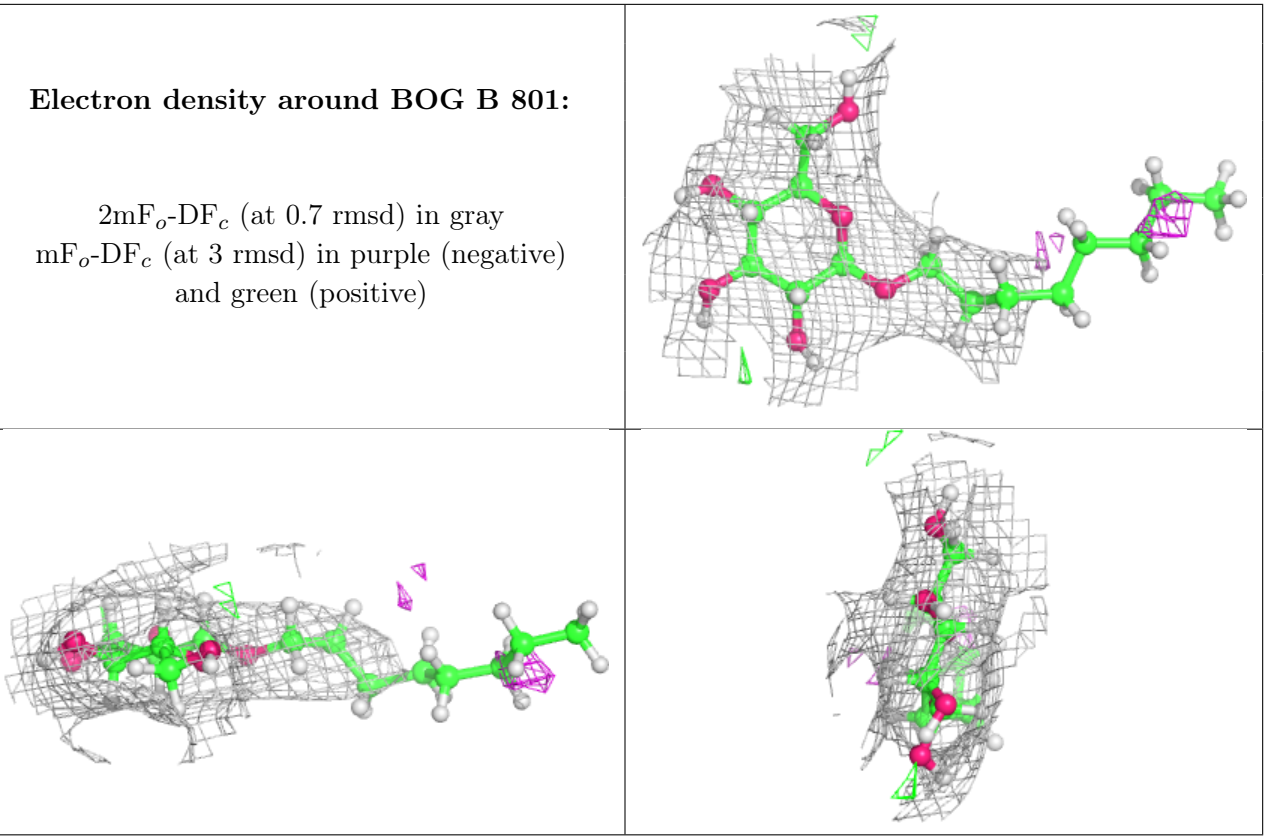
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	BOG	B	801	20/20	0.83	0.35	91,95,107,107	0
2	BOG	A	801	20/20	0.87	0.46	98,101,103,103	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.

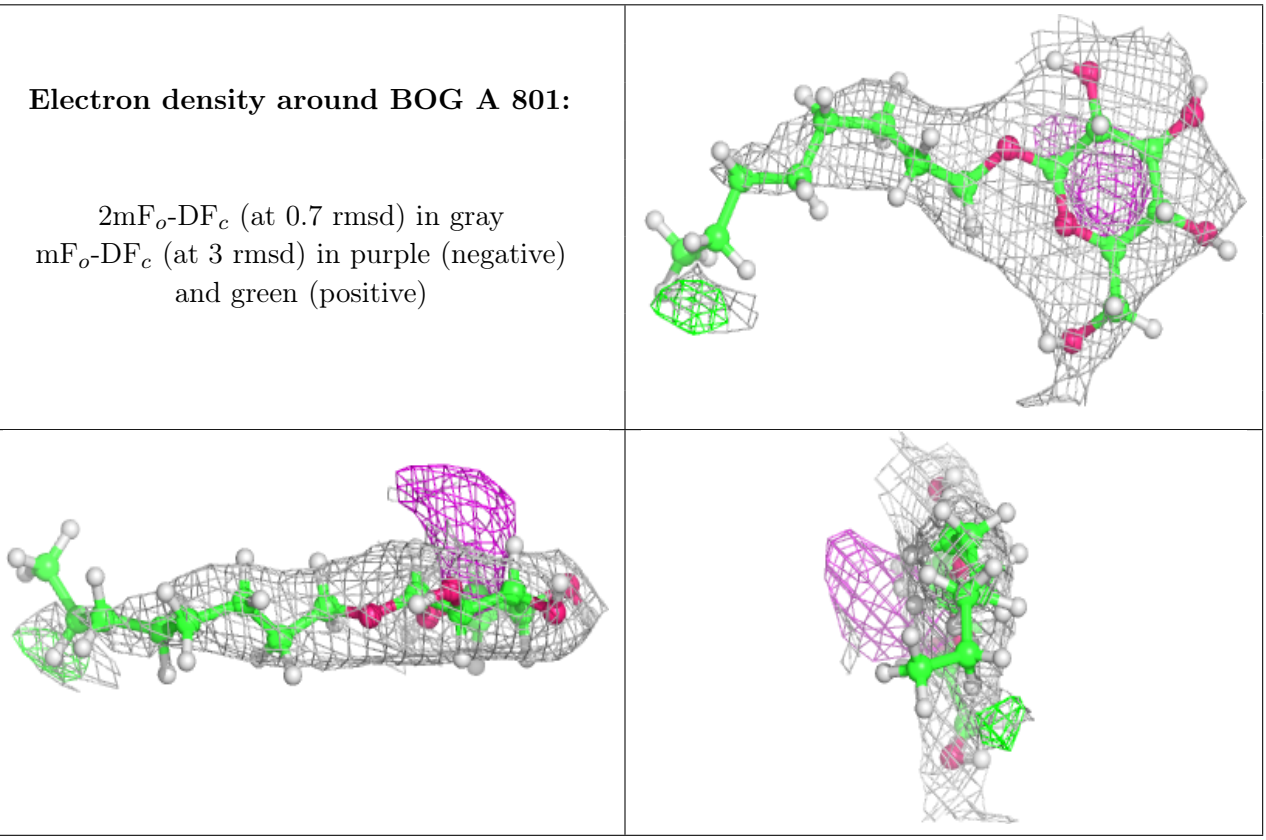
Electron density around BOG B 801:

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



Electron density around BOG A 801:

$2mF_o$-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.