



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 02:02 PM EDT

PDB ID : 6EQ8
Title : Structure of the periplasmic binding protein (PBP) MelB (Atu4661) in complex with galactinol from agrobacterium fabrum C58
Authors : Vigouroux, A.; Morera, S.
Deposited on : 2017-10-12
Resolution : 2.19 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	:	2.37.1
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)	:	2.37.1

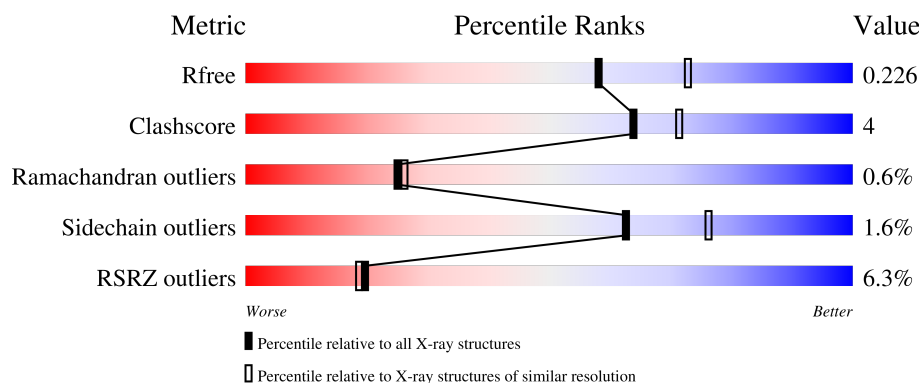
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 $\leq 5\%$. 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	683	<div> <div>7%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div></div> </div> </div>
1	B	683	<div> <div>7%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div></div> </div> </div>
1	C	683	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div></div> </div> </div>
1	D	683	<div> <div>6%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div></div> </div> </div>

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	EDO	A	703	-	-	-	X
2	EDO	C	710	-	-	X	-
8	CL	D	715	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22442 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 Periplasmic alpha-galactoside-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	670	Total	C	N	O	S	0	0	0
			5284	3374	896	998	16			
1	B	670	Total	C	N	O	S	0	0	0
			5285	3374	896	999	16			
1	C	670	Total	C	N	O	S	0	0	0
			5285	3374	896	999	16			
1	A	671	Total	C	N	O	S	0	0	0
			5295	3380	899	1000	16			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	678	HIS	-	expression tag	UNP A0A083ZM57
D	679	HIS	-	expression tag	UNP A0A083ZM57
D	680	HIS	-	expression tag	UNP A0A083ZM57
D	681	HIS	-	expression tag	UNP A0A083ZM57
D	682	HIS	-	expression tag	UNP A0A083ZM57
D	683	HIS	-	expression tag	UNP A0A083ZM57
B	678	HIS	-	expression tag	UNP A0A083ZM57
B	679	HIS	-	expression tag	UNP A0A083ZM57
B	680	HIS	-	expression tag	UNP A0A083ZM57
B	681	HIS	-	expression tag	UNP A0A083ZM57
B	682	HIS	-	expression tag	UNP A0A083ZM57
B	683	HIS	-	expression tag	UNP A0A083ZM57
C	678	HIS	-	expression tag	UNP A0A083ZM57
C	679	HIS	-	expression tag	UNP A0A083ZM57
C	680	HIS	-	expression tag	UNP A0A083ZM57
C	681	HIS	-	expression tag	UNP A0A083ZM57
C	682	HIS	-	expression tag	UNP A0A083ZM57
C	683	HIS	-	expression tag	UNP A0A083ZM57
A	678	HIS	-	expression tag	UNP A0A083ZM57
A	679	HIS	-	expression tag	UNP A0A083ZM57
A	680	HIS	-	expression tag	UNP A0A083ZM57

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Chain	Residue	Modelled	Actual	Comment	Reference
A	681	HIS	-	expression tag	UNP A0A083ZM57
A	682	HIS	-	expression tag	UNP A0A083ZM57
A	683	HIS	-	expression tag	UNP A0A083ZM57

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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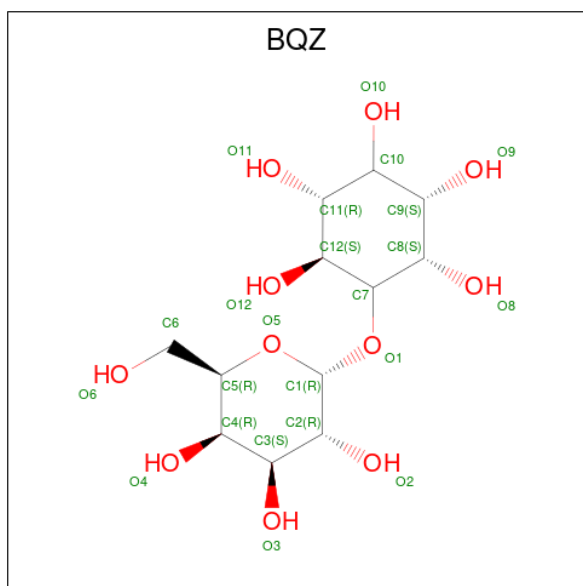
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total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

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

- Molecule 3 is galactinol (three-letter code: BQZ) (formula: C₁₂H₂₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			23	12	11		
3	B	1	Total	C	O	0	0
			23	12	11		
3	C	1	Total	C	O	0	0
			23	12	11		

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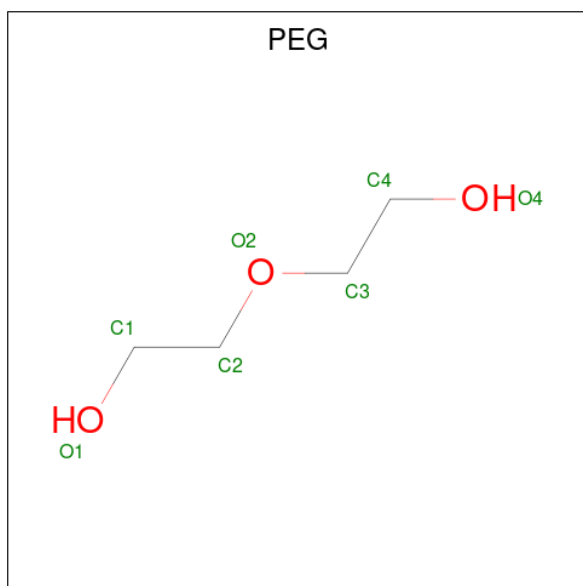
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	12	11		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Ca	0	0
			1	1		
4	B	3	Total	Ca	0	0
			3	3		
4	C	4	Total	Ca	0	0
			4	4		
4	A	5	Total	Ca	0	0
			5	5		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



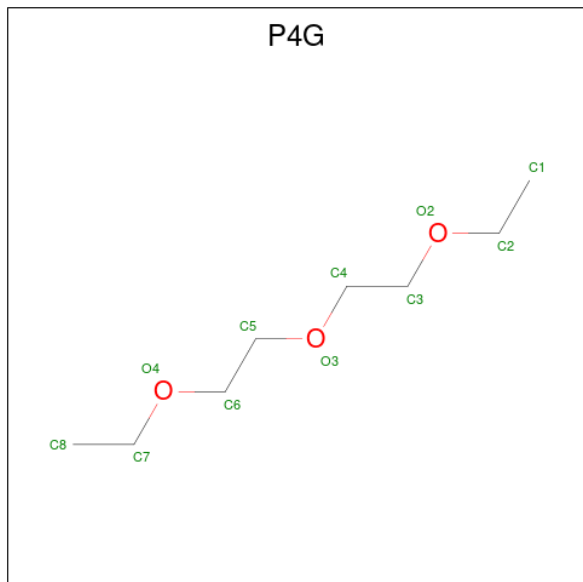
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

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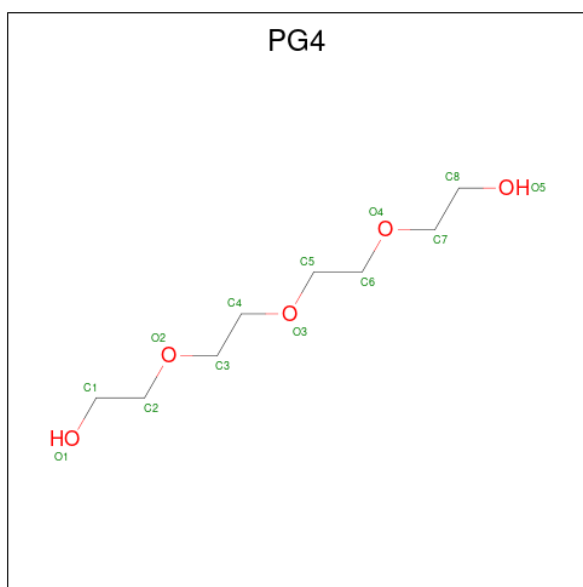
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 1-ETHOXY-2-(2-ETHOXYETHOXY)ETHANE (three-letter code: P4G) (formula: $C_8H_{18}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			11	8	3		
6	C	1	Total	C	O	0	0
			11	8	3		
6	A	1	Total	C	O	0	0
			11	8	3		

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total C O 13 8 5	0	0
7	C	1	Total C O 13 8 5	0	0
7	A	1	Total C O 13 8 5	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	7	Total Cl 7 7	0	0
8	B	11	Total Cl 11 11	0	0
8	C	13	Total Cl 13 13	0	0
8	A	4	Total Cl 4 4	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	170	Total O 170 170	0	0
9	B	172	Total O 172 172	0	0

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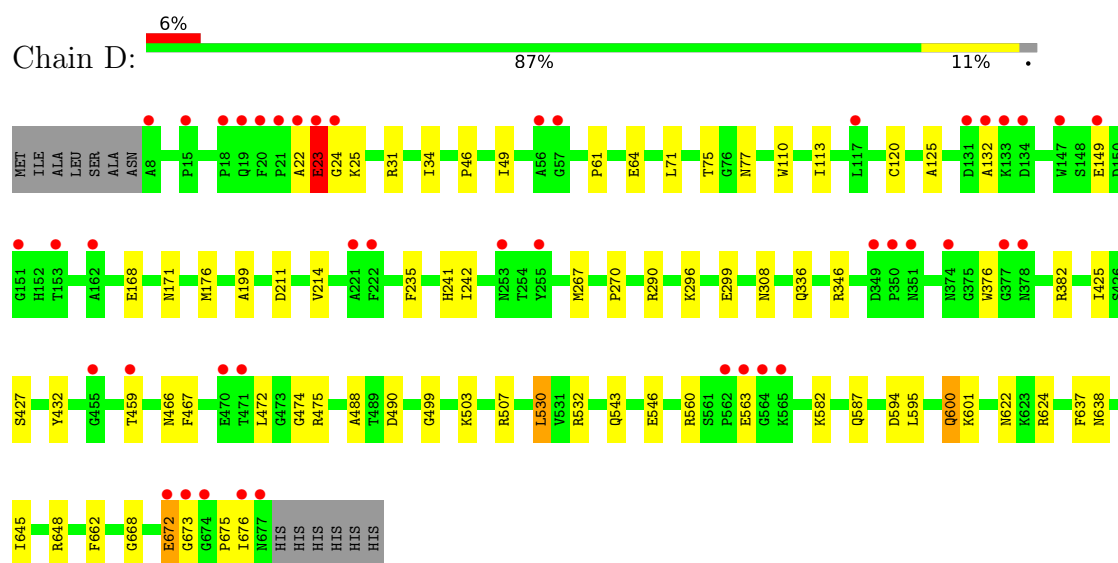
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	260	Total 260	O 260	0	0
9	A	260	Total 260	O 260	0	0

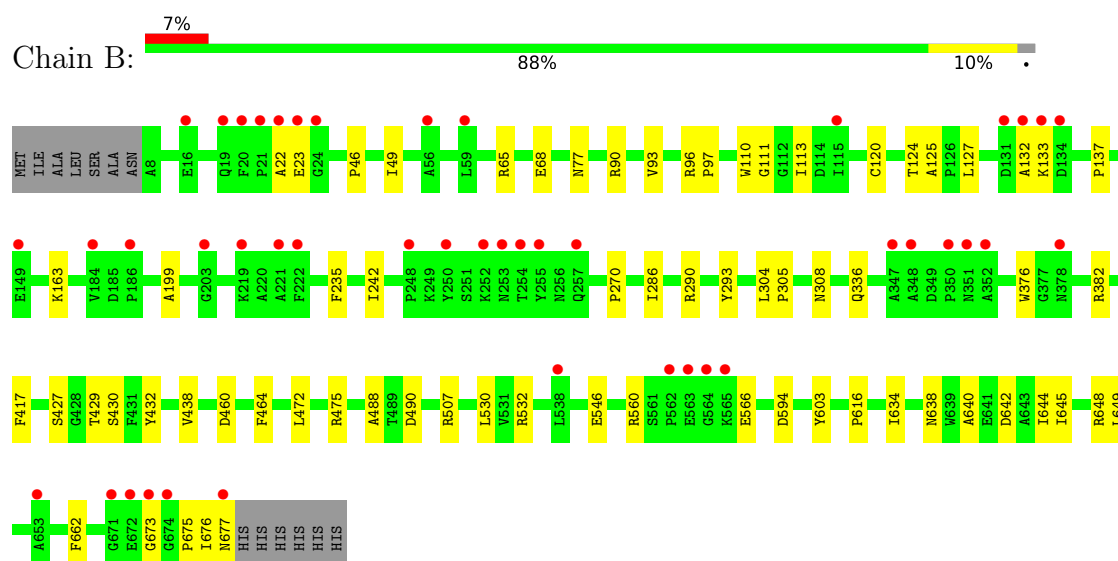
3 Residue-property plots [i](#)

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.

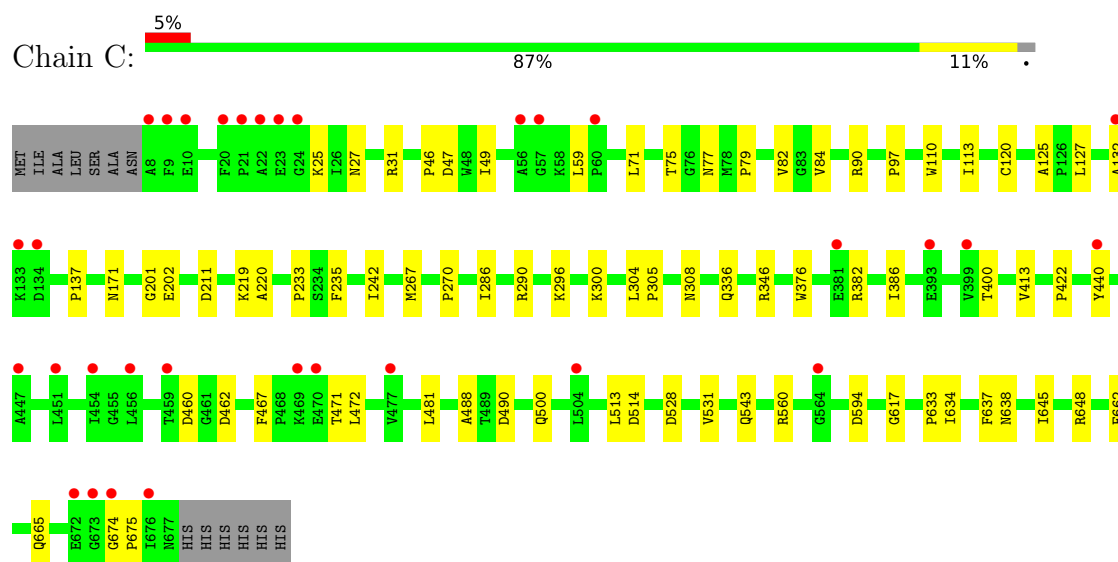
- Molecule 1: Periplasmic alpha-galactoside-binding protein



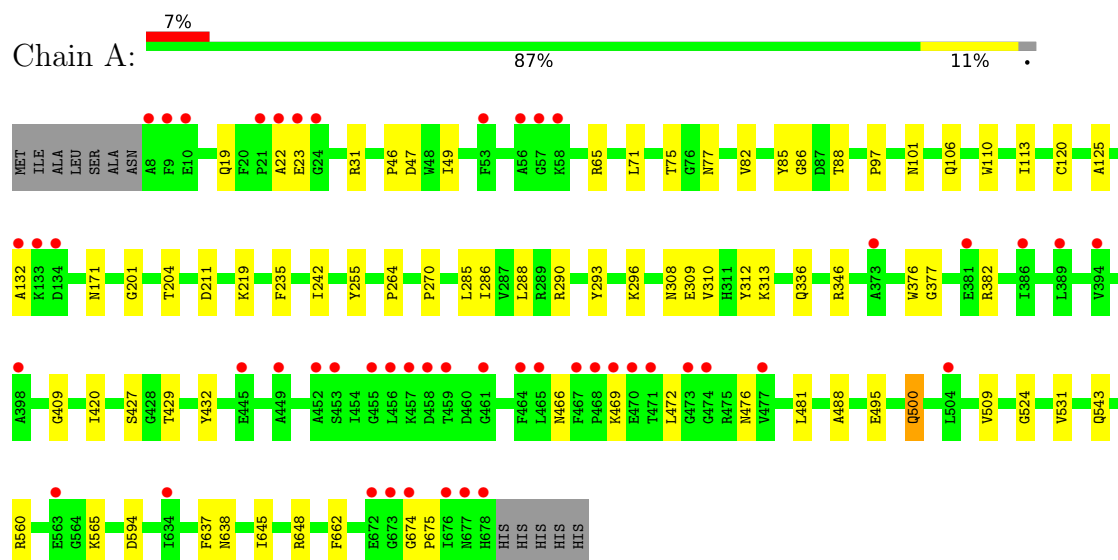
- Molecule 1: Periplasmic alpha-galactoside-binding protein



- Molecule 1: Periplasmic alpha-galactoside-binding protein



- Molecule 1: Periplasmic alpha-galactoside-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	355.26Å 73.66Å 108.08Å 90.00° 105.49° 90.00°	Depositor
Resolution (Å)	32.06 – 2.19 49.09 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.1 (32.06-2.19) 98.8 (49.09-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.18Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.184 , 0.217 0.193 , 0.226	Depositor DCC
R_{free} test set	6882 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22442	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0111e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BQZ, EDO, PEG, CA, P4G, CL, PG4

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	0.52	0/5448	0.67	0/7413
1	B	0.49	0/5437	0.67	1/7398 (0.0%)
1	C	0.52	0/5437	0.68	0/7398
1	D	0.49	0/5436	0.67	1/7396 (0.0%)
All	All	0.51	0/21758	0.67	2/29605 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	672	GLU	C-N-CA	6.13	135.18	122.30
1	B	676	ILE	C-N-CA	5.07	134.37	121.70

There are no chirality outliers.

There are no planarity outliers.

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	5295	0	5112	46	0
1	B	5285	0	5105	35	0
1	C	5285	0	5105	56	0
1	D	5284	0	5104	43	0
2	A	60	0	90	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	20	0	30	3	0
2	C	48	0	72	23	0
2	D	28	0	42	1	0
3	A	23	0	0	0	0
3	B	23	0	0	0	0
3	C	23	0	0	0	0
3	D	23	0	0	0	0
4	A	5	0	0	0	0
4	B	3	0	0	0	0
4	C	4	0	0	0	0
4	D	1	0	0	0	0
5	A	7	0	10	0	0
5	B	7	0	10	0	0
5	C	28	0	40	3	0
5	D	21	0	30	0	0
6	A	11	0	18	0	0
6	C	11	0	18	4	0
6	D	11	0	18	0	0
7	A	13	0	18	0	0
7	C	13	0	18	3	0
7	D	13	0	18	4	0
8	A	4	0	0	1	0
8	B	11	0	0	1	0
8	C	13	0	0	1	0
8	D	7	0	0	2	0
9	A	260	0	0	0	0
9	B	172	0	0	0	0
9	C	260	0	0	3	0
9	D	170	0	0	0	0
All	All	22442	0	20858	179	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 4.

All (179) 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:C:422:PRO:HB3	2:C:710:EDO:H11	1.31	1.10
1:A:420:ILE:HD13	2:A:708:EDO:H11	1.61	0.81
1:A:47:ASP:H	2:A:710:EDO:H22	1.45	0.81
1:C:422:PRO:CB	2:C:710:EDO:H11	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:600:GLN:HE21	1:D:600:GLN:HA	1.45	0.81
1:C:440:TYR:H	2:C:710:EDO:H12	1.47	0.79
1:D:672:GLU:HB3	1:D:673:GLY:HA3	1.65	0.79
1:C:634:ILE:HG23	2:C:711:EDO:H22	1.68	0.76
1:C:46:PRO:HA	5:C:721:PEG:H32	1.68	0.75
1:C:633:PRO:HA	2:C:711:EDO:H11	1.70	0.74
1:A:201:GLY:HA3	2:A:707:EDO:H12	1.69	0.73
1:C:201:GLY:HA3	2:C:706:EDO:H12	1.72	0.71
1:C:400:THR:OG1	2:C:710:EDO:H22	1.91	0.71
1:A:77:ASN:HD22	1:A:648:ARG:HH12	1.39	0.68
1:B:77:ASN:HD22	1:B:648:ARG:HH12	1.41	0.68
1:B:460:ASP:O	1:A:495:GLU:HG2	1.95	0.67
1:C:77:ASN:HD22	1:C:648:ARG:HH12	1.41	0.66
1:C:46:PRO:HD2	1:C:49:ILE:HD12	1.75	0.66
1:A:264:PRO:O	2:A:715:EDO:H22	1.96	0.66
1:C:300:LYS:HB3	2:C:701:EDO:H22	1.78	0.65
1:A:255:TYR:HB2	2:A:706:EDO:H11	1.77	0.65
1:C:422:PRO:HB3	2:C:710:EDO:C1	2.17	0.65
1:D:77:ASN:HD22	1:D:648:ARG:HH12	1.47	0.63
7:D:714:PG4:H11	1:C:462:ASP:HB3	1.80	0.62
1:C:79:PRO:HA	2:C:707:EDO:H22	1.80	0.62
1:C:233:PRO:HG3	2:C:708:EDO:H22	1.83	0.61
1:A:285:LEU:HD13	1:A:313:LYS:HD2	1.82	0.61
1:C:31:ARG:HH22	2:C:705:EDO:H11	1.65	0.61
1:C:400:THR:OG1	2:C:710:EDO:C2	2.49	0.60
2:C:707:EDO:H21	7:C:723:PG4:O4	2.01	0.59
1:D:176:MET:HE3	1:D:214:VAL:HG12	1.85	0.59
1:C:440:TYR:H	2:C:710:EDO:C1	2.15	0.59
1:A:110:TRP:O	1:A:113:ILE:HG22	2.01	0.59
1:A:75:THR:HG22	1:A:82:VAL:HG23	1.85	0.58
1:A:101:ASN:H	1:A:106:GLN:HE21	1.51	0.58
1:D:61:PRO:HD2	1:D:64:GLU:OE2	2.04	0.58
1:A:409:GLY:HA3	2:A:708:EDO:H21	1.86	0.57
1:C:27:ASN:HB2	7:C:723:PG4:H71	1.86	0.56
1:C:413:VAL:HG23	2:C:709:EDO:H12	1.87	0.56
1:C:75:THR:HG22	1:C:82:VAL:HG23	1.87	0.56
1:B:46:PRO:HD2	1:B:49:ILE:HD12	1.88	0.56
1:A:285:LEU:HD13	1:A:313:LYS:CD	2.36	0.55
1:C:400:THR:HG1	2:C:710:EDO:H22	1.70	0.55
1:D:503:LYS:NZ	7:D:714:PG4:H22	2.22	0.55
1:D:499:GLY:HA3	7:D:714:PG4:H41	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LEU:HB3	1:A:296:LYS:HG2	1.89	0.54
1:D:503:LYS:HZ1	7:D:714:PG4:H22	1.72	0.54
1:D:475:ARG:HD3	1:C:513:LEU:HD21	1.90	0.54
1:D:290:ARG:HH11	1:D:308:ASN:HD22	1.57	0.53
1:A:31:ARG:HH12	2:A:705:EDO:H12	1.74	0.53
1:B:290:ARG:HH11	1:B:308:ASN:HD22	1.57	0.53
1:B:530:LEU:CD1	1:B:532:ARG:HB2	2.39	0.53
1:B:642:ASP:HA	2:B:705:EDO:C1	2.39	0.53
1:A:382:ARG:HA	1:A:472:LEU:HD11	1.90	0.53
1:D:425:ILE:H	1:D:600:GLN:HE22	1.56	0.53
1:D:668:GLY:HA2	1:D:676:ILE:HG23	1.91	0.53
1:A:420:ILE:HD13	2:A:708:EDO:C1	2.37	0.53
1:B:336:GLN:HE22	1:B:488:ALA:H	1.56	0.52
1:A:290:ARG:HD2	1:A:308:ASN:HD22	1.74	0.52
1:D:475:ARG:HD3	1:C:513:LEU:CD2	2.38	0.52
1:B:290:ARG:HD2	1:B:308:ASN:HD22	1.74	0.52
6:C:722:P4G:H31	9:C:867:HOH:O	2.10	0.52
1:C:336:GLN:HE22	1:C:488:ALA:H	1.57	0.52
1:C:290:ARG:HD2	1:C:308:ASN:HD22	1.75	0.51
1:A:290:ARG:HH11	1:A:308:ASN:HD22	1.58	0.51
1:D:290:ARG:HD2	1:D:308:ASN:HD22	1.74	0.51
1:A:336:GLN:HE22	1:A:488:ALA:H	1.56	0.51
1:D:472:LEU:HD22	1:D:475:ARG:HH22	1.74	0.51
1:C:290:ARG:HH11	1:C:308:ASN:HD22	1.59	0.51
1:D:382:ARG:HA	1:D:472:LEU:HD11	1.93	0.51
1:B:133:LYS:HD2	1:B:430:SER:OG	2.10	0.51
1:A:288:LEU:HD11	1:A:312:TYR:HE2	1.76	0.51
1:A:31:ARG:HH22	2:A:705:EDO:H21	1.76	0.50
1:A:662:PHE:CD1	1:A:675:PRO:HG2	2.47	0.50
1:B:97:PRO:HG3	1:B:286:ILE:HD11	1.93	0.50
1:A:377:GLY:HA2	1:A:524:GLY:O	2.12	0.50
1:D:336:GLN:HE22	1:D:488:ALA:H	1.59	0.50
1:D:662:PHE:CD1	1:D:675:PRO:HG2	2.46	0.50
2:C:712:EDO:H22	6:C:722:P4G:C8	2.42	0.50
1:B:662:PHE:CD1	1:B:675:PRO:HG2	2.46	0.49
1:B:124:THR:HG22	1:B:137:PRO:HB3	1.95	0.49
1:C:79:PRO:HG3	7:C:723:PG4:H81	1.95	0.49
1:D:459:THR:H	1:D:466:ASN:ND2	2.11	0.49
1:D:75:THR:HG22	1:D:299:GLU:OE1	2.12	0.48
1:C:220:ALA:H	2:C:706:EDO:H22	1.79	0.48
1:A:97:PRO:HG3	1:A:286:ILE:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:622:ASN:HD22	1:D:624:ARG:HG2	1.79	0.48
1:C:346:ARG:HE	6:C:722:P4G:H13	1.78	0.48
1:D:31:ARG:HH22	2:D:701:EDO:H11	1.79	0.47
1:B:120:CYS:HB3	1:B:235:PHE:O	2.14	0.47
1:B:65:ARG:HG2	1:B:293:TYR:CE1	2.50	0.47
1:C:120:CYS:HB3	1:C:235:PHE:O	2.14	0.47
1:D:120:CYS:HB3	1:D:235:PHE:O	2.14	0.47
1:B:242:ILE:HG13	1:B:270:PRO:HG2	1.95	0.47
1:B:464:PHE:CE2	1:A:509:VAL:HG22	2.50	0.47
1:B:507:ARG:HD3	1:A:509:VAL:HG11	1.97	0.47
1:C:662:PHE:CD1	1:C:675:PRO:HG2	2.50	0.47
1:C:171:ASN:HB2	1:C:211:ASP:O	2.15	0.47
1:D:46:PRO:HD2	1:D:49:ILE:HD12	1.97	0.47
1:D:267:MET:HG2	8:D:715:CL:CL	2.52	0.47
1:D:110:TRP:O	1:D:113:ILE:HG22	2.15	0.46
1:B:642:ASP:HA	2:B:705:EDO:H11	1.97	0.46
1:B:644:ILE:HD12	1:B:649:LEU:HD11	1.96	0.46
1:A:46:PRO:HD2	1:A:49:ILE:HD12	1.96	0.46
1:A:120:CYS:HB3	1:A:235:PHE:O	2.16	0.46
1:A:219:LYS:HB2	2:A:707:EDO:H22	1.98	0.46
1:C:125:ALA:HB2	1:C:638:ASN:HB3	1.98	0.46
1:A:77:ASN:ND2	1:A:648:ARG:HH12	2.10	0.46
1:A:171:ASN:HB2	1:A:211:ASP:O	2.15	0.46
1:D:23:GLU:HB3	1:D:24:GLY:H	1.54	0.46
1:B:125:ALA:HB2	1:B:638:ASN:HB3	1.97	0.45
1:C:300:LYS:HD3	5:C:720:PEG:H21	1.98	0.45
1:A:125:ALA:HB2	1:A:638:ASN:HB3	1.99	0.45
1:A:242:ILE:HG13	1:A:270:PRO:HG2	1.99	0.45
1:D:242:ILE:HG13	1:D:270:PRO:HG2	1.98	0.45
1:C:382:ARG:HA	1:C:472:LEU:HD11	1.98	0.45
1:C:500:GLN:HG2	9:C:943:HOH:O	2.15	0.45
1:C:97:PRO:HG3	1:C:286:ILE:HD11	1.99	0.45
2:C:712:EDO:H22	6:C:722:P4G:H81	1.99	0.45
1:D:427:SER:HA	1:D:432:TYR:CG	2.53	0.45
1:A:85:TYR:HD2	2:A:710:EDO:H11	1.82	0.44
1:A:86:GLY:O	8:A:726:CL:CL	2.73	0.44
1:D:168:GLU:HG2	1:D:241:HIS:CG	2.51	0.44
1:A:288:LEU:HD12	1:A:310:VAL:HB	2.00	0.44
1:D:376:TRP:CE2	1:D:560:ARG:HB2	2.53	0.44
1:B:77:ASN:ND2	1:B:648:ARG:HH12	2.12	0.44
1:B:110:TRP:O	1:B:113:ILE:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:ALA:HB2	1:D:638:ASN:HB3	2.00	0.44
1:C:467:PHE:HB3	1:C:471:THR:HB	1.99	0.44
1:A:204:THR:OG1	2:A:707:EDO:C1	2.66	0.44
1:C:77:ASN:ND2	1:C:648:ARG:HH12	2.12	0.43
1:C:84:VAL:O	8:C:724:CL:CL	2.73	0.43
1:D:582:LYS:HD3	1:D:595:LEU:HD21	2.00	0.43
1:B:376:TRP:CE2	1:B:560:ARG:HB2	2.54	0.43
1:A:466:ASN:HA	1:A:476:ASN:HA	2.00	0.43
1:B:127:LEU:HD11	1:B:137:PRO:HA	2.01	0.43
1:B:382:ARG:HA	1:B:472:LEU:HD11	2.00	0.43
1:C:617:GLY:O	2:C:711:EDO:H21	2.19	0.43
1:D:530:LEU:CD1	1:D:532:ARG:HB2	2.49	0.42
1:A:376:TRP:CE2	1:A:560:ARG:HB2	2.54	0.42
1:D:176:MET:HE1	1:D:214:VAL:HG11	2.00	0.42
1:C:127:LEU:HD11	1:C:137:PRO:HA	2.01	0.42
1:D:171:ASN:HB2	1:D:211:ASP:O	2.19	0.42
1:B:634:ILE:HA	1:B:640:ALA:HB2	2.01	0.42
1:C:242:ILE:HG13	1:C:270:PRO:HG2	2.01	0.42
1:C:304:LEU:HB3	1:C:305:PRO:HA	2.02	0.42
1:C:71:LEU:HB3	1:C:296:LYS:HG2	2.01	0.42
1:C:386:ILE:HG21	1:C:528:ASP:HB3	2.01	0.42
1:A:427:SER:HA	1:A:432:TYR:CG	2.53	0.42
1:A:481:LEU:HD11	1:A:531:VAL:HG23	2.01	0.42
1:C:376:TRP:CE2	1:C:560:ARG:HB2	2.54	0.42
1:D:467:PHE:O	1:D:474:GLY:HA2	2.20	0.42
1:B:427:SER:HA	1:B:432:TYR:CG	2.55	0.42
1:D:199:ALA:HA	1:D:546:GLU:HG3	2.01	0.42
1:B:199:ALA:HA	1:B:546:GLU:HG3	2.02	0.41
1:B:438:VAL:HG22	2:B:704:EDO:H21	2.01	0.41
1:B:93:VAL:HG12	1:B:111:GLY:HA3	2.02	0.41
1:A:500:GLN:HE21	1:A:500:GLN:HB2	1.66	0.41
1:B:530:LEU:HD12	1:B:532:ARG:HB2	2.00	0.41
1:C:110:TRP:O	1:C:113:ILE:HG22	2.21	0.41
1:A:65:ARG:HG2	1:A:293:TYR:CE1	2.56	0.41
1:D:176:MET:CE	1:D:214:VAL:HG12	2.49	0.41
1:C:662:PHE:O	1:C:665:GLN:HB2	2.20	0.41
1:B:417:PHE:O	1:B:616:PRO:HD3	2.20	0.41
1:B:304:LEU:HB3	1:B:305:PRO:HA	2.02	0.41
1:A:543:GLN:HG2	1:A:637:PHE:O	2.21	0.41
1:C:481:LEU:HD11	1:C:531:VAL:HG23	2.03	0.40
1:D:34:ILE:HG12	1:D:77:ASN:ND2	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:GLU:H	1:B:68:GLU:HG2	1.67	0.40
1:C:47:ASP:OD2	5:C:721:PEG:H31	2.22	0.40
1:C:219:LYS:HB2	2:C:706:EDO:H22	2.02	0.40
1:C:267:MET:HE3	9:C:987:HOH:O	2.21	0.40
1:C:422:PRO:CA	2:C:710:EDO:H11	2.50	0.40
1:C:543:GLN:HG2	1:C:637:PHE:O	2.21	0.40
1:D:267:MET:CG	8:D:715:CL:CL	3.06	0.40
1:D:543:GLN:HG2	1:D:637:PHE:O	2.21	0.40
1:A:88:THR:HA	1:A:309:GLU:O	2.20	0.40
1:D:71:LEU:HD22	1:D:296:LYS:HD3	2.03	0.40
1:B:96:ARG:HD2	8:B:720:CL:CL	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	669/683 (98%)	634 (95%)	30 (4%)	5 (1%)	22	22
1	B	668/683 (98%)	636 (95%)	27 (4%)	5 (1%)	22	22
1	C	668/683 (98%)	638 (96%)	27 (4%)	3 (0%)	34	37
1	D	668/683 (98%)	637 (95%)	27 (4%)	4 (1%)	25	26
All	All	2673/2732 (98%)	2545 (95%)	111 (4%)	17 (1%)	25	26

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	22	ALA
1	D	23	GLU
1	C	674	GLY
1	B	22	ALA

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Mol	Chain	Res	Type
1	A	674	GLY
1	D	132	ALA
1	B	23	GLU
1	B	132	ALA
1	B	673	GLY
1	C	132	ALA
1	A	22	ALA
1	A	132	ALA
1	A	23	GLU
1	D	645	ILE
1	B	645	ILE
1	C	645	ILE
1	A	645	ILE

5.3.2 Protein sidechains ⓘ

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	558/568 (98%)	551 (99%)	7 (1%)	69	81
1	B	557/568 (98%)	548 (98%)	9 (2%)	62	76
1	C	557/568 (98%)	549 (99%)	8 (1%)	67	80
1	D	556/568 (98%)	544 (98%)	12 (2%)	52	65
All	All	2228/2272 (98%)	2192 (98%)	36 (2%)	62	76

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	23	GLU
1	D	25	LYS
1	D	149	GLU
1	D	346	ARG
1	D	490	ASP
1	D	507	ARG
1	D	530	LEU
1	D	563	GLU

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Mol	Chain	Res	Type
1	D	587	GLN
1	D	594	ASP
1	D	600	GLN
1	D	601	LYS
1	B	90	ARG
1	B	163	LYS
1	B	429	THR
1	B	475	ARG
1	B	490	ASP
1	B	566	GLU
1	B	594	ASP
1	B	603	TYR
1	B	677	ASN
1	C	25	LYS
1	C	59	LEU
1	C	90	ARG
1	C	202	GLU
1	C	460	ASP
1	C	490	ASP
1	C	514	ASP
1	C	594	ASP
1	A	19	GLN
1	A	346	ARG
1	A	429	THR
1	A	469	LYS
1	A	500	GLN
1	A	565	LYS
1	A	594	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	77	ASN
1	D	302	GLN
1	D	303	GLN
1	D	308	ASN
1	D	323	GLN
1	D	336	GLN
1	D	339	ASN
1	D	544	ASN
1	D	600	GLN
1	D	622	ASN

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Mol	Chain	Res	Type
1	B	77	ASN
1	B	302	GLN
1	B	308	ASN
1	B	323	GLN
1	B	336	GLN
1	B	339	ASN
1	B	544	ASN
1	B	622	ASN
1	C	77	ASN
1	C	302	GLN
1	C	303	GLN
1	C	308	ASN
1	C	323	GLN
1	C	336	GLN
1	C	339	ASN
1	C	544	ASN
1	C	622	ASN
1	C	665	GLN
1	A	77	ASN
1	A	106	GLN
1	A	302	GLN
1	A	303	GLN
1	A	308	ASN
1	A	323	GLN
1	A	336	GLN
1	A	339	ASN
1	A	544	ASN
1	A	622	ASN

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 106 ligands modelled in this entry, 48 are monoatomic - leaving 58 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	$\# Z > 2$
2	EDO	C	706	-	3,3,3	0.44	0	2,2,2	0.51	0
2	EDO	A	711	-	3,3,3	0.60	0	2,2,2	0.27	0
2	EDO	D	703	-	3,3,3	0.50	0	2,2,2	0.42	0
2	EDO	A	705	-	3,3,3	0.52	0	2,2,2	0.38	0
2	EDO	A	715	-	3,3,3	0.48	0	2,2,2	0.56	0
6	P4G	C	722	-	10,10,10	0.94	0	9,9,9	0.83	0
2	EDO	A	704	-	3,3,3	0.62	0	2,2,2	0.32	0
2	EDO	A	713	-	3,3,3	0.60	0	2,2,2	0.35	0
2	EDO	B	701	-	3,3,3	0.62	0	2,2,2	0.22	0
2	EDO	A	703	-	3,3,3	0.65	0	2,2,2	0.24	0
2	EDO	A	708	-	3,3,3	0.38	0	2,2,2	0.13	0
2	EDO	B	705	-	3,3,3	0.59	0	2,2,2	0.58	0
3	BQZ	B	706	-	24,24,24	1.14	1 (4%)	36,36,36	0.87	0
5	PEG	D	711	-	6,6,6	0.19	0	5,5,5	0.17	0
2	EDO	A	714	-	3,3,3	0.59	0	2,2,2	0.36	0
2	EDO	C	703	-	3,3,3	0.50	0	2,2,2	0.41	0
2	EDO	C	704	-	3,3,3	0.58	0	2,2,2	0.22	0
2	EDO	A	702	-	3,3,3	0.60	0	2,2,2	0.25	0
2	EDO	D	704	-	3,3,3	0.68	0	2,2,2	0.24	0
3	BQZ	D	708	-	24,24,24	1.03	1 (4%)	36,36,36	0.83	1 (2%)
2	EDO	D	701	-	3,3,3	0.60	0	2,2,2	0.25	0
2	EDO	C	702	-	3,3,3	0.60	0	2,2,2	0.23	0
5	PEG	C	721	-	6,6,6	0.23	0	5,5,5	0.18	0
2	EDO	A	701	-	3,3,3	0.58	0	2,2,2	0.24	0
2	EDO	A	709	-	3,3,3	0.67	0	2,2,2	0.11	0
2	EDO	C	708	-	3,3,3	0.47	0	2,2,2	0.11	0
3	BQZ	C	713	-	24,24,24	1.10	1 (4%)	36,36,36	0.74	0
2	EDO	A	707	-	3,3,3	0.46	0	2,2,2	0.66	0
7	PG4	A	724	-	12,12,12	0.19	0	11,11,11	0.35	0
2	EDO	B	702	-	3,3,3	0.63	0	2,2,2	0.25	0
2	EDO	A	710	-	3,3,3	0.69	0	2,2,2	0.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	712	-	3,3,3	0.67	0	2,2,2	0.14	0
5	PEG	B	710	-	6,6,6	0.08	0	5,5,5	0.07	0
6	P4G	D	713	-	10,10,10	0.95	0	9,9,9	0.38	0
7	PG4	D	714	-	12,12,12	0.14	0	11,11,11	0.11	0
5	PEG	C	720	-	6,6,6	0.18	0	5,5,5	0.21	0
5	PEG	C	718	-	6,6,6	0.22	0	5,5,5	0.16	0
2	EDO	C	705	-	3,3,3	0.72	0	2,2,2	0.12	0
2	EDO	D	707	-	3,3,3	0.65	0	2,2,2	0.26	0
2	EDO	C	710	-	3,3,3	0.60	0	2,2,2	0.82	0
5	PEG	D	710	-	6,6,6	0.13	0	5,5,5	0.16	0
2	EDO	C	709	-	3,3,3	0.79	0	2,2,2	0.12	0
6	P4G	A	723	-	10,10,10	0.93	0	9,9,9	0.53	0
7	PG4	C	723	-	12,12,12	0.33	0	11,11,11	0.47	0
2	EDO	C	712	-	3,3,3	0.48	0	2,2,2	0.28	0
2	EDO	D	702	-	3,3,3	0.68	0	2,2,2	0.11	0
2	EDO	B	704	-	3,3,3	0.64	0	2,2,2	0.13	0
2	EDO	C	707	-	3,3,3	0.49	0	2,2,2	0.50	0
2	EDO	D	705	-	3,3,3	0.56	0	2,2,2	0.31	0
2	EDO	D	706	-	3,3,3	0.57	0	2,2,2	0.38	0
2	EDO	B	703	-	3,3,3	0.60	0	2,2,2	0.29	0
2	EDO	C	711	-	3,3,3	0.63	0	2,2,2	0.63	0
2	EDO	A	706	-	3,3,3	0.70	0	2,2,2	0.06	0
2	EDO	C	701	-	3,3,3	0.59	0	2,2,2	0.25	0
5	PEG	A	722	-	6,6,6	0.27	0	5,5,5	0.21	0
5	PEG	D	712	-	6,6,6	0.21	0	5,5,5	0.13	0
3	BQZ	A	716	-	24,24,24	1.18	3 (12%)	36,36,36	0.85	0
5	PEG	C	719	-	6,6,6	0.19	0	5,5,5	0.17	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	EDO	C	706	-	-	1/1/1/1	-
2	EDO	A	711	-	-	1/1/1/1	-
2	EDO	D	703	-	-	1/1/1/1	-
2	EDO	A	705	-	-	1/1/1/1	-
2	EDO	A	715	-	-	0/1/1/1	-
6	P4G	C	722	-	-	4/8/8/8	-
2	EDO	A	704	-	-	0/1/1/1	-
2	EDO	A	713	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	701	-	-	0/1/1/1	-
2	EDO	A	703	-	-	0/1/1/1	-
2	EDO	A	708	-	-	0/1/1/1	-
2	EDO	B	705	-	-	0/1/1/1	-
3	BQZ	B	706	-	-	0/6/50/50	0/2/2/2
5	PEG	D	711	-	-	2/4/4/4	-
2	EDO	A	714	-	-	1/1/1/1	-
2	EDO	C	703	-	-	0/1/1/1	-
2	EDO	C	704	-	-	0/1/1/1	-
2	EDO	A	702	-	-	1/1/1/1	-
2	EDO	D	704	-	-	1/1/1/1	-
3	BQZ	D	708	-	-	0/6/50/50	0/2/2/2
2	EDO	D	701	-	-	0/1/1/1	-
2	EDO	C	702	-	-	1/1/1/1	-
5	PEG	C	721	-	-	2/4/4/4	-
2	EDO	A	701	-	-	1/1/1/1	-
2	EDO	A	709	-	-	1/1/1/1	-
2	EDO	C	708	-	-	1/1/1/1	-
3	BQZ	C	713	-	-	0/6/50/50	0/2/2/2
2	EDO	A	707	-	-	1/1/1/1	-
7	PG4	A	724	-	-	4/10/10/10	-
2	EDO	B	702	-	-	0/1/1/1	-
2	EDO	A	710	-	-	1/1/1/1	-
2	EDO	A	712	-	-	0/1/1/1	-
5	PEG	B	710	-	-	0/4/4/4	-
6	P4G	D	713	-	-	4/8/8/8	-
7	PG4	D	714	-	-	7/10/10/10	-
5	PEG	C	720	-	-	1/4/4/4	-
5	PEG	C	718	-	-	3/4/4/4	-
2	EDO	C	705	-	-	0/1/1/1	-
2	EDO	D	707	-	-	1/1/1/1	-
2	EDO	C	710	-	-	1/1/1/1	-
5	PEG	D	710	-	-	1/4/4/4	-
2	EDO	C	709	-	-	0/1/1/1	-
6	P4G	A	723	-	-	4/8/8/8	-
7	PG4	C	723	-	-	6/10/10/10	-
2	EDO	C	712	-	-	1/1/1/1	-
2	EDO	D	702	-	-	1/1/1/1	-
2	EDO	B	704	-	-	0/1/1/1	-
2	EDO	C	707	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	D	705	-	-	1/1/1/1	-
2	EDO	D	706	-	-	0/1/1/1	-
2	EDO	B	703	-	-	1/1/1/1	-
2	EDO	C	711	-	-	1/1/1/1	-
2	EDO	A	706	-	-	1/1/1/1	-
2	EDO	C	701	-	-	0/1/1/1	-
5	PEG	A	722	-	-	2/4/4/4	-
5	PEG	D	712	-	-	3/4/4/4	-
3	BQZ	A	716	-	-	0/6/50/50	0/2/2/2
5	PEG	C	719	-	-	0/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	716	BQZ	O8-C8	2.40	1.48	1.43
3	D	708	BQZ	C12-C11	2.31	1.58	1.52
3	B	706	BQZ	C8-C7	2.26	1.58	1.52
3	C	713	BQZ	O8-C8	2.06	1.47	1.43
3	A	716	BQZ	C10-C11	2.01	1.57	1.52
3	A	716	BQZ	O9-C9	-2.01	1.38	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	708	BQZ	C1-O1-C7	-2.01	112.98	117.96

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	722	P4G	O2-C3-C4-O3
7	C	723	PG4	O3-C5-C6-O4
6	D	713	P4G	O2-C3-C4-O3
7	D	714	PG4	O3-C5-C6-O4
7	C	723	PG4	O4-C7-C8-O5
5	C	718	PEG	O2-C3-C4-O4
7	A	724	PG4	O2-C3-C4-O3
2	D	704	EDO	O1-C1-C2-O2
2	D	705	EDO	O1-C1-C2-O2
2	D	707	EDO	O1-C1-C2-O2
2	C	706	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	C	710	EDO	O1-C1-C2-O2
2	A	707	EDO	O1-C1-C2-O2
2	A	710	EDO	O1-C1-C2-O2
6	A	723	P4G	O3-C5-C6-O4
6	A	723	P4G	O2-C3-C4-O3
6	D	713	P4G	C1-C2-O2-C3
2	A	706	EDO	O1-C1-C2-O2
6	D	713	P4G	O3-C5-C6-O4
7	D	714	PG4	C6-C5-O3-C4
7	D	714	PG4	C4-C3-O2-C2
7	A	724	PG4	C5-C6-O4-C7
5	C	718	PEG	C4-C3-O2-C2
5	D	711	PEG	C4-C3-O2-C2
7	C	723	PG4	C6-C5-O3-C4
7	A	724	PG4	C4-C3-O2-C2
6	D	713	P4G	C3-C4-O3-C5
7	D	714	PG4	C8-C7-O4-C6
6	C	722	P4G	C6-C5-O3-C4
7	C	723	PG4	C4-C3-O2-C2
6	A	723	P4G	C4-C3-O2-C2
5	C	718	PEG	C1-C2-O2-C3
5	A	722	PEG	O2-C3-C4-O4
7	C	723	PG4	C3-C4-O3-C5
2	A	702	EDO	O1-C1-C2-O2
7	D	714	PG4	C5-C6-O4-C7
6	A	723	P4G	C5-C6-O4-C7
5	D	712	PEG	O1-C1-C2-O2
5	C	720	PEG	C4-C3-O2-C2
7	D	714	PG4	C1-C2-O2-C3
7	D	714	PG4	O1-C1-C2-O2
2	C	708	EDO	O1-C1-C2-O2
2	A	709	EDO	O1-C1-C2-O2
5	A	722	PEG	C4-C3-O2-C2
6	C	722	P4G	C1-C2-O2-C3
5	D	712	PEG	C1-C2-O2-C3
6	C	722	P4G	C4-C3-O2-C2
2	D	703	EDO	O1-C1-C2-O2
5	D	710	PEG	C1-C2-O2-C3
5	C	721	PEG	C4-C3-O2-C2
7	A	724	PG4	O1-C1-C2-O2
2	D	702	EDO	O1-C1-C2-O2
2	C	702	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	C	711	EDO	O1-C1-C2-O2
2	A	701	EDO	O1-C1-C2-O2
2	A	705	EDO	O1-C1-C2-O2
2	A	711	EDO	O1-C1-C2-O2
2	A	714	EDO	O1-C1-C2-O2
5	D	712	PEG	O2-C3-C4-O4
5	C	721	PEG	O1-C1-C2-O2
2	B	703	EDO	O1-C1-C2-O2
2	C	712	EDO	O1-C1-C2-O2
5	D	711	PEG	O1-C1-C2-O2
7	C	723	PG4	O2-C3-C4-O3

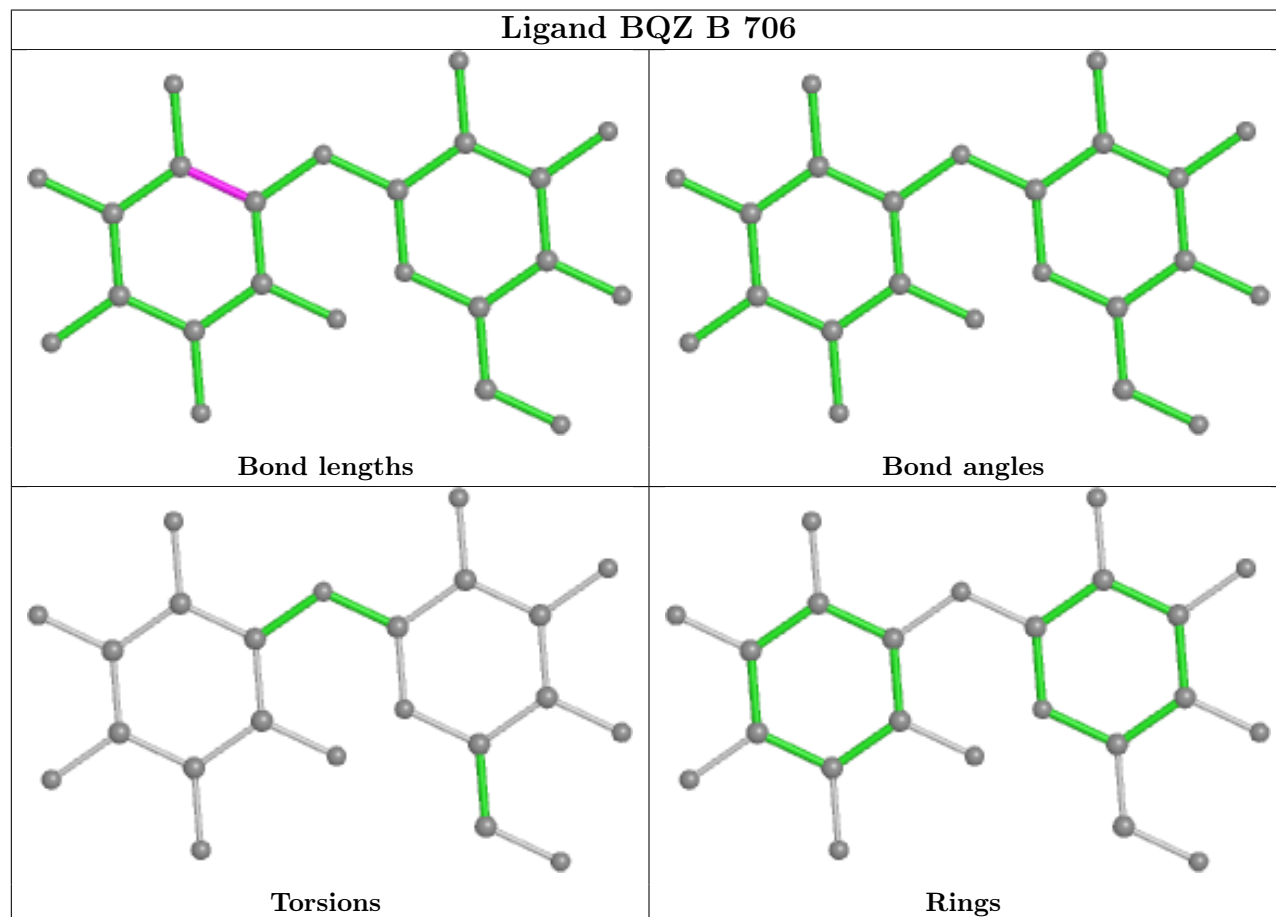
There are no ring outliers.

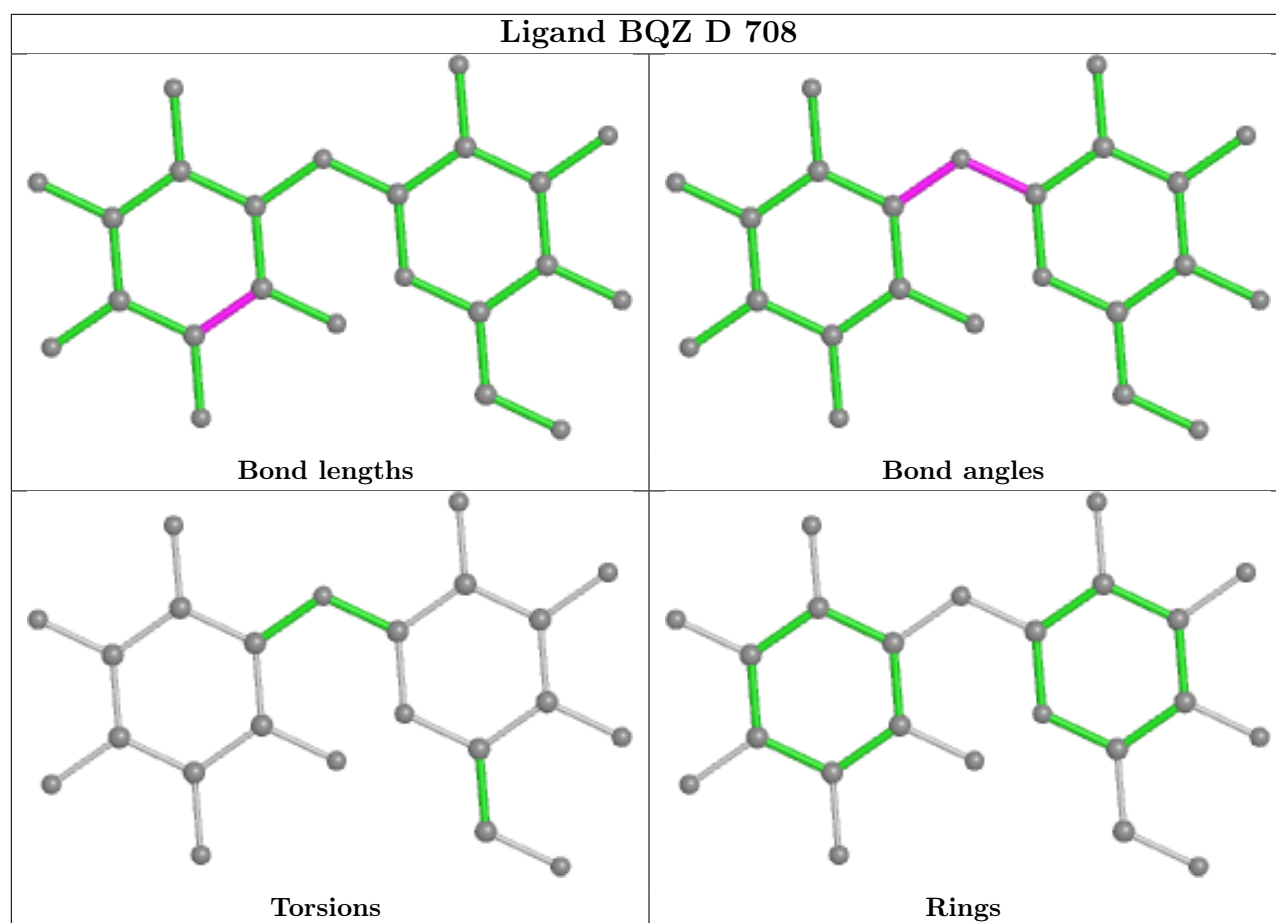
23 monomers are involved in 50 short contacts:

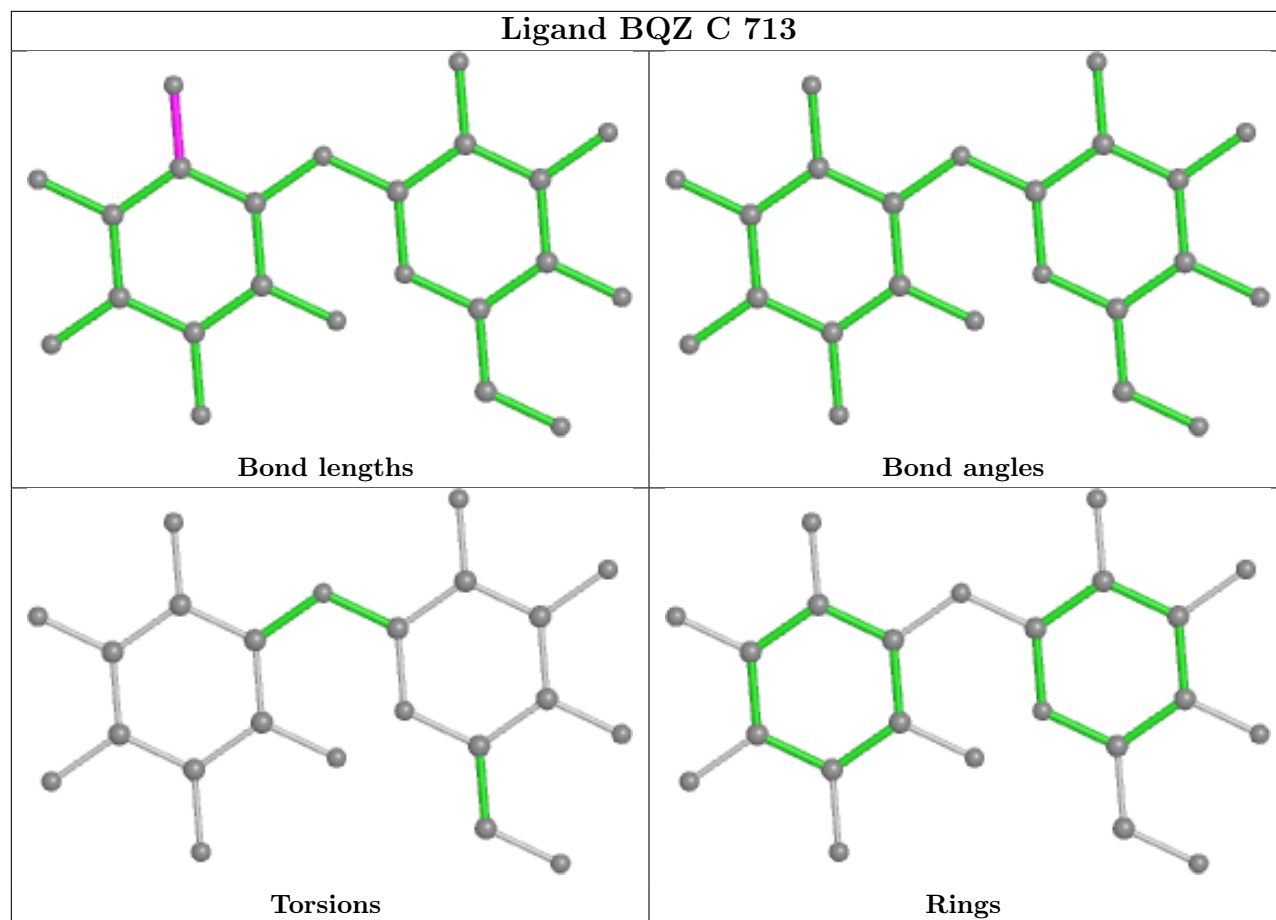
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	706	EDO	3	0
2	A	705	EDO	2	0
2	A	715	EDO	1	0
6	C	722	P4G	4	0
2	A	708	EDO	3	0
2	B	705	EDO	2	0
2	D	701	EDO	1	0
5	C	721	PEG	2	0
2	C	708	EDO	1	0
2	A	707	EDO	3	0
2	A	710	EDO	2	0
7	D	714	PG4	4	0
5	C	720	PEG	1	0
2	C	705	EDO	1	0
2	C	710	EDO	9	0
2	C	709	EDO	1	0
7	C	723	PG4	3	0
2	C	712	EDO	2	0
2	B	704	EDO	1	0
2	C	707	EDO	2	0
2	C	711	EDO	3	0
2	A	706	EDO	1	0
2	C	701	EDO	1	0

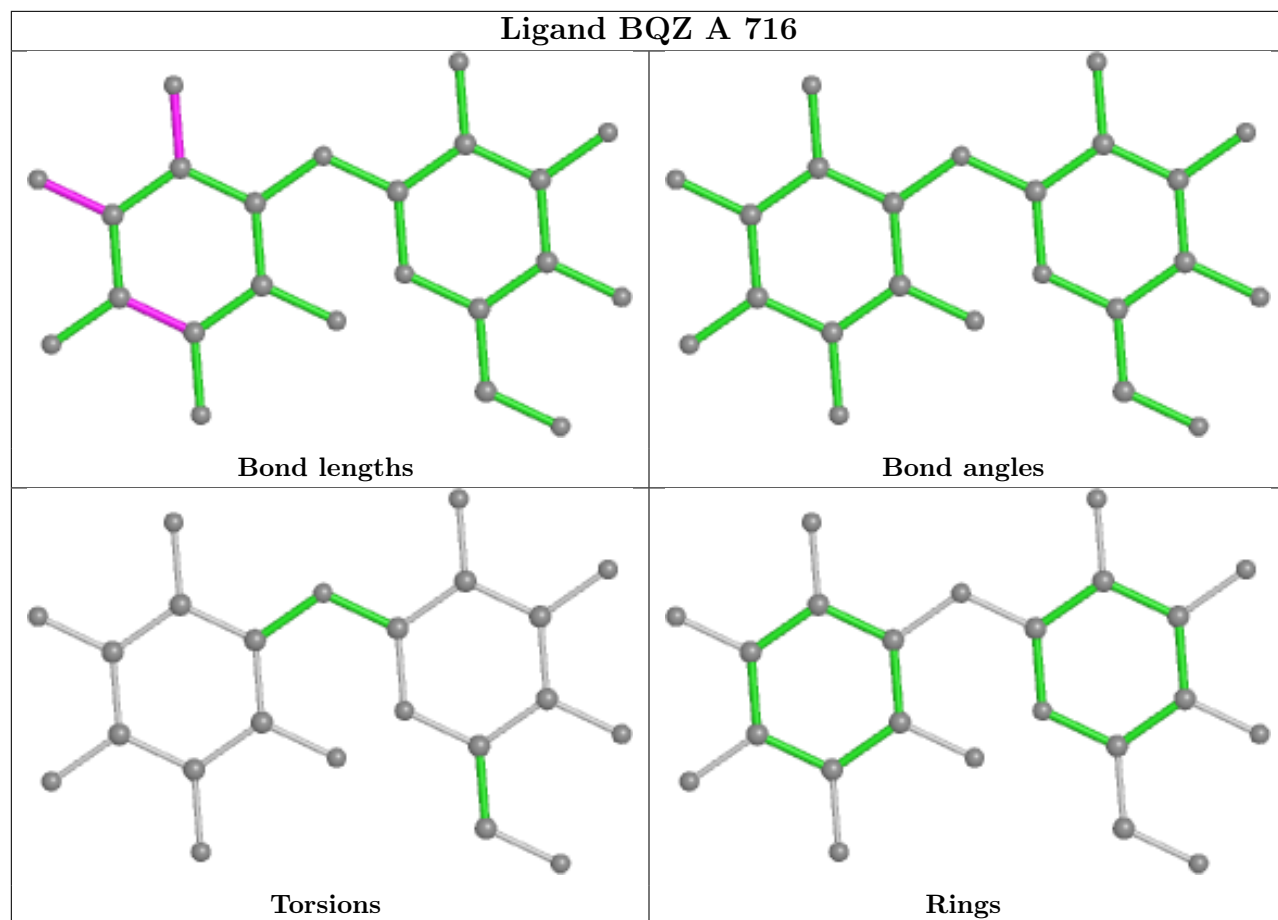
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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, 95th 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	671/683 (98%)	0.48	49 (7%)	15 14	23, 38, 70, 117	0
1	B	670/683 (98%)	0.48	45 (6%)	17 16	30, 45, 75, 102	0
1	C	670/683 (98%)	0.34	32 (4%)	30 29	22, 39, 64, 96	0
1	D	670/683 (98%)	0.57	44 (6%)	18 17	31, 48, 78, 118	0
All	All	2681/2732 (98%)	0.47	170 (6%)	20 19	22, 43, 73, 118	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	674	GLY	9.0
1	B	133	LYS	8.3
1	A	469	LYS	7.9
1	D	21	PRO	7.8
1	D	22	ALA	7.6
1	D	23	GLU	7.3
1	B	22	ALA	7.1
1	A	673	GLY	6.9
1	B	21	PRO	6.8
1	C	673	GLY	6.7
1	A	470	GLU	6.6
1	D	24	GLY	6.5
1	B	24	GLY	6.4
1	D	222	PHE	6.1
1	D	673	GLY	6.1
1	D	149	GLU	6.0
1	C	23	GLU	5.8
1	A	473	GLY	5.6
1	D	350	PRO	5.6
1	A	678	HIS	5.6
1	D	564	GLY	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	452	ALA	5.5
1	C	133	LYS	5.4
1	A	8	ALA	5.3
1	D	133	LYS	5.2
1	D	20	PHE	5.2
1	C	8	ALA	5.1
1	B	350	PRO	5.0
1	B	564	GLY	4.9
1	B	149	GLU	4.9
1	D	563	GLU	4.8
1	D	676	ILE	4.8
1	B	23	GLU	4.6
1	A	23	GLU	4.6
1	D	8	ALA	4.5
1	B	20	PHE	4.5
1	A	381	GLU	4.4
1	B	132	ALA	4.4
1	C	451	LEU	4.3
1	C	676	ILE	4.3
1	B	222	PHE	4.3
1	D	19	GLN	4.3
1	A	468	PRO	4.3
1	B	19	GLN	4.3
1	D	471	THR	4.2
1	D	562	PRO	4.2
1	A	24	GLY	4.1
1	D	674	GLY	4.1
1	C	469	LYS	4.0
1	A	445	GLU	4.0
1	D	131	ASP	4.0
1	A	57	GLY	4.0
1	A	22	ALA	3.9
1	C	674	GLY	3.8
1	A	456	LEU	3.8
1	B	186	PRO	3.7
1	A	21	PRO	3.7
1	D	56	ALA	3.6
1	B	351	ASN	3.6
1	D	134	ASP	3.5
1	B	347	ALA	3.5
1	A	134	ASP	3.4
1	A	504	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	674	GLY	3.4
1	C	470	GLU	3.4
1	D	672	GLU	3.4
1	A	471	THR	3.4
1	A	467	PHE	3.4
1	C	672	GLU	3.4
1	A	389	LEU	3.4
1	C	10	GLU	3.4
1	A	676	ILE	3.4
1	A	373	ALA	3.3
1	D	677	ASN	3.3
1	A	386	ILE	3.3
1	D	374	ASN	3.2
1	D	470	GLU	3.2
1	B	131	ASP	3.2
1	A	461	GLY	3.1
1	C	21	PRO	3.1
1	B	563	GLU	3.1
1	A	53	PHE	3.1
1	A	56	ALA	3.1
1	B	221	ALA	3.0
1	C	564	GLY	3.0
1	C	134	ASP	3.0
1	A	455	GLY	3.0
1	C	22	ALA	3.0
1	D	351	ASN	3.0
1	B	673	GLY	2.9
1	B	254	THR	2.9
1	D	253	ASN	2.9
1	A	474	GLY	2.9
1	A	133	LYS	2.9
1	A	457	LYS	2.9
1	C	504	LEU	2.8
1	A	394	VAL	2.8
1	D	221	ALA	2.8
1	A	453	SER	2.8
1	B	348	ALA	2.7
1	C	447	ALA	2.7
1	C	57	GLY	2.7
1	D	349	ASP	2.7
1	B	219	LYS	2.7
1	D	117	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	456	LEU	2.6
1	B	134	ASP	2.6
1	B	672	GLU	2.6
1	D	378	ASN	2.6
1	D	151	GLY	2.6
1	A	563	GLU	2.6
1	D	565	LYS	2.6
1	D	455	GLY	2.6
1	D	162	ALA	2.5
1	C	381	GLU	2.5
1	B	252	LYS	2.5
1	C	9	PHE	2.5
1	C	56	ALA	2.5
1	B	248	PRO	2.5
1	B	565	LYS	2.5
1	C	459	THR	2.5
1	B	184	VAL	2.5
1	A	477	VAL	2.5
1	B	253	ASN	2.5
1	C	454	ILE	2.5
1	D	132	ALA	2.5
1	B	671	GLY	2.4
1	B	56	ALA	2.4
1	B	352	ALA	2.4
1	A	672	GLU	2.4
1	C	132	ALA	2.4
1	A	459	THR	2.4
1	D	459	THR	2.3
1	D	255	TYR	2.3
1	B	250	TYR	2.3
1	D	377	GLY	2.3
1	B	203	GLY	2.3
1	B	257	GLN	2.3
1	A	10	GLU	2.3
1	B	255	TYR	2.3
1	B	378	ASN	2.3
1	B	562	PRO	2.3
1	C	477	VAL	2.3
1	A	634	ILE	2.3
1	A	9	PHE	2.2
1	D	147	TRP	2.2
1	A	677	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	399	VAL	2.2
1	B	677	ASN	2.2
1	A	449	ALA	2.2
1	B	16	GLU	2.2
1	A	398	ALA	2.1
1	B	538	LEU	2.1
1	B	653	ALA	2.1
1	C	20	PHE	2.1
1	A	58	LYS	2.1
1	B	59	LEU	2.1
1	A	465	LEU	2.1
1	C	393	GLU	2.1
1	D	153	THR	2.1
1	C	24	GLY	2.1
1	B	115	ILE	2.0
1	D	18	PRO	2.0
1	A	132	ALA	2.0
1	A	464	PHE	2.0
1	D	57	GLY	2.0
1	C	440	TYR	2.0
1	A	458	ASP	2.0
1	D	15	PRO	2.0
1	C	60	PRO	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, 95th 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	D	707	4/4	0.50	0.19	68,69,69,69	0
4	CA	C	715	1/1	0.62	0.14	96,96,96,96	0
8	CL	D	716	1/1	0.69	0.08	83,83,83,83	0
5	PEG	C	721	7/7	0.72	0.31	47,52,55,56	0
2	EDO	A	703	4/4	0.72	0.41	66,67,67,67	0
8	CL	C	725	1/1	0.72	0.26	78,78,78,78	0
2	EDO	C	707	4/4	0.74	0.31	54,57,58,58	0
2	EDO	A	711	4/4	0.74	0.24	63,63,64,64	0
5	PEG	D	711	7/7	0.76	0.17	64,69,74,75	0
2	EDO	B	704	4/4	0.78	0.16	74,75,75,75	0
5	PEG	D	710	7/7	0.78	0.19	71,73,75,75	0
8	CL	B	716	1/1	0.79	0.15	81,81,81,81	0
6	P4G	D	713	11/11	0.79	0.21	52,56,64,65	0
2	EDO	A	712	4/4	0.80	0.16	56,56,56,58	0
5	PEG	C	718	7/7	0.81	0.27	53,58,63,63	0
2	EDO	A	709	4/4	0.81	0.15	60,61,62,63	0
2	EDO	A	701	4/4	0.82	0.15	50,51,53,55	0
2	EDO	A	702	4/4	0.82	0.17	60,61,62,62	0
2	EDO	C	705	4/4	0.82	0.20	41,43,46,47	0
6	P4G	C	722	11/11	0.83	0.21	39,42,48,48	0
4	CA	C	716	1/1	0.83	0.08	77,77,77,77	0
8	CL	D	717	1/1	0.83	0.11	74,74,74,74	0
2	EDO	A	710	4/4	0.83	0.23	52,52,53,53	0
2	EDO	C	709	4/4	0.83	0.22	47,49,51,51	0
2	EDO	B	703	4/4	0.84	0.12	59,59,60,61	0
2	EDO	D	706	4/4	0.84	0.31	70,71,71,71	0
4	CA	B	707	1/1	0.84	0.09	75,75,75,75	0
8	CL	C	726	1/1	0.84	0.12	79,79,79,79	0
2	EDO	A	713	4/4	0.85	0.18	76,76,76,77	0
8	CL	B	713	1/1	0.85	0.30	78,78,78,78	0
2	EDO	B	705	4/4	0.85	0.26	41,42,42,43	0
5	PEG	D	712	7/7	0.85	0.15	57,58,59,60	0
4	CA	A	719	1/1	0.85	0.16	82,82,82,82	0
8	CL	B	717	1/1	0.86	0.10	77,77,77,77	0
2	EDO	D	705	4/4	0.86	0.18	52,53,57,59	0
7	PG4	C	723	13/13	0.86	0.20	45,47,52,54	0
2	EDO	C	712	4/4	0.87	0.20	64,64,65,65	0
6	P4G	A	723	11/11	0.87	0.19	39,43,46,48	0
2	EDO	A	714	4/4	0.87	0.14	59,59,60,61	0
5	PEG	A	722	7/7	0.87	0.19	47,50,56,56	0
2	EDO	D	704	4/4	0.87	0.14	50,53,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	D	701	4/4	0.88	0.13	56,56,56,57	0
5	PEG	C	720	7/7	0.88	0.21	57,57,59,60	0
2	EDO	B	701	4/4	0.88	0.17	53,53,54,54	0
2	EDO	B	702	4/4	0.88	0.17	54,54,54,55	0
2	EDO	C	704	4/4	0.88	0.13	60,62,63,64	0
8	CL	B	714	1/1	0.89	0.17	87,87,87,87	0
2	EDO	A	704	4/4	0.89	0.17	52,54,55,57	0
7	PG4	D	714	13/13	0.89	0.17	54,61,66,66	0
8	CL	B	712	1/1	0.89	0.06	76,76,76,76	0
2	EDO	C	701	4/4	0.89	0.12	49,50,50,51	0
2	EDO	A	705	4/4	0.90	0.22	55,55,56,57	0
2	EDO	A	706	4/4	0.90	0.19	40,41,41,42	0
2	EDO	C	702	4/4	0.90	0.26	49,52,54,57	0
2	EDO	A	707	4/4	0.91	0.23	40,41,41,43	0
8	CL	B	721	1/1	0.91	0.11	66,66,66,66	0
5	PEG	C	719	7/7	0.91	0.14	45,47,56,58	0
8	CL	D	715	1/1	0.91	0.16	77,77,77,77	0
8	CL	C	729	1/1	0.91	0.11	66,66,66,66	0
8	CL	C	731	1/1	0.91	0.11	58,58,58,58	0
2	EDO	C	708	4/4	0.92	0.22	48,49,51,54	0
2	EDO	C	703	4/4	0.92	0.11	54,54,55,55	0
2	EDO	C	706	4/4	0.92	0.26	39,43,45,47	0
8	CL	C	728	1/1	0.92	0.09	63,63,63,63	0
2	EDO	D	702	4/4	0.92	0.12	48,48,49,49	0
2	EDO	A	715	4/4	0.92	0.34	50,51,51,51	0
8	CL	C	737	1/1	0.92	0.10	69,69,69,69	0
2	EDO	C	710	4/4	0.93	0.27	28,32,33,35	0
4	CA	A	717	1/1	0.93	0.06	79,79,79,79	0
8	CL	B	718	1/1	0.93	0.11	77,77,77,77	0
7	PG4	A	724	13/13	0.93	0.14	41,45,57,61	0
8	CL	B	715	1/1	0.93	0.13	69,69,69,69	0
5	PEG	B	710	7/7	0.94	0.14	61,63,64,64	0
8	CL	B	720	1/1	0.94	0.10	49,49,49,49	0
8	CL	D	718	1/1	0.94	0.10	63,63,63,63	0
2	EDO	C	711	4/4	0.95	0.21	38,38,41,43	0
4	CA	A	720	1/1	0.95	0.09	74,74,74,74	0
8	CL	C	730	1/1	0.95	0.12	67,67,67,67	0
4	CA	C	717	1/1	0.95	0.04	66,66,66,66	0
3	BQZ	D	708	23/23	0.95	0.15	30,34,41,44	0
8	CL	C	732	1/1	0.96	0.09	60,60,60,60	0
2	EDO	A	708	4/4	0.96	0.19	36,38,43,44	0
4	CA	C	714	1/1	0.97	0.05	57,57,57,57	0

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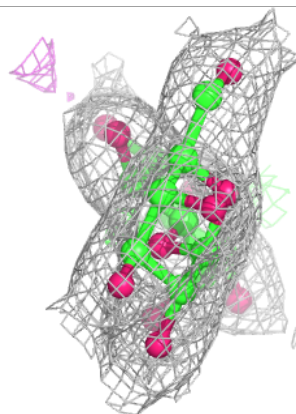
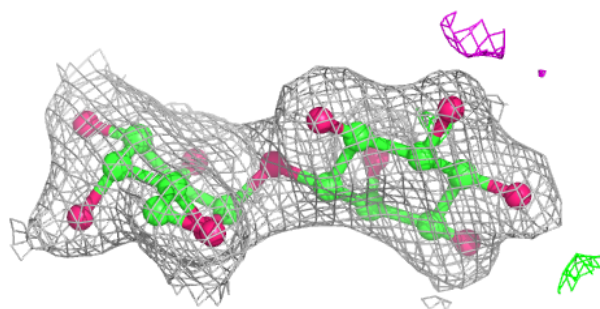
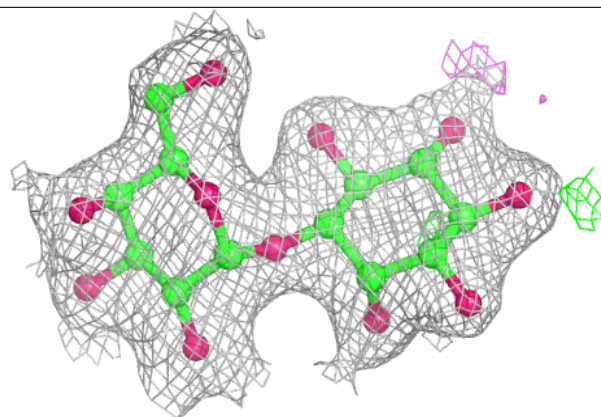
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	CL	C	724	1/1	0.97	0.13	51,51,51,51	0
4	CA	A	721	1/1	0.97	0.15	63,63,63,63	0
3	BQZ	B	706	23/23	0.97	0.15	30,34,44,45	0
3	BQZ	C	713	23/23	0.97	0.18	25,30,34,37	0
3	BQZ	A	716	23/23	0.97	0.17	22,30,34,35	0
2	EDO	D	703	4/4	0.97	0.10	57,58,58,59	0
4	CA	B	709	1/1	0.97	0.11	68,68,68,68	0
8	CL	B	719	1/1	0.97	0.05	52,52,52,52	0
8	CL	D	719	1/1	0.97	0.19	63,63,63,63	0
8	CL	A	726	1/1	0.97	0.16	46,46,46,46	0
4	CA	B	708	1/1	0.98	0.05	40,40,40,40	0
4	CA	D	709	1/1	0.98	0.07	46,46,46,46	0
8	CL	D	720	1/1	0.98	0.07	48,48,48,48	0
8	CL	C	733	1/1	0.98	0.25	60,60,60,60	0
8	CL	C	734	1/1	0.98	0.07	36,36,36,36	0
8	CL	D	721	1/1	0.98	0.07	46,46,46,46	0
8	CL	A	725	1/1	0.98	0.08	48,48,48,48	0
8	CL	B	711	1/1	0.98	0.09	55,55,55,55	0
8	CL	A	727	1/1	0.98	0.14	37,37,37,37	0
8	CL	A	728	1/1	0.98	0.09	56,56,56,56	0
8	CL	C	736	1/1	0.99	0.07	42,42,42,42	0
4	CA	A	718	1/1	0.99	0.09	44,44,44,44	0
8	CL	C	735	1/1	0.99	0.11	34,34,34,34	0

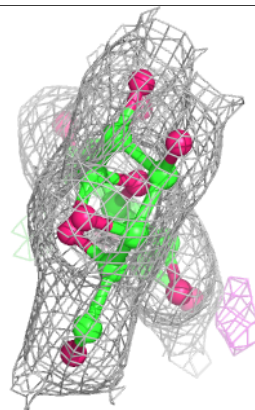
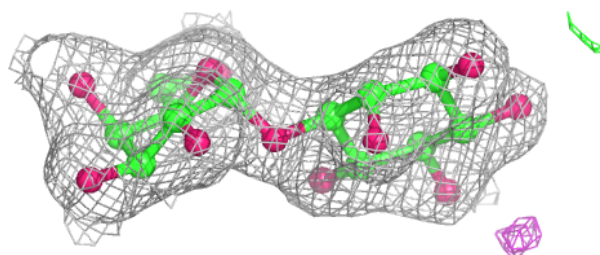
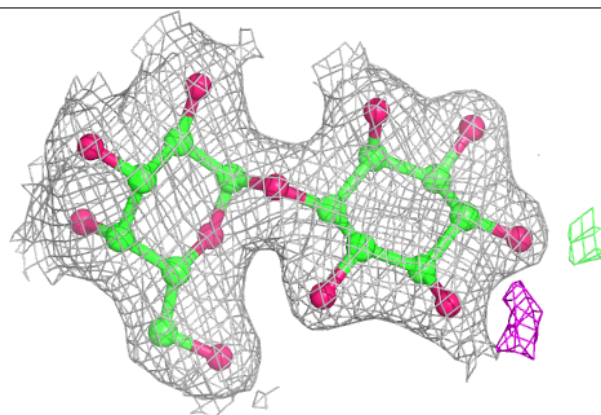
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BQZ D 708:

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

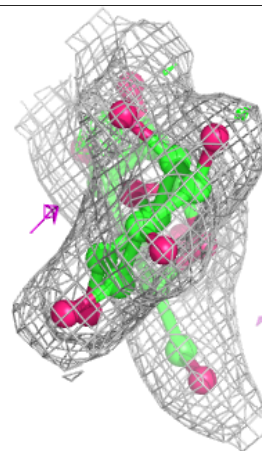
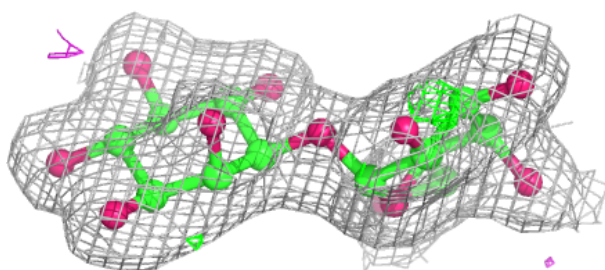
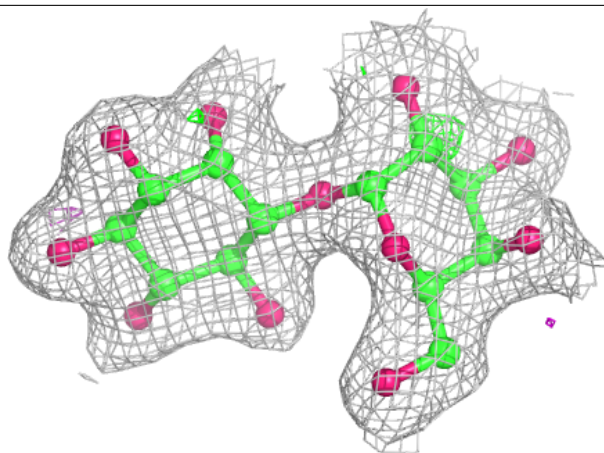
**Electron density around BQZ B 706:**

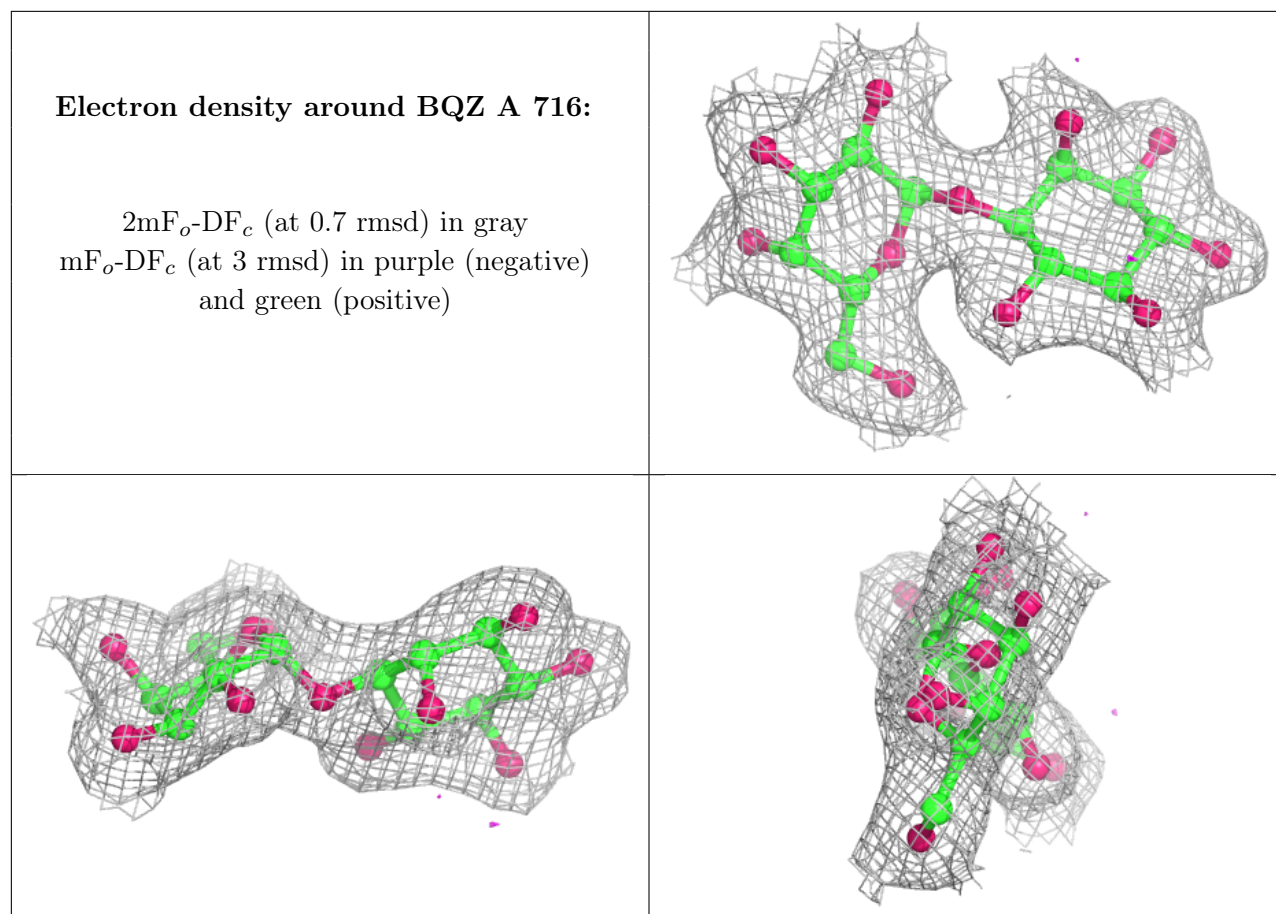
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BQZ C 713:

$2mF_o - DF_c$ (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.