



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:47 AM UTC

PDB ID : 3WF1 / pdb_00003wf1
Title : Crystal structure of human beta-galactosidase in complex with 6S-NBI-GJ
Authors : Suzuki, H.; Ohto, U.; Shimizu, T.
Deposited on : 2013-07-16
Resolution : 2.00 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

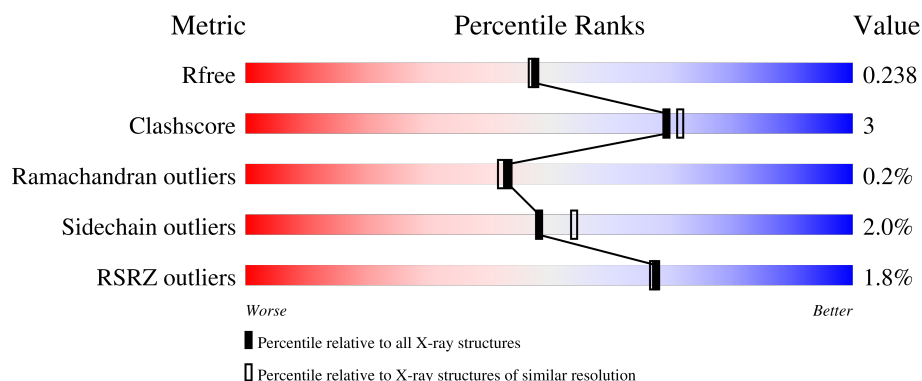
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

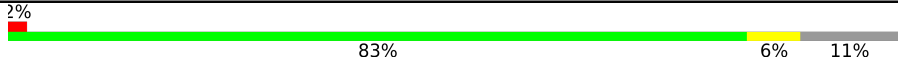
The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	678	 2% 83% 6% 11%
1	B	678	 2% 80% 9% 11%
1	C	678	 2% 79% 9% 11%
1	D	678	 % 79% 9% 11%

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
4	6GJ	B	710	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21271 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	605	Total	C	N	O	S	0	8	0
			4849	3144	805	882	18			
1	B	605	Total	C	N	O	S	0	4	0
			4831	3137	798	879	17			
1	C	603	Total	C	N	O	S	0	6	0
			4815	3126	792	880	17			
1	D	603	Total	C	N	O	S	0	5	0
			4808	3120	791	880	17			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLU	-	expression tag	UNP P16278
A	1	ALA	-	expression tag	UNP P16278
A	2	GLU	-	expression tag	UNP P16278
A	3	ALA	-	expression tag	UNP P16278
A	4	TYR	-	expression tag	UNP P16278
A	5	VAL	-	expression tag	UNP P16278
A	6	GLU	-	expression tag	UNP P16278
A	7	PHE	-	expression tag	UNP P16278
A	8	HIS	-	expression tag	UNP P16278
A	9	HIS	-	expression tag	UNP P16278
A	10	HIS	-	expression tag	UNP P16278
A	11	HIS	-	expression tag	UNP P16278
A	12	HIS	-	expression tag	UNP P16278
A	13	HIS	-	expression tag	UNP P16278
A	14	ASP	-	expression tag	UNP P16278
A	15	TYR	-	expression tag	UNP P16278
A	16	LYS	-	expression tag	UNP P16278
A	17	ASP	-	expression tag	UNP P16278
A	18	ASP	-	expression tag	UNP P16278
A	19	ASP	-	expression tag	UNP P16278
A	20	ASP	-	expression tag	UNP P16278

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Chain	Residue	Modelled	Actual	Comment	Reference
A	21	LYS	-	expression tag	UNP P16278
A	22	THR	-	expression tag	UNP P16278
A	23	SER	-	expression tag	UNP P16278
B	0	GLU	-	expression tag	UNP P16278
B	1	ALA	-	expression tag	UNP P16278
B	2	GLU	-	expression tag	UNP P16278
B	3	ALA	-	expression tag	UNP P16278
B	4	TYR	-	expression tag	UNP P16278
B	5	VAL	-	expression tag	UNP P16278
B	6	GLU	-	expression tag	UNP P16278
B	7	PHE	-	expression tag	UNP P16278
B	8	HIS	-	expression tag	UNP P16278
B	9	HIS	-	expression tag	UNP P16278
B	10	HIS	-	expression tag	UNP P16278
B	11	HIS	-	expression tag	UNP P16278
B	12	HIS	-	expression tag	UNP P16278
B	13	HIS	-	expression tag	UNP P16278
B	14	ASP	-	expression tag	UNP P16278
B	15	TYR	-	expression tag	UNP P16278
B	16	LYS	-	expression tag	UNP P16278
B	17	ASP	-	expression tag	UNP P16278
B	18	ASP	-	expression tag	UNP P16278
B	19	ASP	-	expression tag	UNP P16278
B	20	ASP	-	expression tag	UNP P16278
B	21	LYS	-	expression tag	UNP P16278
B	22	THR	-	expression tag	UNP P16278
B	23	SER	-	expression tag	UNP P16278
C	0	GLU	-	expression tag	UNP P16278
C	1	ALA	-	expression tag	UNP P16278
C	2	GLU	-	expression tag	UNP P16278
C	3	ALA	-	expression tag	UNP P16278
C	4	TYR	-	expression tag	UNP P16278
C	5	VAL	-	expression tag	UNP P16278
C	6	GLU	-	expression tag	UNP P16278
C	7	PHE	-	expression tag	UNP P16278
C	8	HIS	-	expression tag	UNP P16278
C	9	HIS	-	expression tag	UNP P16278
C	10	HIS	-	expression tag	UNP P16278
C	11	HIS	-	expression tag	UNP P16278
C	12	HIS	-	expression tag	UNP P16278
C	13	HIS	-	expression tag	UNP P16278
C	14	ASP	-	expression tag	UNP P16278

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Chain	Residue	Modelled	Actual	Comment	Reference
C	15	TYR	-	expression tag	UNP P16278
C	16	LYS	-	expression tag	UNP P16278
C	17	ASP	-	expression tag	UNP P16278
C	18	ASP	-	expression tag	UNP P16278
C	19	ASP	-	expression tag	UNP P16278
C	20	ASP	-	expression tag	UNP P16278
C	21	LYS	-	expression tag	UNP P16278
C	22	THR	-	expression tag	UNP P16278
C	23	SER	-	expression tag	UNP P16278
D	0	GLU	-	expression tag	UNP P16278
D	1	ALA	-	expression tag	UNP P16278
D	2	GLU	-	expression tag	UNP P16278
D	3	ALA	-	expression tag	UNP P16278
D	4	TYR	-	expression tag	UNP P16278
D	5	VAL	-	expression tag	UNP P16278
D	6	GLU	-	expression tag	UNP P16278
D	7	PHE	-	expression tag	UNP P16278
D	8	HIS	-	expression tag	UNP P16278
D	9	HIS	-	expression tag	UNP P16278
D	10	HIS	-	expression tag	UNP P16278
D	11	HIS	-	expression tag	UNP P16278
D	12	HIS	-	expression tag	UNP P16278
D	13	HIS	-	expression tag	UNP P16278
D	14	ASP	-	expression tag	UNP P16278
D	15	TYR	-	expression tag	UNP P16278
D	16	LYS	-	expression tag	UNP P16278
D	17	ASP	-	expression tag	UNP P16278
D	18	ASP	-	expression tag	UNP P16278
D	19	ASP	-	expression tag	UNP P16278
D	20	ASP	-	expression tag	UNP P16278
D	21	LYS	-	expression tag	UNP P16278
D	22	THR	-	expression tag	UNP P16278
D	23	SER	-	expression tag	UNP P16278

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

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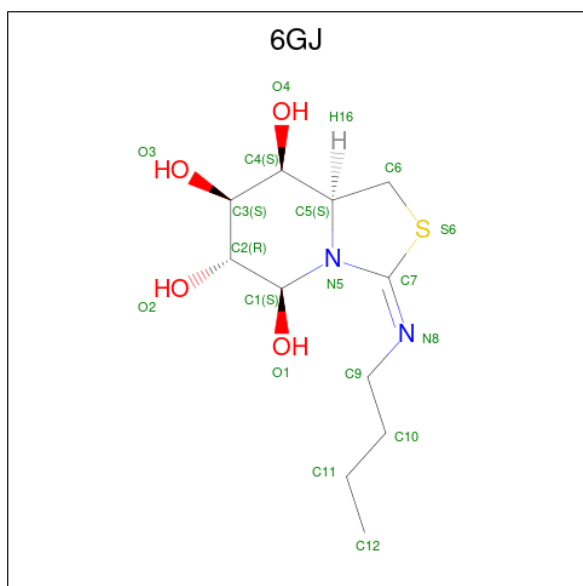
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		

- Molecule 4 is (3E,5S,6R,7S,8S,8aS)-3-(butylimino)hexahydro[1,3]thiazolo[3,4-a]pyridine-5,6,7,8-tetrol (CCD ID: 6GJ) (formula: C₁₁H₂₀N₂O₄S).



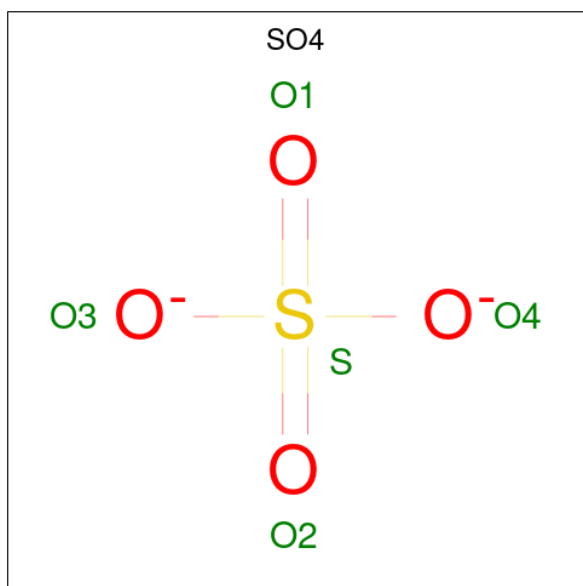
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			18	11	2	4	1		
4	B	1	Total	C	N	O	S	0	0
			18	11	2	4	1		
4	C	1	Total	C	N	O	S	0	0
			18	11	2	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	S	0	0
			18	11	2	4	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

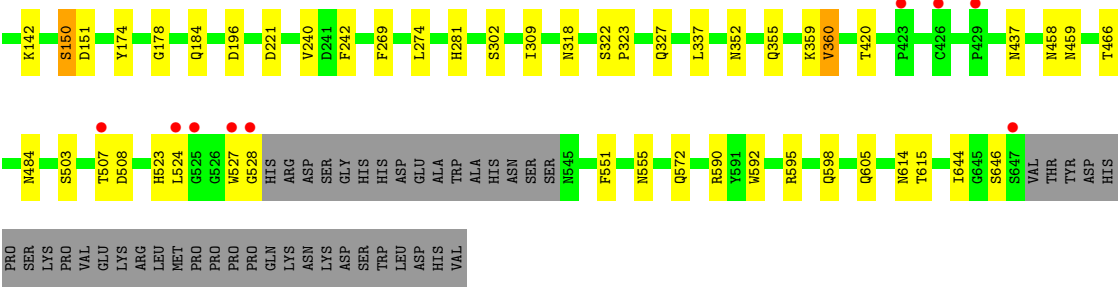
- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



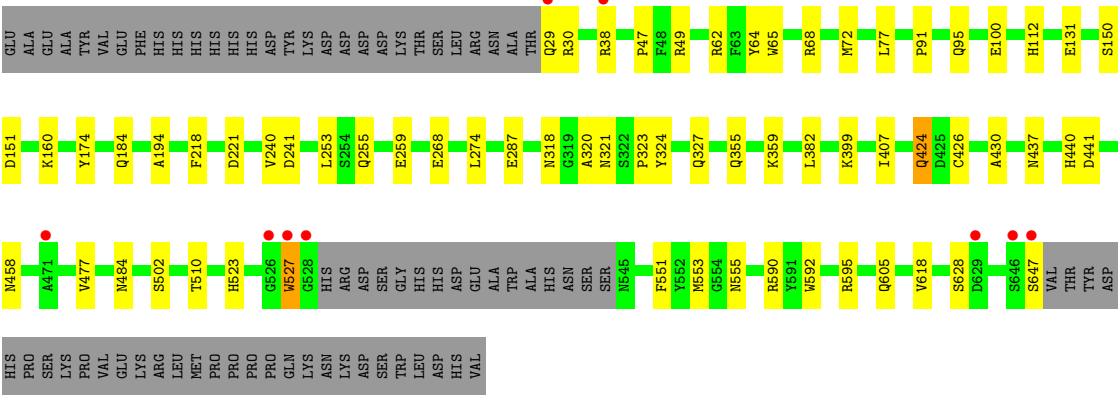
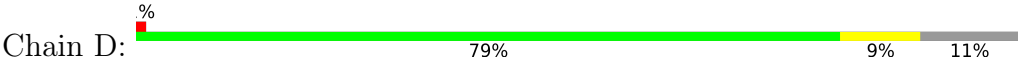
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	414	Total	O	0	0
			414	414		
7	B	446	Total	O	0	0
			446	446		
7	C	379	Total	O	0	0
			379	379		
7	D	357	Total	O	0	0
			357	357		



● Molecule 1: Beta-galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.91Å 116.01Å 140.57Å 90.00° 92.28° 90.00°	Depositor
Resolution (Å)	25.90 – 2.00 25.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.4 (25.90-2.00) 97.4 (25.90-2.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.186 , 0.232 0.194 , 0.238	Depositor DCC
R_{free} test set	10030 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.054 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21271	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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: NAG, 6GJ, CL, SO4, EDO

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	0.99	1/5041 (0.0%)	0.96	3/6873 (0.0%)
1	B	0.98	2/5002 (0.0%)	0.99	5/6822 (0.1%)
1	C	0.91	1/4995 (0.0%)	0.95	2/6814 (0.0%)
1	D	0.92	0/4981	0.96	4/6796 (0.1%)
All	All	0.95	4/20019 (0.0%)	0.97	14/27305 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	TYR	C-O	-5.86	1.15	1.23
1	B	607	ILE	C-O	-5.33	1.18	1.24
1	A	450	ILE	CA-C	5.32	1.57	1.53
1	C	142	LYS	CA-C	5.26	1.59	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	407	ILE	CB-CA-C	-6.21	103.76	112.14
1	B	335	ALA	CA-C-N	6.07	126.24	119.32
1	B	335	ALA	C-N-CA	6.07	126.24	119.32
1	A	459	ASN	N-CA-C	5.71	118.71	111.69
1	B	459	ASN	N-CA-C	5.60	117.46	111.36
1	B	49	ARG	CG-CD-NE	-5.59	99.69	112.00
1	D	477	VAL	N-CA-C	5.29	115.92	108.36
1	D	49	ARG	CG-CD-NE	-5.26	100.43	112.00
1	C	49	ARG	CG-CD-NE	-5.21	100.53	112.00
1	C	79	ALA	N-CA-C	5.15	116.67	108.79
1	B	486	GLY	N-CA-C	-5.14	105.12	111.70
1	A	279	GLN	CA-C-N	-5.12	114.44	119.92
1	A	279	GLN	C-N-CA	-5.12	114.44	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	194	ALA	N-CA-C	5.11	116.93	111.36

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	4849	0	4723	23	0
1	B	4831	0	4701	39	0
1	C	4815	0	4688	30	0
1	D	4808	0	4682	42	0
2	A	56	0	50	0	0
2	B	56	0	51	0	0
2	C	56	0	52	0	0
2	D	56	0	52	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	18	0	20	1	0
4	B	18	0	20	7	0
4	C	18	0	19	0	0
4	D	18	0	20	0	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
5	C	10	0	0	0	0
5	D	10	0	0	0	0
6	A	8	0	12	0	0
6	B	8	0	12	3	0
6	C	8	0	12	0	0
6	D	8	0	12	0	0
7	A	414	0	0	5	0
7	B	446	0	0	7	0
7	C	379	0	0	1	0
7	D	357	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	21271	0	19126	135	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 (135) 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:259:GLU:HB2	7:D:1103:HOH:O	1.64	0.96
1:D:555:ASN:HB2	2:D:704:NAG:O5	1.70	0.90
1:B:437:ASN:HD21	1:B:458:ASN:H	1.15	0.88
1:A:327:GLN:HE22	1:A:484:ASN:HD21	1.29	0.81
1:A:437:ASN:HD21	1:A:458:ASN:H	1.29	0.80
1:D:437:ASN:HD21	1:D:458:ASN:H	1.33	0.75
1:B:382:LEU:HD23	1:B:524:LEU:HD12	1.73	0.70
4:B:710:6GJ:H6	4:B:710:6GJ:O1	1.91	0.69
4:B:710:6GJ:O1	4:B:710:6GJ:C9	2.41	0.69
1:B:327:GLN:HE22	1:B:484:ASN:HD21	1.40	0.69
1:C:437:ASN:HD21	1:C:458:ASN:H	1.41	0.69
1:D:426:CYS:SG	7:D:1101:HOH:O	2.50	0.68
1:A:105:GLU:O	1:A:109[A]:ARG:HG3	1.93	0.68
1:C:615:THR:HG22	7:C:904:HOH:O	1.93	0.67
1:C:327:GLN:HE22	1:C:484:ASN:HD21	1.42	0.65
1:A:112:HIS:HD2	7:A:1048:HOH:O	1.79	0.64
1:B:109[A]:ARG:NH1	1:B:113:GLU:OE2	2.30	0.63
1:D:112:HIS:HD2	7:D:1104:HOH:O	1.80	0.63
1:B:273:TRP:CZ3	4:B:710:6GJ:S6	2.94	0.60
1:B:273:TRP:CH2	4:B:710:6GJ:S6	2.97	0.57
1:D:327:GLN:HE22	1:D:484:ASN:HD21	1.51	0.57
1:D:555:ASN:CB	2:D:704:NAG:O5	2.50	0.56
1:A:234[B]:GLN:HE21	1:A:235:GLY:N	2.04	0.55
1:D:255:GLN:HG2	7:D:1103:HOH:O	2.07	0.55
1:A:382:LEU:HD23	1:A:524:LEU:HD12	1.89	0.55
1:C:318:ASN:HD21	1:C:590:ARG:HH21	1.54	0.54
1:C:83:TYR:CE2	1:C:128:ALA:HB2	2.43	0.53
1:C:35:ASP:OD2	1:C:38:ARG:HB2	2.09	0.53
1:A:318:ASN:HD21	1:A:590:ARG:HH21	1.57	0.52
1:D:426:CYS:CB	7:D:1101:HOH:O	2.58	0.51
1:C:281:HIS:CE1	1:C:644:ILE:HD12	2.46	0.51
1:B:109[A]:ARG:NE	7:B:1086:HOH:O	2.44	0.50
1:C:523:HIS:CE1	1:C:527:TRP:CZ2	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:437:ASN:ND2	1:D:458:ASN:H	2.07	0.50
1:D:553:MET:CE	7:D:1116:HOH:O	2.60	0.50
1:B:106:TYR:HA	1:B:109[B]:ARG:HE	1.75	0.50
1:B:243:GLY:H	6:B:708:EDO:C2	2.25	0.50
1:A:327:GLN:HE22	1:A:484:ASN:ND2	2.05	0.50
1:A:598:GLN:NE2	7:A:1214:HOH:O	2.45	0.50
1:B:397:PRO:HD2	1:D:527:TRP:CD2	2.47	0.49
1:A:275:ASP:HB2	7:A:1179:HOH:O	2.12	0.49
1:B:629:ASP:O	1:B:631:PRO:HD3	2.12	0.49
1:D:184:GLN:HB2	1:D:218:PHE:CZ	2.48	0.49
1:D:30:ARG:HB3	1:D:174:TYR:CE2	2.48	0.49
1:D:112:HIS:CD2	7:D:1104:HOH:O	2.62	0.48
1:B:318:ASN:HD21	1:B:590:ARG:HE	1.60	0.48
1:D:320:ALA:H	1:D:484:ASN:HD22	1.60	0.48
1:A:644:ILE:HD12	7:A:1097:HOH:O	2.13	0.48
4:B:710:6GJ:H5	4:B:710:6GJ:C1	2.44	0.48
1:D:523:HIS:HA	7:D:1116:HOH:O	2.14	0.48
1:B:273:TRP:N	7:B:1155:HOH:O	2.46	0.48
1:B:553:MET:SD	1:B:617:THR:HG23	2.54	0.48
4:B:710:6GJ:C9	4:B:710:6GJ:C1	2.92	0.47
1:C:524:LEU:HD21	1:C:551:PHE:CD1	2.49	0.47
1:D:424:GLN:HE22	1:D:502:SER:HB2	1.78	0.47
1:A:310:GLY:HA3	1:A:331:TYR:O	2.15	0.47
1:D:527:TRP:HA	1:D:527:TRP:CE3	2.49	0.47
1:B:268:GLU:OE1	4:B:710:6GJ:H1	2.13	0.47
1:D:430:ALA:CB	7:D:1101:HOH:O	2.62	0.47
1:C:352[A]:ASN:OD1	1:C:355:GLN:NE2	2.47	0.47
1:B:318:ASN:ND2	1:B:590:ARG:HE	2.14	0.46
1:B:88:PHE:O	1:B:102:HIS:HD2	1.96	0.46
1:A:397:PRO:HD2	1:C:527:TRP:CG	2.50	0.46
1:B:170:LYS:N	1:B:171:PRO:HD2	2.31	0.46
1:D:91:PRO:HD2	1:D:95:GLN:O	2.15	0.46
1:D:318:ASN:HD21	1:D:590:ARG:HH21	1.62	0.46
1:D:551:PHE:HA	1:D:618:VAL:O	2.16	0.46
1:A:381:LYS:HB2	1:A:552:TYR:CE2	2.52	0.45
1:C:598:GLN:HA	1:C:644:ILE:HA	1.99	0.45
1:B:572[A]:GLN:HG3	1:B:637:THR:HB	1.97	0.45
1:B:243:GLY:H	6:B:708:EDO:H21	1.80	0.45
1:C:242:PHE:O	1:C:269:PHE:HA	2.16	0.45
1:D:440:HIS:HA	1:D:441:ASP:HA	1.79	0.45
1:D:62:ARG:HA	1:D:65:TRP:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:ASP:O	1:D:240:VAL:HA	2.17	0.44
1:B:327:GLN:HE22	1:B:484:ASN:ND2	2.13	0.44
1:C:91:PRO:HD2	1:C:95:GLN:O	2.17	0.44
1:C:507:THR:O	1:C:508:ASP:HB2	2.17	0.44
1:C:309:ILE:HB	1:C:337:LEU:HB2	1.99	0.44
1:B:318:ASN:HD21	1:B:590:ARG:HH21	1.66	0.44
1:C:221:ASP:O	1:C:240:VAL:HA	2.18	0.43
1:A:305:LEU:HD12	1:A:305:LEU:N	2.32	0.43
1:A:112:HIS:CD2	7:A:1048:HOH:O	2.63	0.43
1:B:381:LYS:HB2	1:B:552:TYR:CE2	2.54	0.43
1:A:72:MET:HE2	1:A:80:ILE:HG22	1.99	0.43
1:B:310:GLY:HA3	1:B:331:TYR:O	2.19	0.43
1:D:253:LEU:HD23	1:D:253:LEU:HA	1.92	0.43
1:D:430:ALA:N	7:D:1101:HOH:O	2.51	0.43
1:B:95:GLN:HG2	7:B:1181:HOH:O	2.19	0.43
1:A:598:GLN:HA	1:A:644:ILE:HA	2.01	0.43
1:D:150:SER:O	1:D:151:ASP:C	2.62	0.42
1:B:321:ASN:ND2	1:B:327:GLN:HE21	2.17	0.42
1:B:440:HIS:HA	1:B:441:ASP:HA	1.78	0.42
1:A:273:TRP:CH2	4:A:706:6GJ:S6	3.12	0.42
1:B:299:ARG:HD3	7:B:1045:HOH:O	2.18	0.42
1:C:29:GLN:HE21	1:C:29:GLN:HA	1.84	0.42
1:B:190:GLY:HA3	1:B:227:PHE:O	2.19	0.42
1:B:383:LYS:NZ	1:D:100:GLU:OE2	2.51	0.42
1:D:424:GLN:HE22	1:D:502:SER:CB	2.33	0.42
1:C:76:GLY:HA3	1:C:360:VAL:HG22	2.01	0.42
1:D:62:ARG:HA	1:D:65:TRP:CG	2.54	0.42
2:D:701:NAG:O6	2:D:701:NAG:O4	2.32	0.42
1:A:399:LYS:HE2	1:C:528:GLY:O	2.20	0.42
1:C:151:ASP:C	1:C:151:ASP:OD1	2.63	0.42
1:D:323:PRO:O	1:D:324:TYR:C	2.63	0.42
1:A:52:SER:HA	1:A:79:ALA:O	2.20	0.41
1:B:95:GLN:NE2	7:B:1083:HOH:O	2.54	0.41
1:B:555:ASN:HA	1:B:614:ASN:O	2.21	0.41
1:D:318:ASN:HD21	1:D:590:ARG:HE	1.68	0.41
1:D:321:ASN:ND2	1:D:327:GLN:HE21	2.18	0.41
1:D:430:ALA:HB2	7:D:1101:HOH:O	2.19	0.41
1:D:592:TRP:CE2	1:D:595:ARG:HG3	2.55	0.41
1:B:205:LYS:HD2	7:B:1187:HOH:O	2.20	0.41
1:B:579:GLY:HA3	1:B:619:LEU:O	2.21	0.41
1:C:49:ARG:HB2	1:C:302:SER:OG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:PRO:HD2	1:C:184:GLN:O	2.21	0.41
1:C:174:TYR:HA	1:C:178:GLY:O	2.21	0.41
1:B:125:TYR:CE2	1:B:148:ARG:CZ	3.04	0.41
1:A:564:ASP:O	1:A:567:GLN:HG3	2.21	0.41
1:B:598:GLN:HA	1:B:644:ILE:HA	2.03	0.41
1:C:322:SER:HA	1:C:323:PRO:C	2.46	0.41
1:D:64:TYR:O	1:D:68:ARG:HG2	2.20	0.41
1:D:72:MET:HB3	1:D:77:LEU:HD12	2.03	0.41
1:B:275:ASP:HB2	7:B:1218:HOH:O	2.20	0.41
1:C:555:ASN:HA	1:C:614:ASN:O	2.21	0.41
1:D:241:ASP:HB2	1:D:268:GLU:HB2	2.03	0.41
1:A:415:PHE:CD1	1:A:415:PHE:N	2.89	0.40
1:B:243:GLY:N	6:B:708:EDO:H22	2.35	0.40
1:D:399:LYS:HE3	1:D:510:THR:HG23	2.03	0.40
1:C:437:ASN:CG	1:C:437:ASN:O	2.62	0.40
1:B:174:TYR:HA	1:B:178:GLY:O	2.22	0.40
1:C:592:TRP:CE2	1:C:595:ARG:HG3	2.56	0.40
1:C:62:ARG:HA	1:C:65:TRP:CD2	2.57	0.40
1:C:150:SER:OG	1:C:196:ASP:OD2	2.39	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	609/678 (90%)	587 (96%)	20 (3%)	2 (0%)	36	35
1	B	605/678 (89%)	585 (97%)	19 (3%)	1 (0%)	43	42
1	C	605/678 (89%)	584 (96%)	20 (3%)	1 (0%)	43	42
1	D	604/678 (89%)	579 (96%)	25 (4%)	0	100	100
All	All	2423/2712 (89%)	2335 (96%)	84 (4%)	4 (0%)	43	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	611	SER
1	A	628	SER
1	C	503	SER
1	B	630	ASP

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	526/585 (90%)	520 (99%)	6 (1%)	65	73
1	B	522/585 (89%)	514 (98%)	8 (2%)	57	64
1	C	522/585 (89%)	506 (97%)	16 (3%)	35	37
1	D	521/585 (89%)	507 (97%)	14 (3%)	39	42
All	All	2091/2340 (89%)	2047 (98%)	44 (2%)	48	52

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	274	LEU
1	A	309	ILE
1	A	360	VAL
1	A	503	SER
1	A	553	MET
1	A	605	GLN
1	B	40	SER
1	B	47	PRO
1	B	131	GLU
1	B	234	GLN
1	B	274	LEU
1	B	358	GLU
1	B	605	GLN
1	B	628	SER
1	C	29	GLN
1	C	35	ASP

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Mol	Chain	Res	Type
1	C	40	SER
1	C	104	VAL
1	C	150	SER
1	C	274	LEU
1	C	359	LYS
1	C	360	VAL
1	C	420	THR
1	C	459[A]	ASN
1	C	459[B]	ASN
1	C	466	THR
1	C	572[A]	GLN
1	C	572[B]	GLN
1	C	605	GLN
1	C	646	SER
1	D	29	GLN
1	D	38	ARG
1	D	47	PRO
1	D	131	GLU
1	D	160	LYS
1	D	274	LEU
1	D	287	GLU
1	D	359	LYS
1	D	382	LEU
1	D	424	GLN
1	D	527	TRP
1	D	605	GLN
1	D	628	SER
1	D	647	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	97	GLN
1	A	112	HIS
1	A	204	GLN
1	A	279	GLN
1	A	318	ASN
1	A	321	ASN
1	A	355	GLN
1	A	437	ASN
1	A	484	ASN

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Mol	Chain	Res	Type
1	B	46	GLN
1	B	102	HIS
1	B	204	GLN
1	B	318	ASN
1	B	321	ASN
1	B	355	GLN
1	B	437	ASN
1	B	484	ASN
1	B	523	HIS
1	B	529	HIS
1	B	605	GLN
1	C	29	GLN
1	C	46	GLN
1	C	279	GLN
1	C	318	ASN
1	C	321	ASN
1	C	355	GLN
1	C	424	GLN
1	C	437	ASN
1	C	484	ASN
1	C	523	HIS
1	C	605	GLN
1	D	102	HIS
1	D	204	GLN
1	D	279	GLN
1	D	318	ASN
1	D	321	ASN
1	D	355	GLN
1	D	424	GLN
1	D	437	ASN
1	D	484	ASN
1	D	605	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](#)

Of 40 ligands modelled in this entry, 4 are monoatomic - leaving 36 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	C	706	-	4,4,4	0.47	0	6,6,6	0.29	0
2	NAG	B	704	1	14,14,15	0.57	0	17,19,21	0.95	1 (5%)
2	NAG	C	703	1	14,14,15	0.49	0	17,19,21	1.08	2 (11%)
4	6GJ	B	710	-	18,19,19	1.55	3 (16%)	15,27,27	2.83	5 (33%)
6	EDO	A	710	-	3,3,3	0.44	0	2,2,2	0.88	0
6	EDO	A	709	-	3,3,3	0.24	0	2,2,2	1.29	0
6	EDO	C	710	-	3,3,3	0.50	0	2,2,2	1.15	0
4	6GJ	C	705	-	18,19,19	1.76	4 (22%)	15,27,27	4.38	6 (40%)
6	EDO	D	708	-	3,3,3	0.12	0	2,2,2	1.16	0
2	NAG	A	702	1	14,14,15	1.05	1 (7%)	17,19,21	2.94	7 (41%)
6	EDO	B	709	-	3,3,3	0.47	0	2,2,2	0.56	0
2	NAG	D	704	1	14,14,15	0.60	0	17,19,21	2.16	3 (17%)
2	NAG	C	701	1	14,14,15	0.30	0	17,19,21	0.56	0
2	NAG	C	702	1	14,14,15	0.52	0	17,19,21	1.47	1 (5%)
5	SO4	B	706	-	4,4,4	0.48	0	6,6,6	0.30	0
5	SO4	C	707	-	4,4,4	0.40	0	6,6,6	0.30	0
4	6GJ	D	702	-	18,19,19	1.72	4 (22%)	15,27,27	4.37	3 (20%)
2	NAG	A	704	1	14,14,15	0.56	0	17,19,21	0.83	0
2	NAG	B	703	1	14,14,15	0.70	0	17,19,21	2.17	8 (47%)
5	SO4	D	710	-	4,4,4	0.44	0	6,6,6	0.61	0
2	NAG	C	704	1	14,14,15	0.66	0	17,19,21	0.95	1 (5%)
2	NAG	B	701	1	14,14,15	0.57	0	17,19,21	1.49	2 (11%)
6	EDO	B	708	-	3,3,3	0.45	0	2,2,2	0.24	0
2	NAG	D	703	1	14,14,15	0.48	0	17,19,21	1.26	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	D	709	-	4,4,4	0.43	0	6,6,6	0.41	0
2	NAG	A	703	1	14,14,15	1.16	1 (7%)	17,19,21	2.45	8 (47%)
2	NAG	D	701	1	14,14,15	0.94	1 (7%)	17,19,21	1.59	5 (29%)
2	NAG	A	701	1	14,14,15	0.46	0	17,19,21	1.39	3 (17%)
5	SO4	A	707	-	4,4,4	0.53	0	6,6,6	0.34	0
2	NAG	D	705	1	14,14,15	0.74	0	17,19,21	1.27	2 (11%)
2	NAG	B	702	1	14,14,15	1.05	0	17,19,21	2.19	6 (35%)
6	EDO	C	709	-	3,3,3	0.38	0	2,2,2	0.80	0
4	6GJ	A	706	-	18,19,19	1.54	3 (16%)	15,27,27	4.52	7 (46%)
5	SO4	B	707	-	4,4,4	0.47	0	6,6,6	0.32	0
5	SO4	A	708	-	4,4,4	0.56	0	6,6,6	0.37	0
6	EDO	D	707	-	3,3,3	0.44	0	2,2,2	0.69	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	NAG	B	704	1	-	0/6/23/26	0/1/1/1
2	NAG	C	703	1	-	0/6/23/26	0/1/1/1
4	6GJ	B	710	-	-	3/5/38/38	0/2/2/2
6	EDO	A	710	-	-	1/1/1/1	-
6	EDO	A	709	-	-	1/1/1/1	-
6	EDO	C	710	-	-	1/1/1/1	-
4	6GJ	C	705	-	-	3/5/38/38	0/2/2/2
6	EDO	D	708	-	-	0/1/1/1	-
2	NAG	A	702	1	-	2/6/23/26	0/1/1/1
6	EDO	B	709	-	-	0/1/1/1	-
2	NAG	D	704	1	-	2/6/23/26	0/1/1/1
2	NAG	C	701	1	-	5/6/23/26	0/1/1/1
2	NAG	C	702	1	-	0/6/23/26	0/1/1/1
4	6GJ	D	702	-	-	3/5/38/38	0/2/2/2
2	NAG	A	704	1	-	0/6/23/26	0/1/1/1
2	NAG	B	703	1	-	2/6/23/26	0/1/1/1
2	NAG	C	704	1	-	0/6/23/26	0/1/1/1
2	NAG	B	701	1	-	1/6/23/26	0/1/1/1
6	EDO	B	708	-	-	0/1/1/1	-
2	NAG	D	703	1	-	0/6/23/26	0/1/1/1
2	NAG	A	703	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	701	1	-	1/6/23/26	0/1/1/1
2	NAG	A	701	1	-	1/6/23/26	0/1/1/1
2	NAG	D	705	1	-	0/6/23/26	0/1/1/1
2	NAG	B	702	1	-	2/6/23/26	0/1/1/1
6	EDO	C	709	-	-	1/1/1/1	-
4	6GJ	A	706	-	-	4/5/38/38	0/2/2/2
6	EDO	D	707	-	-	1/1/1/1	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	702	6GJ	C7-S6	-4.97	1.67	1.75
4	C	705	6GJ	C7-S6	-4.67	1.68	1.75
4	B	710	6GJ	C7-N8	3.87	1.32	1.26
4	A	706	6GJ	C7-S6	-3.77	1.69	1.75
4	C	705	6GJ	O1-C1	3.24	1.44	1.40
4	D	702	6GJ	O1-C1	3.07	1.44	1.40
4	B	710	6GJ	C6-S6	-3.06	1.74	1.81
4	D	702	6GJ	C7-N8	3.04	1.31	1.26
4	B	710	6GJ	C7-S6	-2.79	1.71	1.75
4	A	706	6GJ	O1-C1	2.76	1.44	1.40
4	C	705	6GJ	C6-S6	-2.72	1.74	1.81
2	A	703	NAG	C2-N2	2.67	1.50	1.46
4	A	706	6GJ	C7-N8	2.65	1.30	1.26
4	C	705	6GJ	C7-N8	2.56	1.30	1.26
2	A	702	NAG	O3-C3	-2.53	1.36	1.43
2	D	701	NAG	C1-C2	2.52	1.55	1.52
4	D	702	6GJ	C6-S6	-2.40	1.75	1.81

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	702	6GJ	C9-N8-C7	15.21	141.54	117.83
4	A	706	6GJ	C9-N8-C7	14.24	140.03	117.83
4	C	705	6GJ	C9-N8-C7	13.81	139.37	117.83
2	A	702	NAG	C1-O5-C5	9.05	124.32	112.19
4	A	706	6GJ	C3-C2-C1	7.04	120.74	109.01
4	C	705	6GJ	C3-C2-C1	6.86	120.45	109.01
4	B	710	6GJ	C9-N8-C7	6.72	128.31	117.83
2	D	704	NAG	O5-C1-C2	6.38	121.16	111.29
4	B	710	6GJ	O1-C1-N5	-5.37	99.87	111.40
2	A	702	NAG	C6-C5-C4	-5.15	100.38	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	703	NAG	O5-C1-C2	-5.04	103.50	111.29
2	D	704	NAG	C1-O5-C5	4.93	118.79	112.19
4	D	702	6GJ	O1-C1-N5	-4.91	100.85	111.40
4	B	710	6GJ	C10-C9-N8	4.88	119.31	110.67
2	B	702	NAG	C1-O5-C5	4.56	118.30	112.19
2	C	702	NAG	C1-O5-C5	4.44	118.14	112.19
4	D	702	6GJ	C5-C6-S6	-4.25	98.59	106.31
4	C	705	6GJ	O2-C2-C3	4.15	120.15	110.38
2	B	702	NAG	O6-C6-C5	-4.10	97.37	111.33
2	B	701	NAG	C1-O5-C5	3.97	117.50	112.19
2	A	703	NAG	O7-C7-C8	-3.86	115.18	122.05
2	B	703	NAG	O5-C1-C2	-3.75	105.49	111.29
2	A	703	NAG	O3-C3-C4	-3.71	101.64	110.38
2	A	703	NAG	C8-C7-N2	3.56	122.01	116.12
2	A	703	NAG	O3-C3-C2	3.54	116.75	109.40
4	A	706	6GJ	O1-C1-N5	-3.54	103.81	111.40
2	B	703	NAG	C1-O5-C5	3.53	116.92	112.19
2	B	703	NAG	C4-C3-C2	-3.50	105.89	111.02
4	C	705	6GJ	O1-C1-N5	-3.43	104.04	111.40
2	B	702	NAG	C6-C5-C4	-3.42	104.63	113.02
4	A	706	6GJ	C5-C6-S6	-3.24	100.42	106.31
2	A	702	NAG	O6-C6-C5	-3.17	100.52	111.33
4	B	710	6GJ	C3-C4-C5	-3.17	106.01	111.37
2	D	705	NAG	O7-C7-C8	-3.06	116.61	122.05
2	B	703	NAG	C1-C2-N2	3.05	115.23	110.43
4	A	706	6GJ	C3-C4-C5	-2.91	106.45	111.37
4	A	706	6GJ	O2-C2-C3	2.91	117.23	110.38
2	B	702	NAG	C4-C3-C2	-2.86	106.82	111.02
4	C	705	6GJ	C5-C6-S6	-2.82	101.19	106.31
2	B	702	NAG	O3-C3-C4	-2.81	103.76	110.38
2	A	701	NAG	C1-C2-N2	-2.76	106.08	110.43
2	A	702	NAG	C1-C2-N2	-2.74	106.12	110.43
2	B	701	NAG	O6-C6-C5	-2.72	102.08	111.33
2	C	703	NAG	C1-O5-C5	2.70	115.81	112.19
2	B	703	NAG	C6-C5-C4	-2.64	106.53	113.02
2	B	703	NAG	O3-C3-C4	-2.57	104.31	110.38
2	D	701	NAG	O5-C5-C6	2.55	112.63	107.66
2	B	704	NAG	C1-C2-N2	-2.53	106.44	110.43
2	A	702	NAG	O4-C4-C5	-2.53	103.09	109.32
2	A	702	NAG	O5-C5-C4	2.52	116.95	110.83
2	D	701	NAG	O5-C1-C2	2.45	115.09	111.29
2	D	705	NAG	C8-C7-N2	2.45	120.18	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	703	NAG	O5-C5-C6	2.45	112.43	107.66
2	A	703	NAG	C4-C3-C2	-2.42	107.47	111.02
2	A	701	NAG	O6-C6-C5	-2.40	103.16	111.33
4	A	706	6GJ	O4-C4-C3	2.35	115.92	110.38
2	A	703	NAG	C1-O5-C5	2.34	115.32	112.19
2	B	703	NAG	O7-C7-N2	2.33	126.11	121.98
2	D	701	NAG	O5-C5-C4	-2.29	105.27	110.83
4	C	705	6GJ	C10-C9-N8	-2.27	106.65	110.67
4	B	710	6GJ	C5-C6-S6	-2.25	102.21	106.31
2	A	703	NAG	C1-C2-N2	2.21	113.92	110.43
2	A	701	NAG	O3-C3-C2	-2.21	104.81	109.40
2	A	702	NAG	O3-C3-C4	-2.19	105.20	110.38
2	C	704	NAG	O4-C4-C3	-2.17	105.26	110.38
2	D	701	NAG	C1-C2-N2	2.16	113.84	110.43
2	D	703	NAG	C2-N2-C7	-2.13	120.04	122.90
2	D	704	NAG	O7-C7-C8	-2.08	118.35	122.05
2	B	702	NAG	C1-C2-N2	-2.06	107.18	110.43
2	C	703	NAG	O3-C3-C2	-2.06	105.13	109.40
2	B	703	NAG	O7-C7-C8	-2.03	118.44	122.05
2	D	701	NAG	O7-C7-C8	-2.02	118.46	122.05

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	701	NAG	C1-C2-N2-C7
4	A	706	6GJ	N5-C7-N8-C9
4	A	706	6GJ	S6-C7-N8-C9
4	B	710	6GJ	N5-C7-N8-C9
4	B	710	6GJ	S6-C7-N8-C9
4	C	705	6GJ	N5-C7-N8-C9
4	C	705	6GJ	S6-C7-N8-C9
4	D	702	6GJ	N5-C7-N8-C9
4	D	702	6GJ	S6-C7-N8-C9
2	D	704	NAG	C4-C5-C6-O6
2	B	703	NAG	O5-C5-C6-O6
2	B	702	NAG	C4-C5-C6-O6
2	A	702	NAG	C4-C5-C6-O6
2	D	704	NAG	O5-C5-C6-O6
2	B	702	NAG	O5-C5-C6-O6
2	C	701	NAG	C8-C7-N2-C2
4	B	710	6GJ	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
4	D	702	6GJ	C11-C10-C9-N8
2	D	701	NAG	O5-C5-C6-O6
6	C	709	EDO	O1-C1-C2-O2
6	C	710	EDO	O1-C1-C2-O2
6	D	707	EDO	O1-C1-C2-O2
2	A	702	NAG	O5-C5-C6-O6
2	C	701	NAG	O7-C7-N2-C2
6	A	710	EDO	O1-C1-C2-O2
4	A	706	6GJ	C11-C10-C9-N8
4	A	706	6GJ	C9-C10-C11-C12
4	C	705	6GJ	C11-C10-C9-N8
2	B	703	NAG	C4-C5-C6-O6
2	C	701	NAG	C3-C2-N2-C7
2	B	701	NAG	C4-C5-C6-O6
6	A	709	EDO	O1-C1-C2-O2
2	A	701	NAG	C4-C5-C6-O6
2	C	701	NAG	C4-C5-C6-O6

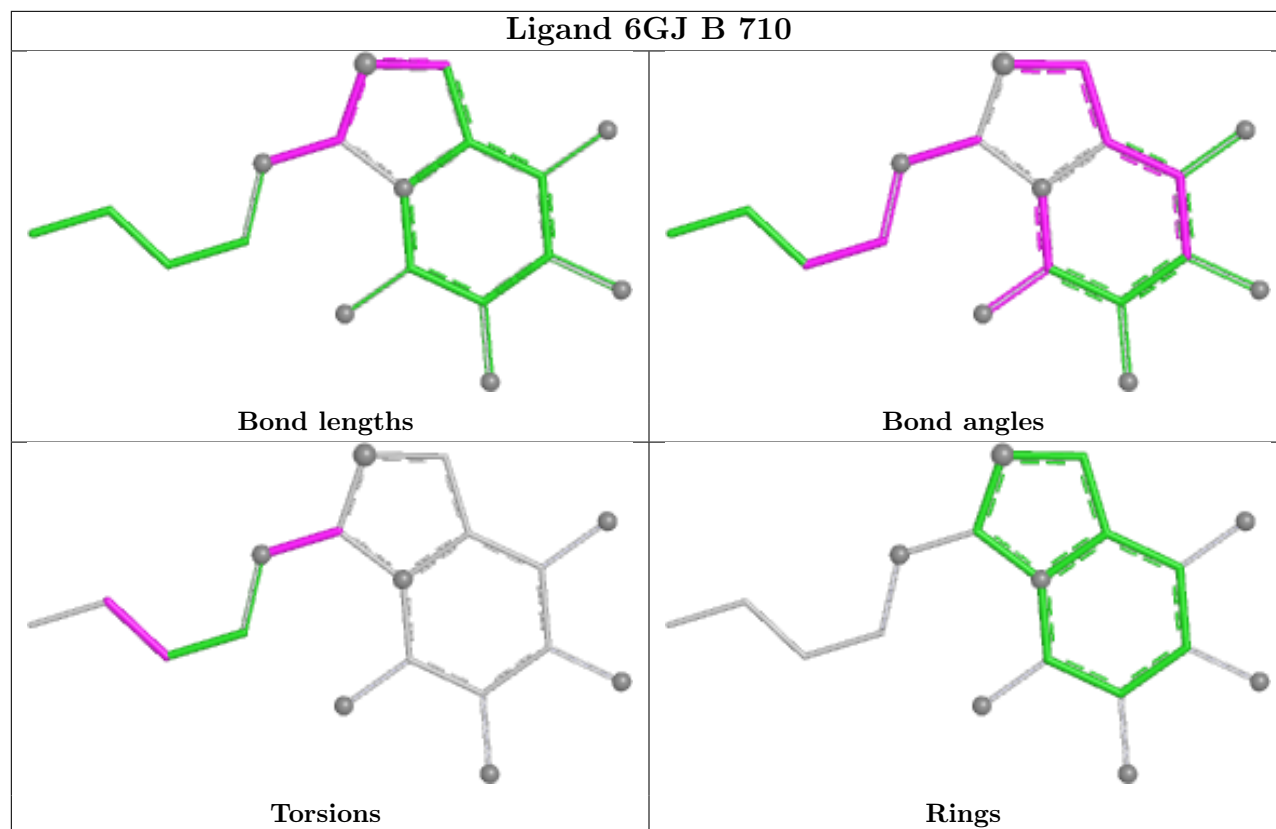
There are no ring outliers.

5 monomers are involved in 14 short contacts:

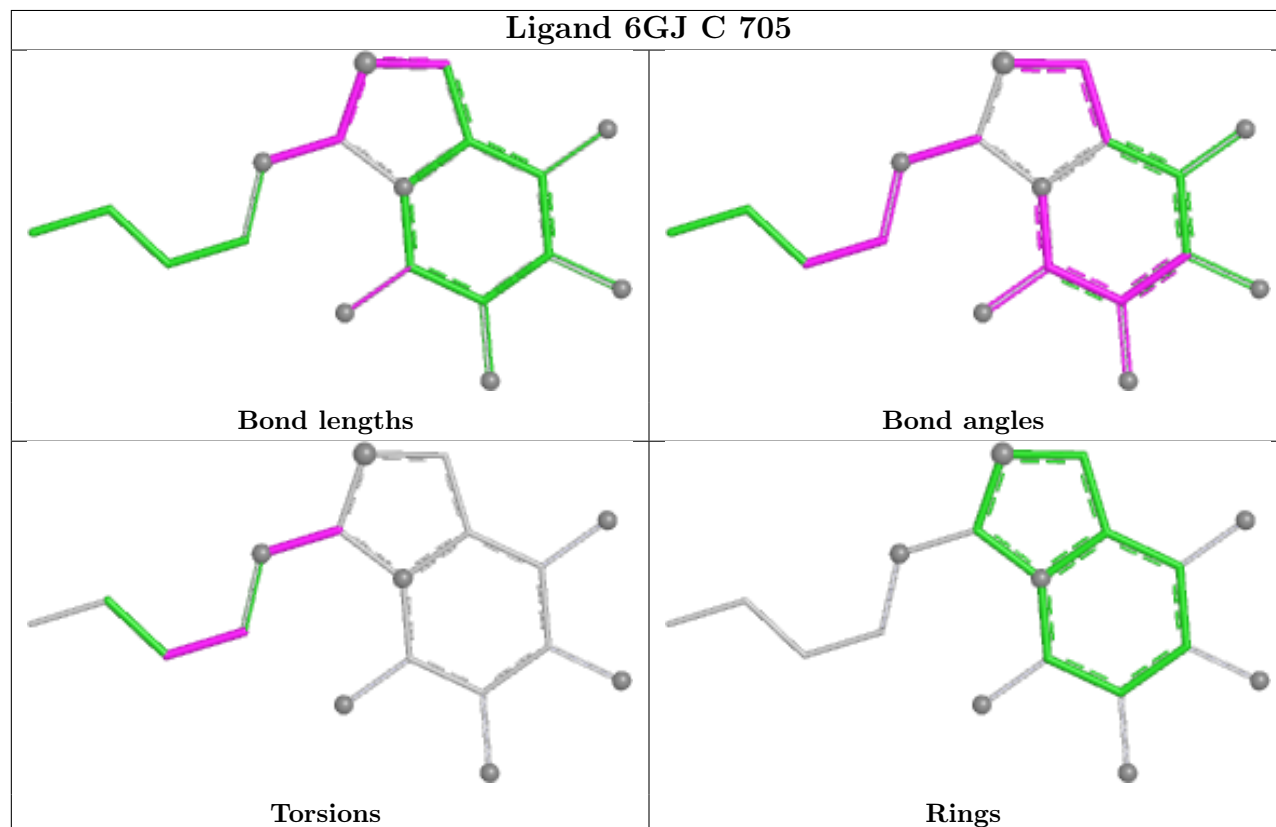
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	710	6GJ	7	0
2	D	704	NAG	2	0
6	B	708	EDO	3	0
2	D	701	NAG	1	0
4	A	706	6GJ	1	0

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.

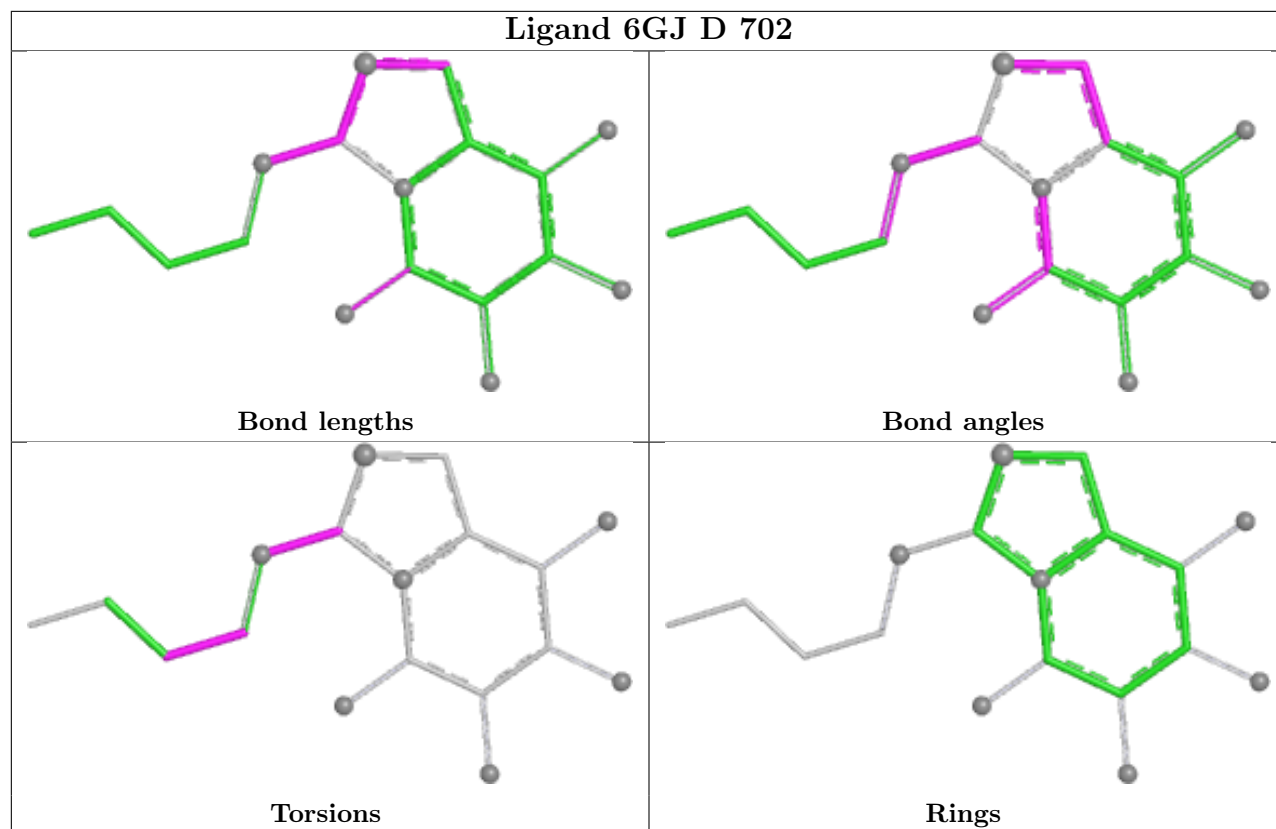
Ligand 6GJ B 710



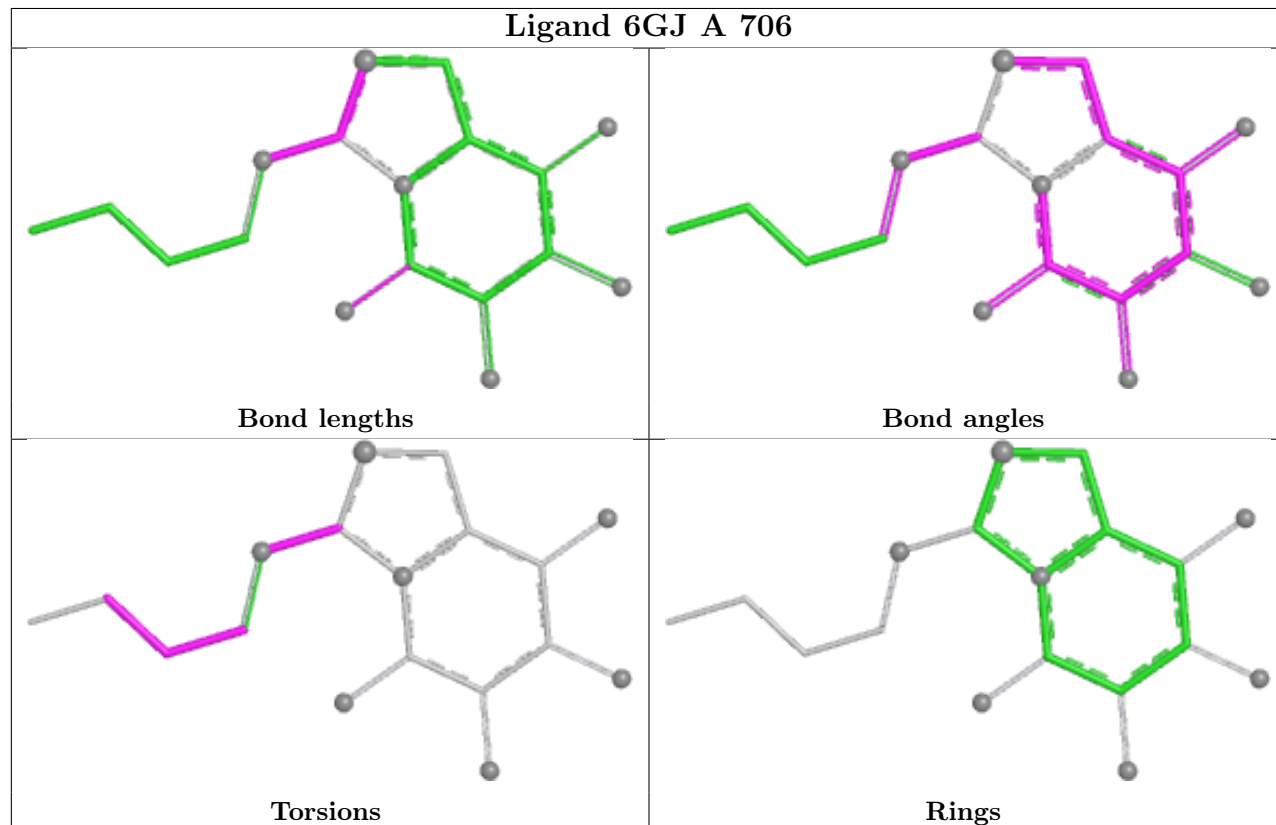
Ligand 6GJ C 705



Ligand 6GJ D 702



Ligand 6GJ A 706



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	605/678 (89%)	-0.04	11 (1%) 67 67	14, 25, 41, 91	8 (1%)
1	B	605/678 (89%)	-0.14	11 (1%) 67 67	12, 24, 41, 87	4 (0%)
1	C	603/678 (88%)	-0.00	12 (1%) 65 64	15, 26, 50, 77	6 (0%)
1	D	603/678 (88%)	0.07	9 (1%) 72 71	17, 28, 52, 87	5 (0%)
All	All	2416/2712 (89%)	-0.03	43 (1%) 67 67	12, 26, 46, 91	23 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	527	TRP	6.8
1	C	527	TRP	5.3
1	B	646	SER	4.9
1	D	528	GLY	4.7
1	A	646	SER	4.1
1	B	643	VAL	3.9
1	A	644	ILE	3.9
1	C	528	GLY	3.8
1	A	647	SER	3.7
1	D	526	GLY	3.7
1	A	645	GLY	3.6
1	B	611	SER	3.5
1	C	525	GLY	3.0
1	D	29	GLN	3.0
1	B	645	GLY	3.0
1	B	644	ILE	2.8
1	D	629	ASP	2.8
1	C	429	PRO	2.7
1	D	38	ARG	2.6
1	A	643	VAL	2.6
1	A	629	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	109[A]	ARG	2.5
1	D	646	SER	2.5
1	C	647	SER	2.4
1	B	283	THR	2.4
1	B	629	ASP	2.3
1	C	35	ASP	2.3
1	D	647	SER	2.3
1	B	360	VAL	2.3
1	A	282	SER	2.2
1	D	471	ALA	2.2
1	B	647	SER	2.2
1	A	280	PRO	2.2
1	A	628	SER	2.2
1	C	29	GLN	2.1
1	C	524	LEU	2.1
1	C	423	PRO	2.1
1	A	586[A]	PHE	2.1
1	B	29	GLN	2.0
1	C	507	THR	2.0
1	B	627	SER	2.0
1	C	31	MET	2.0
1	C	426	CYS	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 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, 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	704	14/15	0.47	0.17	75,85,89,91	0

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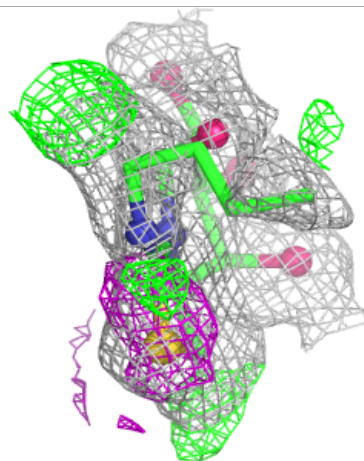
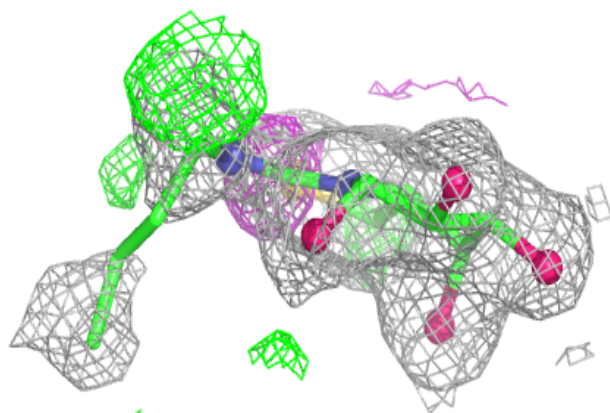
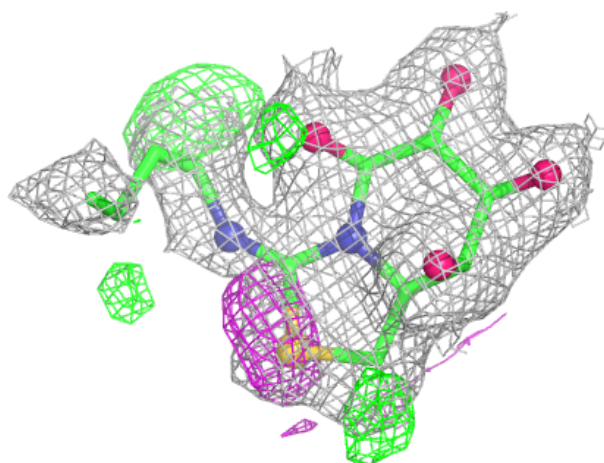
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	C	701	14/15	0.48	0.20	79,88,98,103	0
2	NAG	D	701	14/15	0.56	0.18	69,76,92,92	0
2	NAG	A	703	14/15	0.68	0.16	36,41,51,52	0
2	NAG	A	704	14/15	0.74	0.13	49,55,63,67	0
2	NAG	C	702	14/15	0.78	0.12	40,47,54,58	0
5	SO4	A	707	5/5	0.78	0.10	60,60,63,63	0
6	EDO	C	710	4/4	0.78	0.18	31,31,35,42	0
2	NAG	B	703	14/15	0.79	0.15	36,43,57,61	0
2	NAG	D	703	14/15	0.81	0.11	41,44,51,53	0
5	SO4	D	709	5/5	0.82	0.10	67,70,74,74	0
2	NAG	B	704	14/15	0.82	0.11	46,49,52,58	0
2	NAG	C	703	14/15	0.83	0.11	35,46,49,50	0
6	EDO	A	709	4/4	0.84	0.16	44,48,49,54	0
6	EDO	D	708	4/4	0.84	0.17	38,40,43,45	0
6	EDO	B	708	4/4	0.86	0.15	37,43,43,45	0
4	6GJ	D	702	18/18	0.86	0.14	24,31,56,57	0
4	6GJ	A	706	18/18	0.86	0.15	20,31,63,64	0
6	EDO	A	710	4/4	0.87	0.12	29,31,32,40	0
2	NAG	A	702	14/15	0.87	0.10	24,30,35,35	0
5	SO4	C	706	5/5	0.89	0.08	61,62,64,65	0
2	NAG	B	702	14/15	0.89	0.08	25,28,32,35	0
5	SO4	D	710	5/5	0.89	0.12	52,53,54,54	0
6	EDO	D	707	4/4	0.89	0.13	28,33,36,37	0
4	6GJ	C	705	18/18	0.89	0.12	23,31,54,54	0
6	EDO	C	709	4/4	0.90	0.14	29,35,36,39	0
4	6GJ	B	710	18/18	0.90	0.14	19,26,59,61	0
2	NAG	B	701	14/15	0.90	0.09	21,28,36,36	0
5	SO4	B	706	5/5	0.90	0.07	64,67,70,71	0
2	NAG	C	704	14/15	0.92	0.08	25,31,33,36	0
2	NAG	A	701	14/15	0.92	0.08	23,27,32,41	0
5	SO4	C	707	5/5	0.93	0.12	44,52,54,56	0
6	EDO	B	709	4/4	0.93	0.10	28,29,31,33	0
5	SO4	A	708	5/5	0.94	0.10	38,47,49,52	0
2	NAG	D	705	14/15	0.94	0.06	27,31,34,36	0
5	SO4	B	707	5/5	0.96	0.09	31,39,44,44	0
3	CL	A	705	1/1	0.99	0.04	21,21,21,21	0
3	CL	B	705	1/1	0.99	0.03	20,20,20,20	0
3	CL	C	708	1/1	0.99	0.03	22,22,22,22	0
3	CL	D	706	1/1	0.99	0.03	21,21,21,21	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.

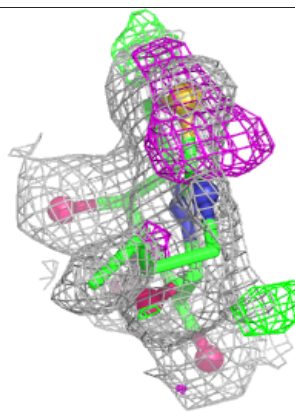
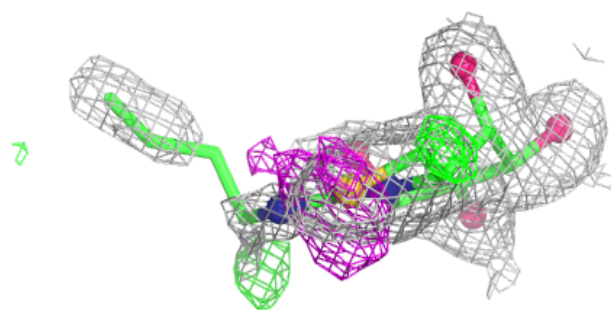
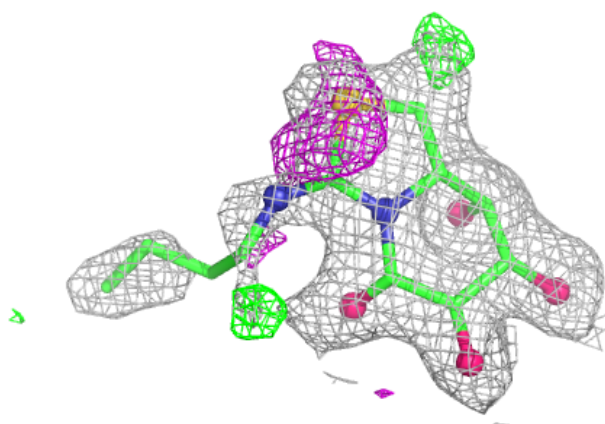
Electron density around 6GJ D 702:

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



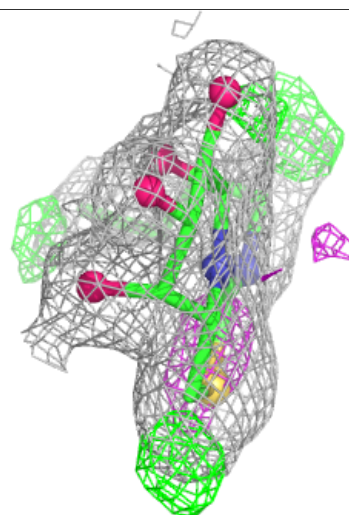
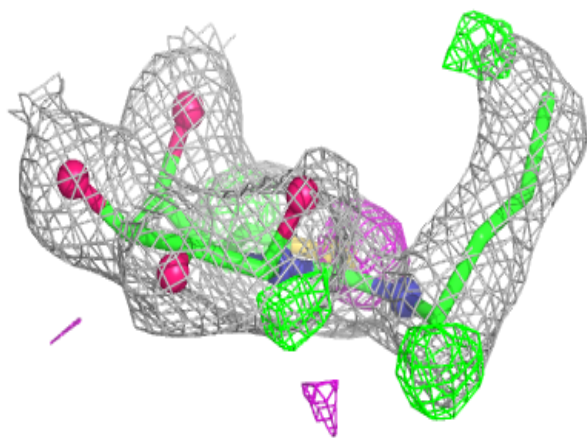
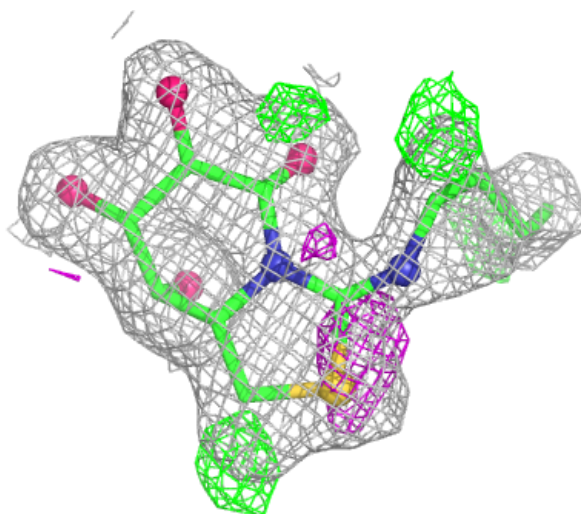
Electron density around 6GJ A 706:

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



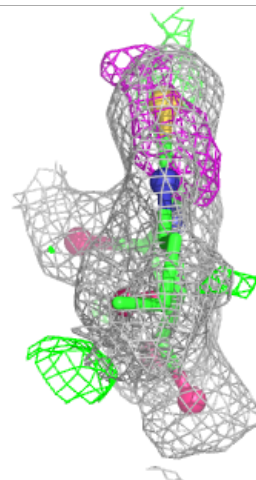
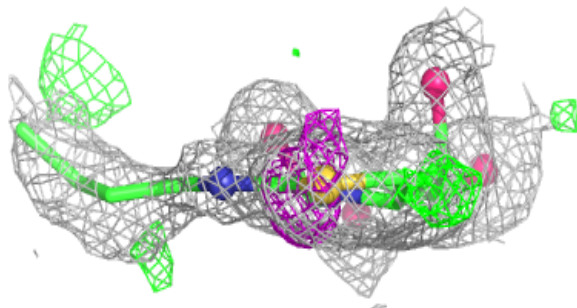
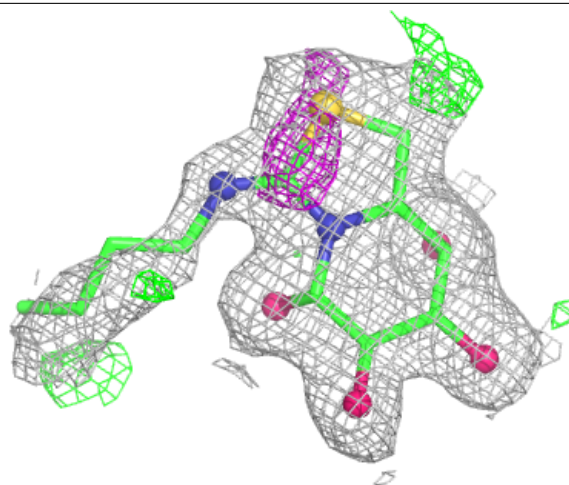
Electron density around 6GJ C 705:

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



Electron density around 6GJ B 710:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.