



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2022 – 07:28 PM JST

PDB ID : 7VZZ
Title : The structure of GdmN in complex with the natural tetrahedral intermediate, carbamoyl adenylate, and 20-O-methyl-19-chloroproansamitocin
Authors : Wei, J.; Zheng, J.; Zhou, J.; Kang, Q.; Bai, L.
Deposited on : 2021-11-17
Resolution : 2.85 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	:	2.31.2
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)	:	2.31.2

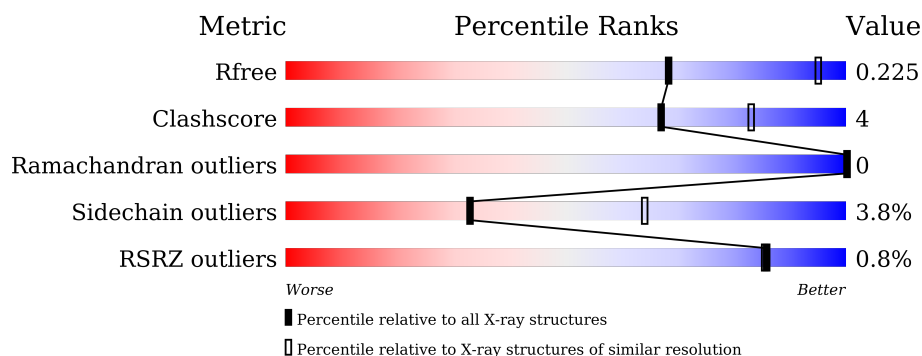
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	702	 86% 9% . .
1	B	702	 84% 11% . .

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10632 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 GdmN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	674	Total	C	N	O	S	0	0	0
			5193	3291	913	980	9			
1	B	677	Total	C	N	O	S	0	0	0
			5214	3302	916	987	9			

There are 40 discrepancies between the modelled and reference sequences:

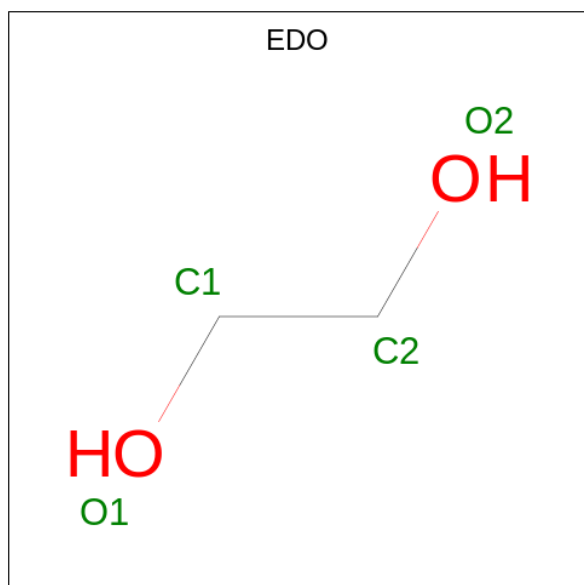
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q84G19
A	-18	GLY	-	expression tag	UNP Q84G19
A	-17	SER	-	expression tag	UNP Q84G19
A	-16	SER	-	expression tag	UNP Q84G19
A	-15	HIS	-	expression tag	UNP Q84G19
A	-14	HIS	-	expression tag	UNP Q84G19
A	-13	HIS	-	expression tag	UNP Q84G19
A	-12	HIS	-	expression tag	UNP Q84G19
A	-11	HIS	-	expression tag	UNP Q84G19
A	-10	HIS	-	expression tag	UNP Q84G19
A	-9	SER	-	expression tag	UNP Q84G19
A	-8	SER	-	expression tag	UNP Q84G19
A	-7	GLY	-	expression tag	UNP Q84G19
A	-6	LEU	-	expression tag	UNP Q84G19
A	-5	VAL	-	expression tag	UNP Q84G19
A	-4	PRO	-	expression tag	UNP Q84G19
A	-3	ARG	-	expression tag	UNP Q84G19
A	-2	GLY	-	expression tag	UNP Q84G19
A	-1	SER	-	expression tag	UNP Q84G19
A	0	HIS	-	expression tag	UNP Q84G19
B	-19	MET	-	initiating methionine	UNP Q84G19
B	-18	GLY	-	expression tag	UNP Q84G19
B	-17	SER	-	expression tag	UNP Q84G19
B	-16	SER	-	expression tag	UNP Q84G19
B	-15	HIS	-	expression tag	UNP Q84G19

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q84G19
B	-13	HIS	-	expression tag	UNP Q84G19
B	-12	HIS	-	expression tag	UNP Q84G19
B	-11	HIS	-	expression tag	UNP Q84G19
B	-10	HIS	-	expression tag	UNP Q84G19
B	-9	SER	-	expression tag	UNP Q84G19
B	-8	SER	-	expression tag	UNP Q84G19
B	-7	GLY	-	expression tag	UNP Q84G19
B	-6	LEU	-	expression tag	UNP Q84G19
B	-5	VAL	-	expression tag	UNP Q84G19
B	-4	PRO	-	expression tag	UNP Q84G19
B	-3	ARG	-	expression tag	UNP Q84G19
B	-2	GLY	-	expression tag	UNP Q84G19
B	-1	SER	-	expression tag	UNP Q84G19
B	0	HIS	-	expression tag	UNP Q84G19

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



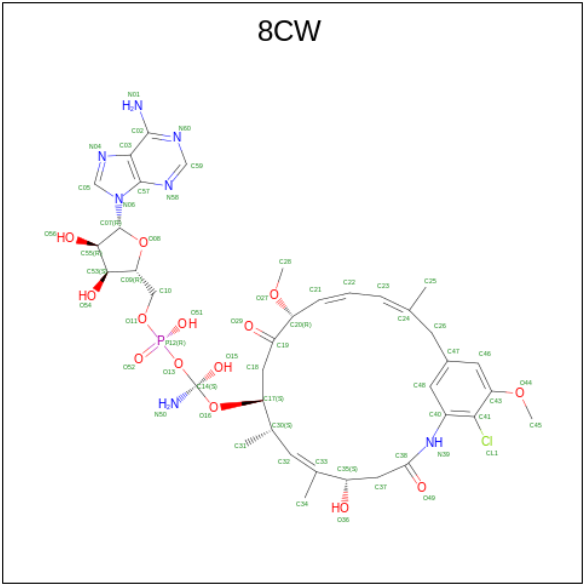
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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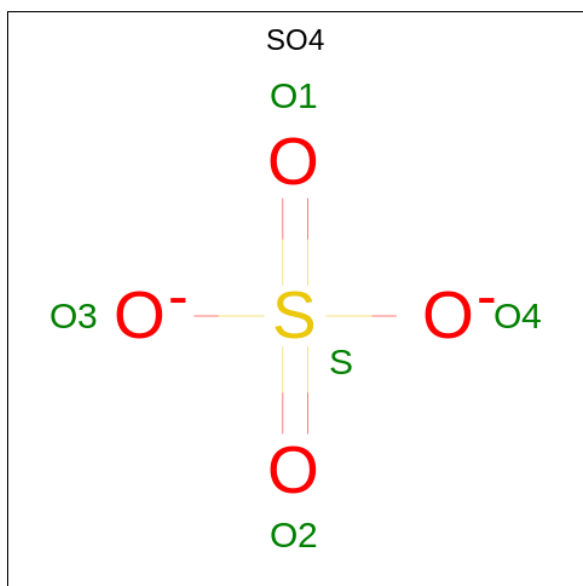
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total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

- Molecule 3 is [(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methyl [({S})-azanyl-[(5 {S},6 {E},8 {S},9 {S},12 {R},13 {E},15 {E})-21-chloranyl-12,20-dimethoxy-6,8,16-trimethyl-5-oxidanyl-3,11-bis(oxidanylidene)-2-azabicyclo[16.3.1]docosa-1(21),6,13,15,18(22),19-hexaen-9-yl]oxy]-oxidanyl-methyl] hydrogen phosphate (three-letter code: 8CW) (formula: C₃₇H₄₉ClN₇O₁₄P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	P	0	0
			60	37	1	7	14	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



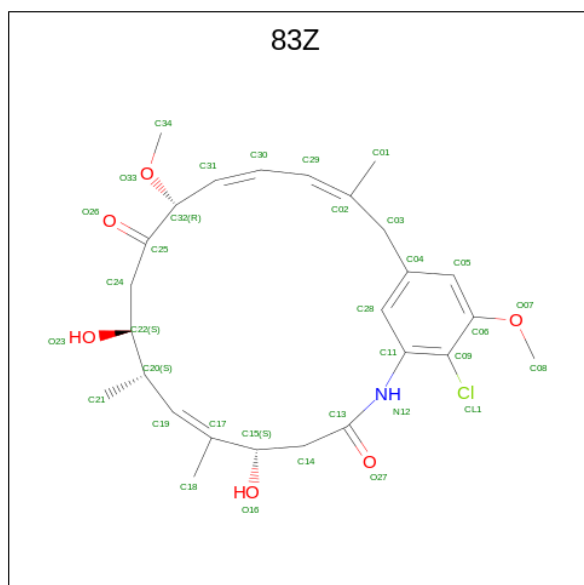
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Fe	0	0
			1	1		
5	B	1	Total	Fe	0	0
			1	1		

- # CA0
-
- The chemical structure of CA0 is a complex molecule. It features a purine-like base (N1, N3, N7, N9, C2, C4, C6, C8) with an amino group (NH2) at N6. This base is connected to a ribose sugar (C1', C2', C3', C4', C5') via a glycosidic bond. The ribose sugar is further connected to a phosphate group (P, O1A, O2A, O3A, O1B, O2B) via a phosphodiester bond. The phosphate group is also connected to a terminal group (O1B, O2B) via a phosphodiester bond. The structure is labeled with atom names and numbers, and includes stereochemical indicators (wedges and dashes) for the ribose sugar and phosphate group.
- NC1=NC2=C(N1)N=CN=C2[C@H]3O[C@@H](COP(=O)(O)OP(=O)(O)O)[C@H](O)[C@@H](O)[C@H]3O

- Molecule 7 is (5 {S},6 {E},8 {S},9 {S},12 {R},15 {E})-21-chloranyl-12,20-dimethoxy-6,8,16-trimethyl-5,9-bis(oxidanyl)-2-azabicyclo[16.3.1]docosa-1(21),6,15,18(22),19-pentaene-3,11-dione (three-letter code: 83Z) (formula: C₂₆H₃₄ClNO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	Cl	N	O	0	0
			34	26	1	1	6		


- Molecule 8 is water.

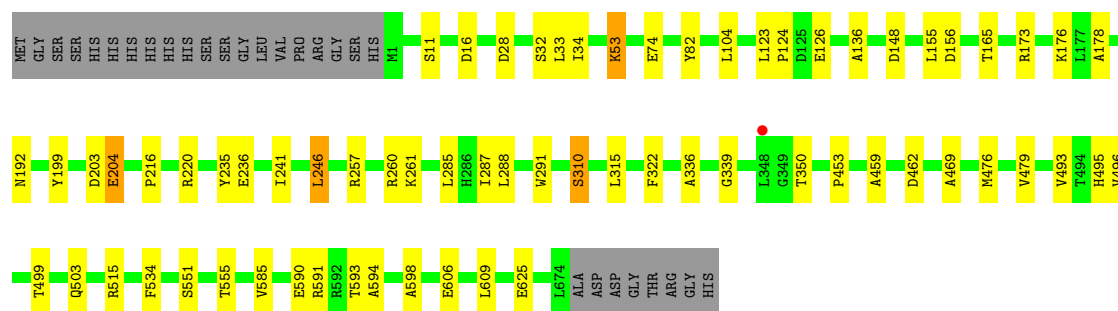
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	7	Total	O	0	0
			7	7		
8	B	9	Total	O	0	0
			9	9		

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.

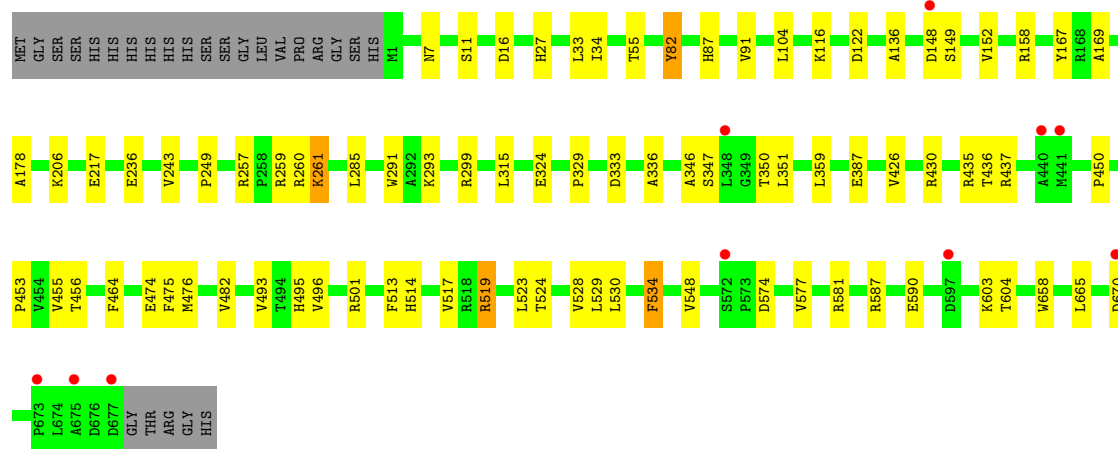
• Molecule 1: GdmN

Chain A: 



• Molecule 1: GdmN

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.86Å 111.86Å 231.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.70 – 2.85 25.70 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (25.70-2.85) 99.8 (25.70-2.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.50 (at 2.85Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.175 , 0.225 0.175 , 0.225	Depositor DCC
R_{free} test set	1976 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10632	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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: FE, SO4, CA0, EDO, 83Z, 8CW

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	0.47	0/5314	0.67	2/7227 (0.0%)
1	B	0.45	0/5335	0.65	0/7256
All	All	0.46	0/10649	0.66	2/14483 (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	A	156	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	155	LEU	CB-CG-CD1	-5.14	102.25	111.00

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	5193	0	5101	37	0
1	B	5214	0	5114	49	0
2	A	36	0	54	0	0
2	B	16	0	24	1	0
3	A	60	0	0	2	0
4	A	25	0	0	0	0
4	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	B	26	0	14	1	0
7	B	34	0	0	0	0
8	A	7	0	0	0	0
8	B	9	0	0	0	0
All	All	10632	0	10307	81	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 (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ARG:HH22	1:B:261:LYS:NZ	1.81	0.79
1:B:259:ARG:HH22	1:B:261:LYS:HZ3	1.32	0.73
1:A:192:ASN:ND2	1:A:246:LEU:H	1.95	0.65
1:A:591:ARG:NH1	1:A:606:GLU:OE1	2.34	0.60
1:B:299:ARG:HG2	1:B:324:GLU:HB2	1.87	0.56
1:B:430:ARG:NH1	1:B:524:THR:HB	2.21	0.56
1:A:593:THR:HG22	1:A:594:ALA:O	2.06	0.55
1:A:260:ARG:N	1:A:260:ARG:HD2	2.21	0.54
1:B:11:SER:HB3	1:B:16:ASP:HA	1.89	0.54
1:B:587:ARG:HG3	2:B:702:EDO:H22	1.89	0.54
1:B:136:ALA:HB1	1:B:336:ALA:O	2.08	0.53
1:A:310:SER:HB2	1:A:479:VAL:HG23	1.89	0.53
1:B:285:LEU:HD11	1:B:315:LEU:HG	1.90	0.53
1:B:513:PHE:O	1:B:517:VAL:HG23	2.10	0.51
3:A:706:8CW:CL1	1:B:243:VAL:HG12	2.47	0.51
1:A:126:GLU:H	1:A:126:GLU:CD	2.15	0.50
1:A:285:LEU:HD11	1:A:315:LEU:HD23	1.94	0.50
1:B:243:VAL:HG22	1:B:249:PRO:HG3	1.93	0.50
1:A:257:ARG:HB3	1:B:104:LEU:CD1	2.42	0.50
1:A:285:LEU:HD11	1:A:315:LEU:CD2	2.43	0.49
1:A:28:ASP:OD1	1:A:53:LYS:HE3	2.12	0.49
1:B:152:VAL:HB	1:B:167:TYR:HB2	1.95	0.48
1:B:346:ALA:HB2	1:B:351:LEU:HD12	1.96	0.48
1:A:453:PRO:HB3	1:A:493:VAL:HG21	1.96	0.47
1:B:27:HIS:HA	1:B:55:THR:HG22	1.97	0.47
1:A:33:LEU:HD23	1:A:33:LEU:HA	1.78	0.47
1:B:178:ALA:HB2	1:B:291:TRP:CZ2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:TYR:CE1	1:A:287:ILE:HD11	2.50	0.46
1:B:574:ASP:O	1:B:577:VAL:HG22	2.15	0.46
1:A:192:ASN:HD22	1:A:246:LEU:H	1.63	0.46
1:B:658:TRP:NE1	1:B:665:LEU:HB2	2.32	0.45
1:A:136:ALA:HB1	1:A:336:ALA:O	2.16	0.45
1:B:456:THR:HG22	1:B:514:HIS:CD2	2.51	0.45
1:B:450:PRO:HG3	1:B:495:HIS:CD2	2.52	0.45
1:B:476:MET:HB3	1:B:501:ARG:HG2	1.99	0.45
1:A:598:ALA:HB1	1:B:581:ARG:HB3	1.98	0.45
1:A:585:VAL:HG23	1:A:609:LEU:HD22	1.98	0.45
1:A:590:GLU:HB3	1:B:590:GLU:HB3	1.99	0.45
1:B:260:ARG:N	1:B:260:ARG:HD2	2.31	0.45
1:B:464:PHE:CE1	1:B:482:VAL:HG22	2.52	0.45
1:A:178:ALA:HB2	1:A:291:TRP:CZ2	2.51	0.45
1:B:426:VAL:HG21	1:B:529:LEU:HD13	1.99	0.45
1:A:11:SER:HB3	1:A:16:ASP:HA	1.99	0.44
1:B:27:HIS:CD2	1:B:27:HIS:H	2.35	0.44
1:A:165:THR:HG23	1:A:176:LYS:HD2	2.00	0.44
1:B:455:VAL:HG23	1:B:528:VAL:HG22	2.00	0.44
1:A:476:MET:HG3	1:A:503:GLN:HB2	2.00	0.43
1:B:453:PRO:HB3	1:B:493:VAL:HG21	1.99	0.43
1:A:136:ALA:O	1:A:339:GLY:HA3	2.19	0.43
1:B:261:LYS:HD2	1:B:261:LYS:HA	1.58	0.43
1:B:359:LEU:HD12	1:B:474:GLU:HG2	2.01	0.43
1:A:123:LEU:HD12	1:A:124:PRO:HD2	2.01	0.43
1:A:204:GLU:H	1:A:204:GLU:HG2	1.20	0.43
1:B:495:HIS:ND1	1:B:496:VAL:HG12	2.34	0.43
1:B:517:VAL:HG22	1:B:529:LEU:HD12	2.01	0.43
1:B:519:ARG:NH1	1:B:523:LEU:HD21	2.34	0.43
1:A:104:LEU:CD1	1:B:257:ARG:HB3	2.49	0.42
1:A:459:ALA:O	1:A:462:ASP:HB2	2.19	0.42
1:A:260:ARG:HD3	1:B:104:LEU:HG	2.01	0.42
1:B:329:PRO:HD3	1:B:475:PHE:CE2	2.55	0.42
1:A:322:PHE:O	1:A:469:ALA:HB2	2.20	0.42
1:B:519:ARG:HH12	1:B:523:LEU:HD21	1.85	0.42
1:B:87:HIS:O	1:B:91:VAL:HG23	2.20	0.41
1:A:199:TYR:HB3	1:A:203:ASP:HB2	2.00	0.41
1:B:464:PHE:CD1	1:B:482:VAL:HG22	2.56	0.41
1:A:479:VAL:HG13	1:A:499:THR:HB	2.03	0.41
1:B:519:ARG:HD2	1:B:519:ARG:HA	1.82	0.41
1:A:74:GLU:H	1:A:74:GLU:CD	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:PHE:CE2	1:B:548:VAL:HG13	2.56	0.41
1:A:216:PRO:O	1:A:220:ARG:HB2	2.20	0.41
1:A:593:THR:CG2	1:A:594:ALA:N	2.84	0.41
1:B:259:ARG:HH22	1:B:261:LYS:HZ2	1.65	0.41
1:B:665:LEU:HD23	1:B:665:LEU:HA	1.73	0.41
1:A:551:SER:O	1:A:555:THR:HG23	2.20	0.41
1:B:149:SER:HA	1:B:169:ALA:O	2.22	0.40
1:A:288:LEU:HD23	1:A:288:LEU:HA	1.92	0.40
1:A:204:GLU:OE1	3:A:706:8CW:O56	2.40	0.40
1:B:7:ASN:HB2	1:B:82:TYR:CE2	2.56	0.40
1:B:33:LEU:HD23	1:B:33:LEU:HA	1.85	0.40
1:B:333:ASP:OD1	6:B:708:CA0:O3A	2.39	0.40
1:B:7:ASN:HB2	1:B:82:TYR:CD2	2.56	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	672/702 (96%)	651 (97%)	21 (3%)	0	100	100
1	B	675/702 (96%)	646 (96%)	29 (4%)	0	100	100
All	All	1347/1404 (96%)	1297 (96%)	50 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	537/559 (96%)	519 (97%)	18 (3%)	37	67
1	B	539/559 (96%)	516 (96%)	23 (4%)	29	59
All	All	1076/1118 (96%)	1035 (96%)	41 (4%)	33	64

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	SER
1	A	34	ILE
1	A	53	LYS
1	A	82	TYR
1	A	148	ASP
1	A	173	ARG
1	A	204	GLU
1	A	236	GLU
1	A	241	ILE
1	A	246	LEU
1	A	261	LYS
1	A	310	SER
1	A	350	THR
1	A	495	HIS
1	A	496	VAL
1	A	515	ARG
1	A	534	PHE
1	A	625	GLU
1	B	34	ILE
1	B	82	TYR
1	B	116	LYS
1	B	122	ASP
1	B	148	ASP
1	B	158	ARG
1	B	206	LYS
1	B	217	GLU
1	B	236	GLU
1	B	261	LYS
1	B	293	LYS
1	B	347	SER
1	B	350	THR
1	B	387	GLU
1	B	435	ARG

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Mol	Chain	Res	Type
1	B	436	THR
1	B	437	ARG
1	B	519	ARG
1	B	530	LEU
1	B	534	PHE
1	B	603	LYS
1	B	604	THR
1	B	670	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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	B	701	-	3,3,3	0.97	0	2,2,2	0.34	0
4	SO4	A	708	-	4,4,4	1.04	0	6,6,6	0.59	0
2	EDO	A	715	-	3,3,3	1.04	0	2,2,2	0.31	0
2	EDO	A	705	-	3,3,3	0.95	0	2,2,2	0.51	0
4	SO4	A	707	-	4,4,4	0.73	0	6,6,6	0.62	0
6	CA0	B	708	5	24,28,28	3.91	12 (50%)	26,42,42	1.77	8 (30%)
4	SO4	B	706	-	4,4,4	1.06	0	6,6,6	0.25	0
2	EDO	B	703	-	3,3,3	0.61	0	2,2,2	0.80	0
4	SO4	A	709	-	4,4,4	1.35	0	6,6,6	0.49	0
4	SO4	A	710	-	4,4,4	0.87	0	6,6,6	0.73	0
4	SO4	B	705	-	4,4,4	0.58	0	6,6,6	1.25	1 (16%)
2	EDO	B	702	-	3,3,3	1.08	0	2,2,2	0.20	0
2	EDO	A	713	-	3,3,3	1.26	0	2,2,2	0.48	0
7	83Z	B	709	-	33,35,35	1.88	6 (18%)	39,48,48	2.10	13 (33%)
4	SO4	A	711	-	4,4,4	1.21	0	6,6,6	0.45	0
2	EDO	A	716	-	3,3,3	0.83	0	2,2,2	0.21	0
3	8CW	A	706	5	57,64,64	3.72	24 (42%)	62,94,94	2.13	19 (30%)
2	EDO	A	714	-	3,3,3	0.99	0	2,2,2	0.45	0
2	EDO	A	703	-	3,3,3	0.84	0	2,2,2	0.64	0
2	EDO	A	702	-	3,3,3	0.86	0	2,2,2	0.53	0
2	EDO	A	704	-	3,3,3	1.22	0	2,2,2	0.23	0
2	EDO	B	704	-	3,3,3	1.15	0	2,2,2	0.19	0
2	EDO	A	701	-	3,3,3	0.91	0	2,2,2	0.71	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	A	714	-	-	1/1/1/1	-
2	EDO	B	701	-	-	1/1/1/1	-
2	EDO	B	702	-	-	1/1/1/1	-
6	CA0	B	708	5	-	2/9/31/31	0/3/3/3
2	EDO	A	713	-	-	1/1/1/1	-
2	EDO	B	703	-	-	0/1/1/1	-
2	EDO	A	703	-	-	0/1/1/1	-
7	83Z	B	709	-	-	11/42/42/42	0/1/2/2
2	EDO	A	716	-	-	0/1/1/1	-
2	EDO	A	715	-	-	1/1/1/1	-
2	EDO	A	702	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	705	-	-	1/1/1/1	-
2	EDO	A	704	-	-	0/1/1/1	-
2	EDO	B	704	-	-	0/1/1/1	-
3	8CW	A	706	5	-	17/48/79/79	0/4/5/5
2	EDO	A	701	-	-	1/1/1/1	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	706	8CW	C55-C07	-14.39	1.31	1.53
3	A	706	8CW	O08-C07	12.57	1.58	1.41
6	B	708	CA0	C2'-C1'	8.93	1.67	1.53
3	A	706	8CW	C53-C09	-8.31	1.31	1.53
6	B	708	CA0	C3'-C2'	-7.96	1.31	1.53
6	B	708	CA0	O4'-C1'	-7.59	1.30	1.41
6	B	708	CA0	CB-N2B	6.56	1.45	1.33
3	A	706	8CW	O08-C09	5.87	1.58	1.45
7	B	709	83Z	C13-N12	5.69	1.48	1.35
3	A	706	8CW	C38-N39	5.36	1.47	1.35
3	A	706	8CW	C26-C47	5.35	1.60	1.51
6	B	708	CA0	O4'-C4'	5.23	1.56	1.45
3	A	706	8CW	C02-N01	5.10	1.52	1.34
3	A	706	8CW	P12-O13	4.95	1.73	1.60
3	A	706	8CW	C34-C33	4.92	1.59	1.50
3	A	706	8CW	C55-C53	4.88	1.66	1.53
3	A	706	8CW	O44-C43	4.67	1.44	1.37
6	B	708	CA0	PA-O3A	4.47	1.69	1.60
3	A	706	8CW	C22-C23	4.37	1.57	1.43
6	B	708	CA0	O3'-C3'	4.06	1.52	1.43
6	B	708	CA0	C5'-C4'	-3.98	1.39	1.51
7	B	709	83Z	C32-C31	3.85	1.54	1.50
3	A	706	8CW	C41-CL1	3.68	1.80	1.72
7	B	709	83Z	O07-C06	3.68	1.43	1.37
3	A	706	8CW	C20-C21	3.65	1.54	1.50
7	B	709	83Z	C09-CL1	3.52	1.80	1.72
6	B	708	CA0	C6-N6	3.52	1.46	1.34
7	B	709	83Z	C30-C29	3.50	1.54	1.43
7	B	709	83Z	C11-N12	3.40	1.48	1.41
3	A	706	8CW	C30-C32	3.32	1.58	1.51
3	A	706	8CW	C25-C24	3.24	1.59	1.50
3	A	706	8CW	C35-C33	3.14	1.56	1.51
3	A	706	8CW	C32-C33	3.13	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	706	8CW	C18-C19	2.98	1.58	1.51
3	A	706	8CW	C26-C24	2.66	1.54	1.51
6	B	708	CA0	C3'-C4'	2.59	1.59	1.53
3	A	706	8CW	C46-C43	2.58	1.43	1.38
6	B	708	CA0	O2'-C2'	2.48	1.48	1.43
6	B	708	CA0	PA-O5'	2.35	1.68	1.59
3	A	706	8CW	P12-O11	2.15	1.68	1.59
3	A	706	8CW	C40-N39	2.10	1.45	1.41
3	A	706	8CW	C37-C38	2.01	1.56	1.51

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	706	8CW	C18-C17-C30	-6.63	99.96	115.45
3	A	706	8CW	C40-C41-CL1	-6.05	115.10	119.52
7	B	709	83Z	O07-C06-C09	4.79	121.21	115.53
3	A	706	8CW	O51-P12-O13	4.60	125.05	106.43
7	B	709	83Z	C22-C20-C19	-4.45	101.39	110.64
3	A	706	8CW	C23-C22-C21	-4.23	114.27	124.53
7	B	709	83Z	C11-C09-CL1	-3.98	116.61	119.52
3	A	706	8CW	N58-C59-N60	-3.87	122.62	128.68
7	B	709	83Z	C04-C03-C02	-3.74	99.74	114.47
3	A	706	8CW	C47-C26-C24	-3.74	99.76	114.47
3	A	706	8CW	C37-C38-N39	3.71	119.59	114.50
7	B	709	83Z	O16-C15-C14	3.59	118.86	110.05
6	B	708	CA0	O1B-CB-N2B	-3.54	119.68	125.51
7	B	709	83Z	C18-C17-C15	3.39	121.43	115.22
7	B	709	83Z	C01-C02-C03	3.21	121.66	114.88
6	B	708	CA0	N3-C2-N1	-3.17	123.72	128.68
6	B	708	CA0	O3A-PA-O5'	3.15	112.10	102.92
3	A	706	8CW	O29-C19-C18	-2.91	117.49	121.41
3	A	706	8CW	C48-C47-C46	2.91	122.97	118.98
3	A	706	8CW	C25-C24-C26	2.90	121.00	114.88
6	B	708	CA0	C4-C5-N7	-2.84	106.44	109.40
7	B	709	83Z	C22-C24-C25	-2.81	107.80	114.19
6	B	708	CA0	O2'-C2'-C3'	2.81	120.92	111.82
7	B	709	83Z	O16-C15-C17	-2.77	104.18	110.81
6	B	708	CA0	O3'-C3'-C4'	-2.67	103.33	111.05
7	B	709	83Z	C24-C22-C20	-2.58	109.22	114.03
6	B	708	CA0	O1A-PA-O3A	2.56	112.48	104.14
3	A	706	8CW	C31-C30-C17	-2.50	108.07	111.80
7	B	709	83Z	C28-C04-C05	2.45	122.35	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	706	8CW	O44-C43-C41	2.45	118.43	115.53
3	A	706	8CW	O13-P12-O52	-2.43	100.39	109.29
4	B	705	SO4	O4-S-O1	2.40	121.85	109.31
3	A	706	8CW	O51-P12-O52	-2.40	100.37	112.24
6	B	708	CA0	O5'-C5'-C4'	-2.34	100.92	108.99
7	B	709	83Z	C05-C06-C09	-2.31	117.87	120.76
3	A	706	8CW	C28-O27-C20	-2.28	109.81	112.93
3	A	706	8CW	O49-C38-N39	-2.24	119.54	123.63
3	A	706	8CW	C37-C35-C33	-2.23	104.83	113.13
7	B	709	83Z	C21-C20-C19	-2.13	106.50	110.05
3	A	706	8CW	C43-C46-C47	-2.09	116.92	120.05
3	A	706	8CW	C30-C32-C33	-2.07	122.30	127.73

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	706	8CW	C18-C17-C30-C31
3	A	706	8CW	C18-C17-C30-C32
3	A	706	8CW	O16-C17-C30-C31
3	A	706	8CW	C10-O11-P12-O52
7	B	709	83Z	O23-C22-C24-C25
3	A	706	8CW	O49-C38-N39-C40
7	B	709	83Z	O27-C13-N12-C11
3	A	706	8CW	C37-C38-N39-C40
7	B	709	83Z	C14-C13-N12-C11
2	A	702	EDO	O1-C1-C2-O2
7	B	709	83Z	C31-C32-O33-C34
2	B	702	EDO	O1-C1-C2-O2
3	A	706	8CW	O16-C17-C18-C19
3	A	706	8CW	C30-C17-C18-C19
3	A	706	8CW	C10-O11-P12-O13
6	B	708	CA0	CB-O3A-PA-O2A
7	B	709	83Z	C30-C31-C32-C25
2	A	701	EDO	O1-C1-C2-O2
3	A	706	8CW	C21-C22-C23-C24
3	A	706	8CW	C21-C20-O27-C28
3	A	706	8CW	O16-C17-C30-C32
2	A	713	EDO	O1-C1-C2-O2
2	A	714	EDO	O1-C1-C2-O2
2	A	715	EDO	O1-C1-C2-O2
7	B	709	83Z	C28-C11-N12-C13

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Mol	Chain	Res	Type	Atoms
3	A	706	8CW	C18-C19-C20-O27
7	B	709	83Z	C24-C25-C32-O33
3	A	706	8CW	C34-C33-C35-O36
3	A	706	8CW	C32-C33-C35-O36
7	B	709	83Z	O16-C15-C17-C19
7	B	709	83Z	O16-C15-C17-C18
3	A	706	8CW	C48-C40-N39-C38
7	B	709	83Z	C02-C29-C30-C31
3	A	706	8CW	O29-C19-C20-O27
2	A	705	EDO	O1-C1-C2-O2
2	B	701	EDO	O1-C1-C2-O2
7	B	709	83Z	C09-C11-N12-C13
6	B	708	CA0	CB-O3A-PA-O5'

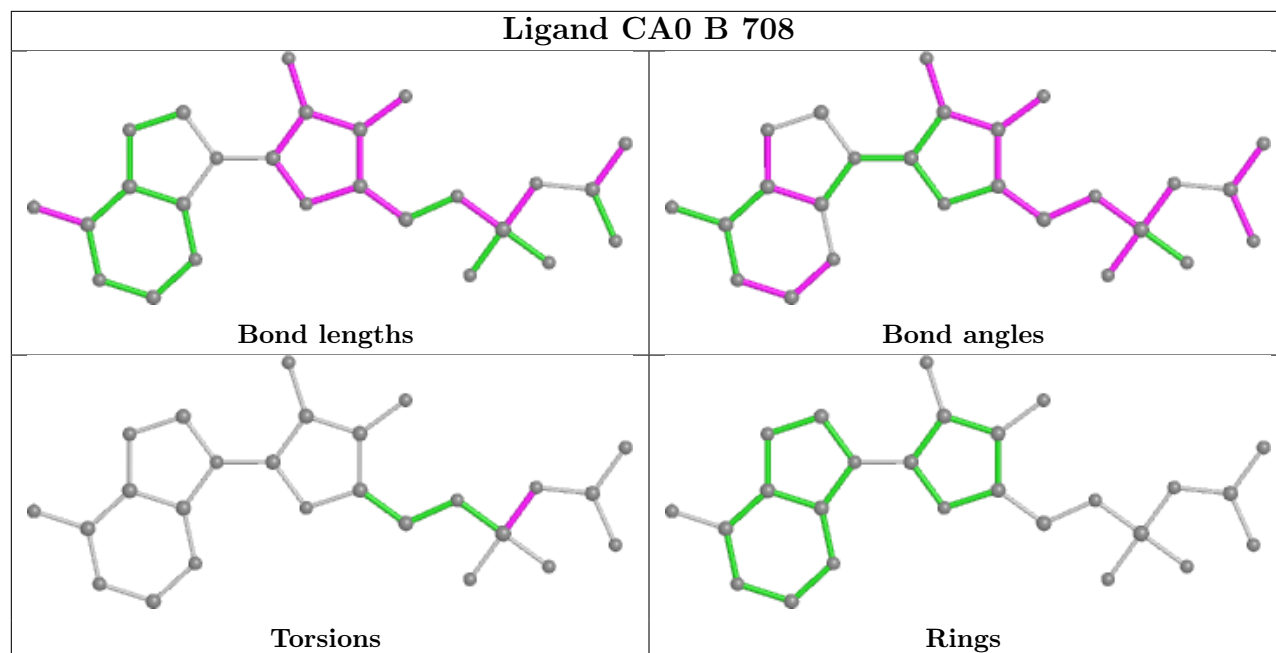
There are no ring outliers.

3 monomers are involved in 4 short contacts:

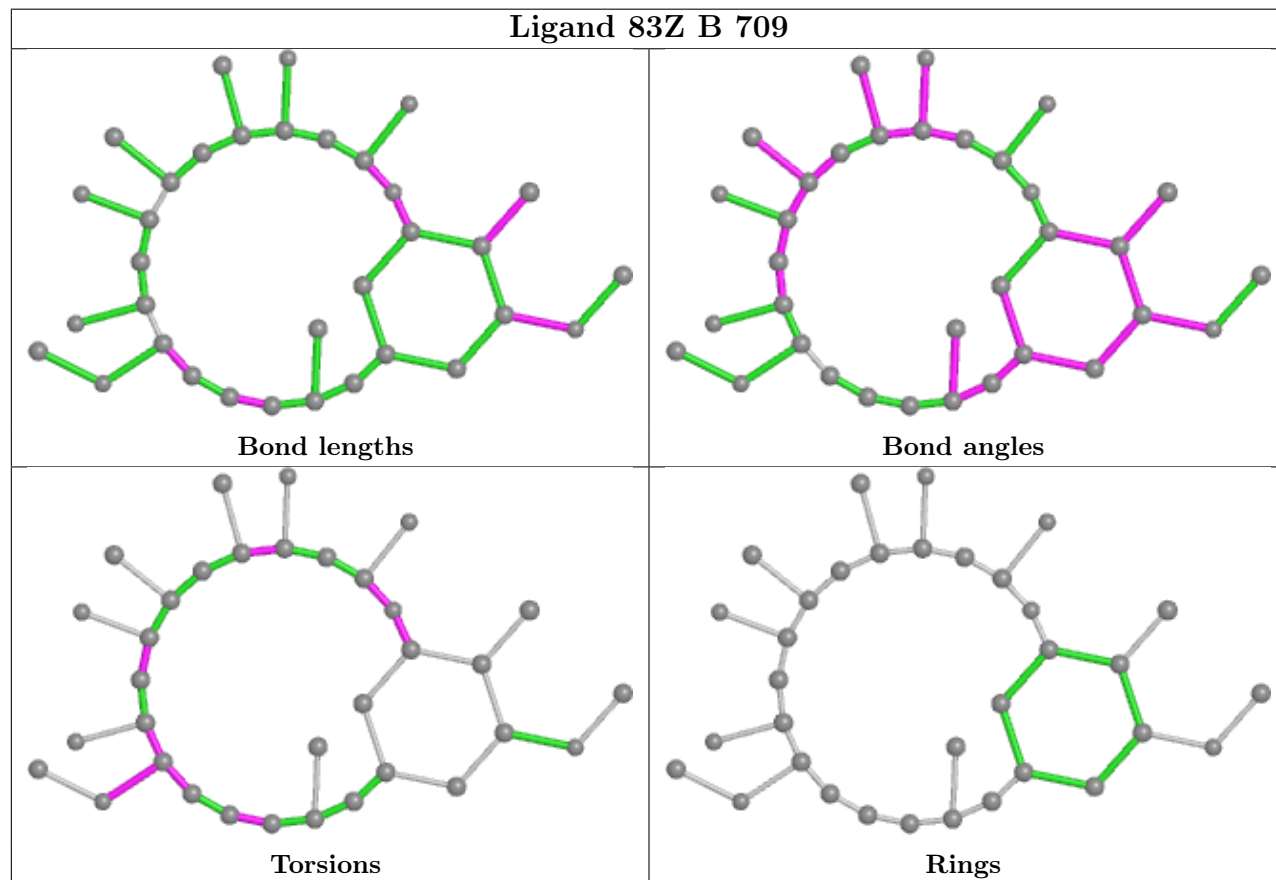
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	708	CA0	1	0
2	B	702	EDO	1	0
3	A	706	8CW	2	0

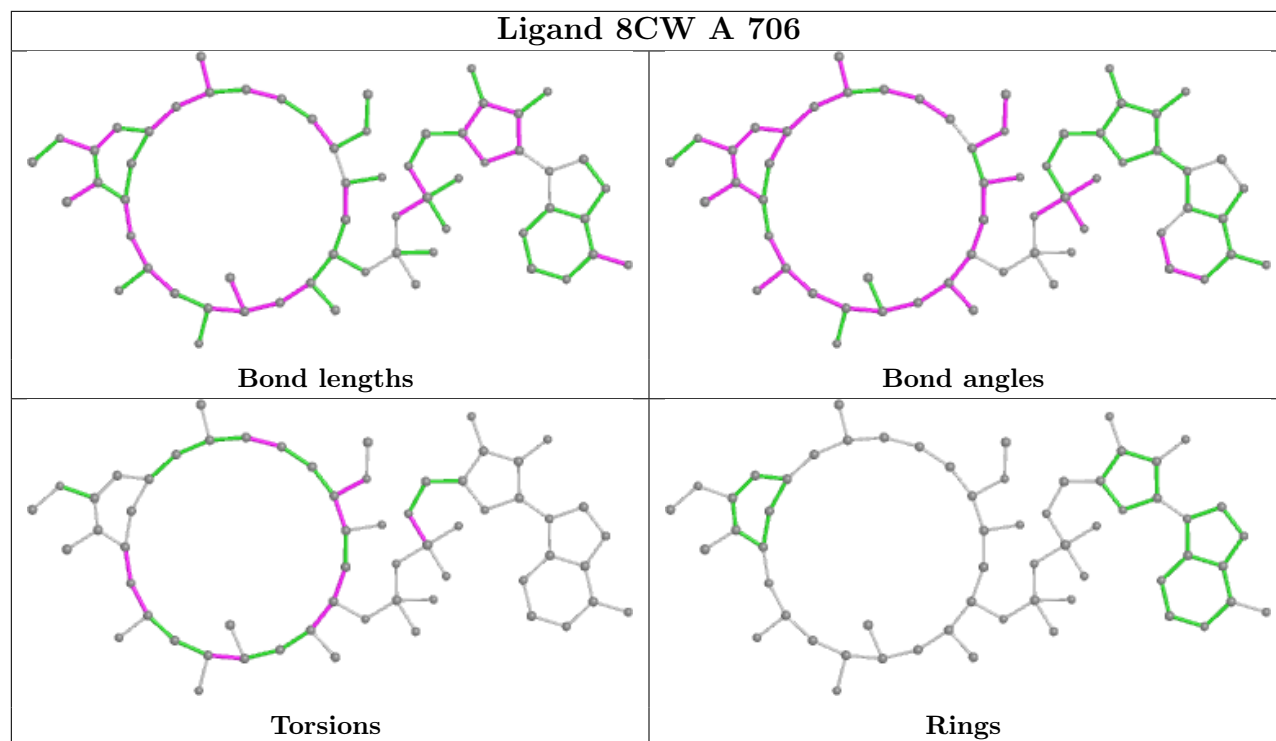
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 CA0 B 708



Ligand 83Z B 709





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	674/702 (96%)	-0.42	1 (0%) 95 96	19, 31, 47, 61	0
1	B	677/702 (96%)	-0.23	10 (1%) 73 72	27, 40, 64, 83	0
All	All	1351/1404 (96%)	-0.32	11 (0%) 86 85	19, 35, 59, 83	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	440	ALA	4.4
1	B	348	LEU	3.3
1	B	673	PRO	3.1
1	B	675	ALA	2.9
1	B	677	ASP	2.6
1	B	441	MET	2.5
1	B	148	ASP	2.4
1	B	670	ASP	2.3
1	A	348	LEU	2.3
1	B	572	SER	2.2
1	B	597	ASP	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 ⓘ

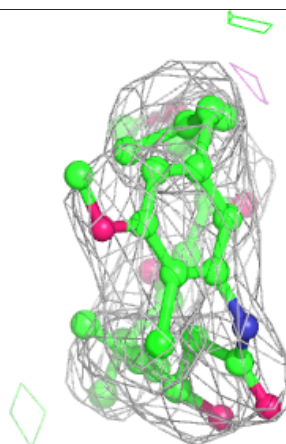
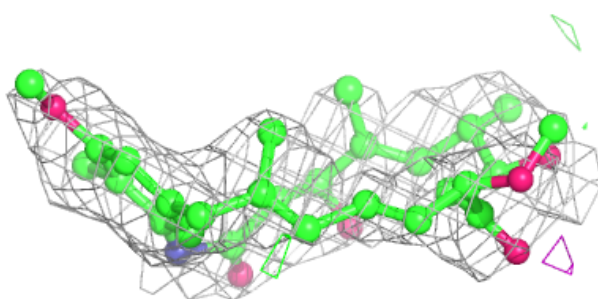
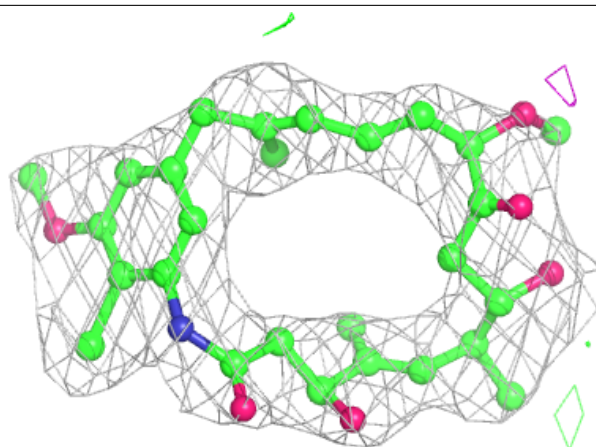
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	EDO	A	713	4/4	0.81	0.15	49,50,55,56	0
2	EDO	A	702	4/4	0.82	0.39	48,49,54,60	0
2	EDO	A	714	4/4	0.85	0.21	46,49,49,50	0
2	EDO	A	703	4/4	0.86	0.35	47,61,62,69	0
2	EDO	B	701	4/4	0.86	0.19	35,46,48,51	0
2	EDO	B	702	4/4	0.87	0.30	43,53,55,61	0
2	EDO	A	704	4/4	0.88	0.26	41,47,51,51	0
2	EDO	A	715	4/4	0.89	0.52	41,46,51,54	0
2	EDO	B	703	4/4	0.89	0.35	41,41,44,45	0
2	EDO	B	704	4/4	0.89	0.29	35,44,47,52	0
2	EDO	A	701	4/4	0.91	0.21	28,38,41,44	0
2	EDO	A	716	4/4	0.93	0.15	30,33,36,37	0
7	83Z	B	709	34/34	0.93	0.24	37,44,52,60	0
4	SO4	A	709	5/5	0.94	0.27	56,60,66,66	0
3	8CW	A	706	60/60	0.94	0.20	24,42,48,53	0
2	EDO	A	705	4/4	0.95	0.11	35,43,49,49	0
4	SO4	A	708	5/5	0.95	0.18	39,42,47,56	0
5	FE	B	707	1/1	0.96	0.17	43,43,43,43	0
4	SO4	A	710	5/5	0.96	0.23	54,61,63,74	0
5	FE	A	712	1/1	0.97	0.11	33,33,33,33	0
4	SO4	A	711	5/5	0.97	0.20	38,48,52,54	0
4	SO4	B	705	5/5	0.97	0.16	45,46,62,64	0
6	CA0	B	708	26/26	0.98	0.11	30,35,40,41	1
4	SO4	A	707	5/5	0.98	0.09	35,35,35,38	0
4	SO4	B	706	5/5	0.99	0.14	44,44,54,57	0

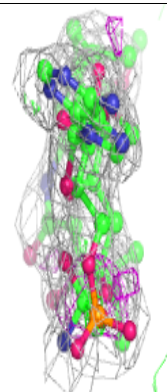
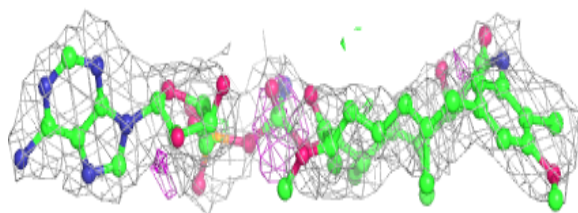
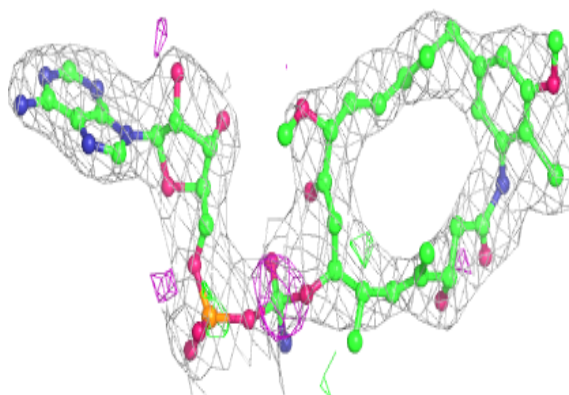
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

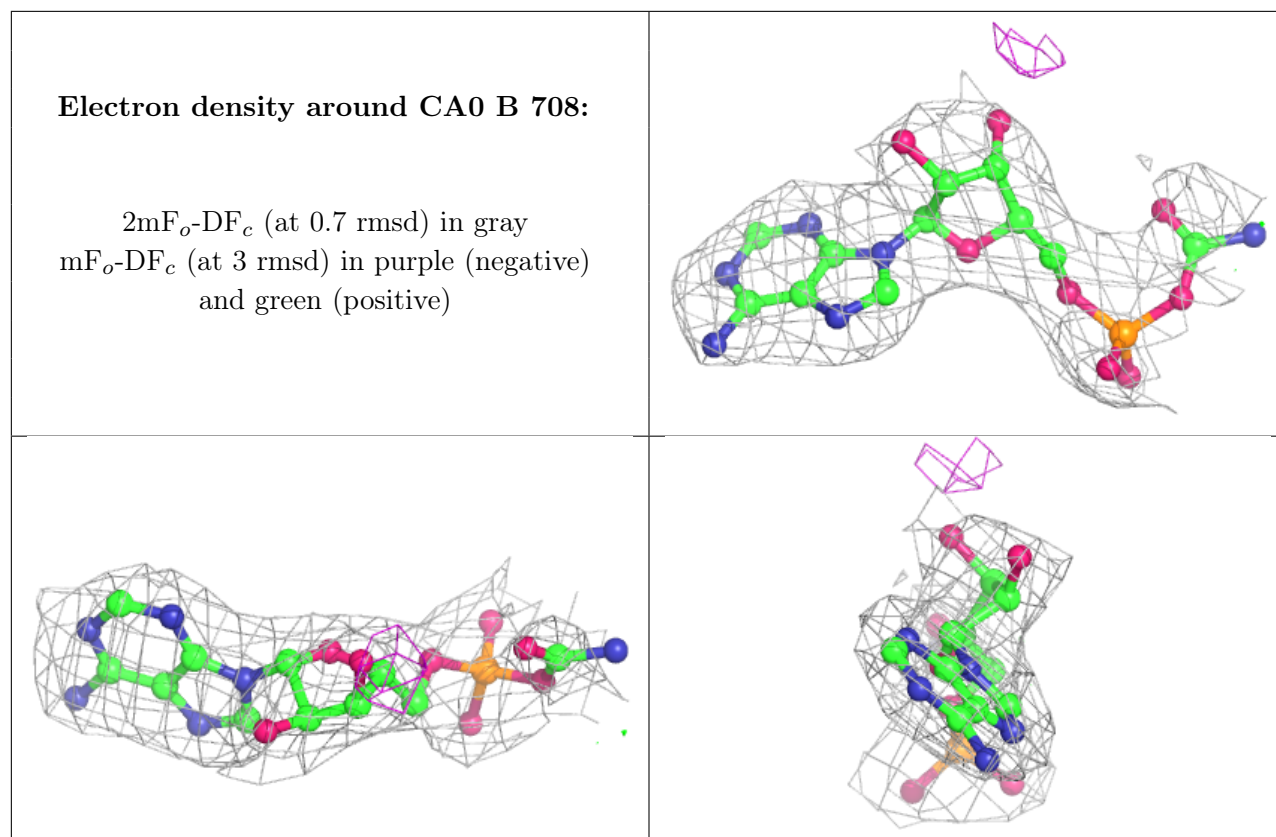
Electron density around 83Z B 709:

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

**Electron density around 8CW 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.