



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2022 – 07:32 PM JST

PDB ID : 7VZY
Title : The structure of GdmN complex with AMP and 20-O-methyl-19-chloroproan
samitocin
Authors : Wei, J.; Zheng, J.; Zhou, J.; Kang, Q.; Bai, L.
Deposited on : 2021-11-17
Resolution : 2.81 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

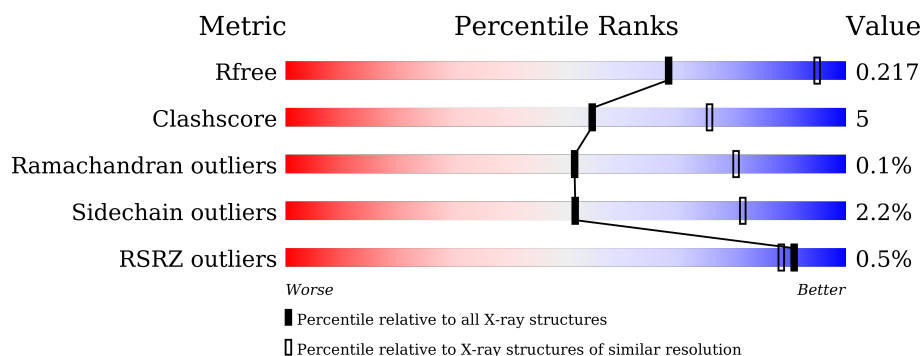
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	
1	B	702	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10634 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	1	0
			5201	3297	914	981	9			
1	B	678	Total	C	N	O	S	0	2	0
			5237	3316	922	990	9			

There are 40 discrepancies between the modelled and reference sequences:

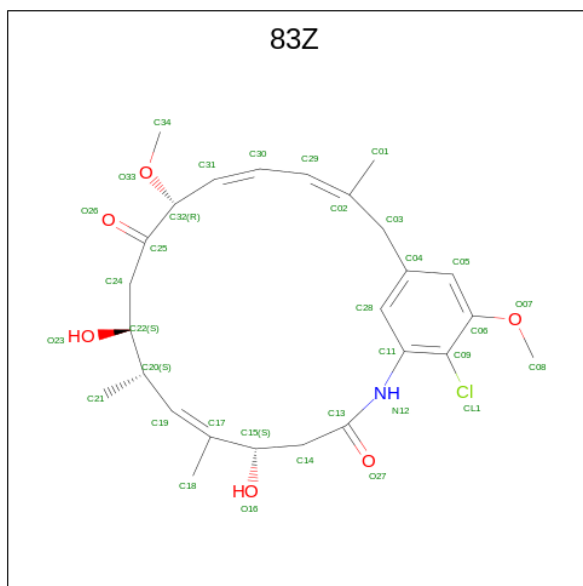
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q84G19
A	-18	GLY	-	expression tag	UNP Q84G19
A	-17	SER	-	expression tag	UNP Q84G19
A	-16	SER	-	expression tag	UNP Q84G19
A	-15	HIS	-	expression tag	UNP Q84G19
A	-14	HIS	-	expression tag	UNP Q84G19
A	-13	HIS	-	expression 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 (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).

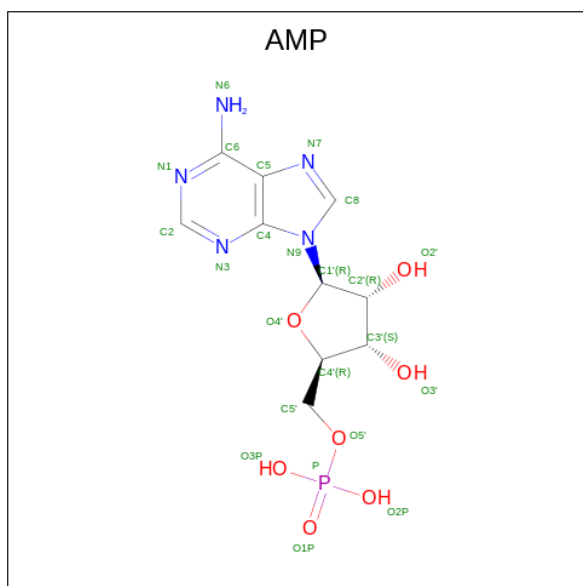


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			34	26	1	1	6		
2	B	1	Total	C	Cl	N	O	0	0
			34	26	1	1	6		

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P) (labeled as "Ligand of Interest" by depositor).



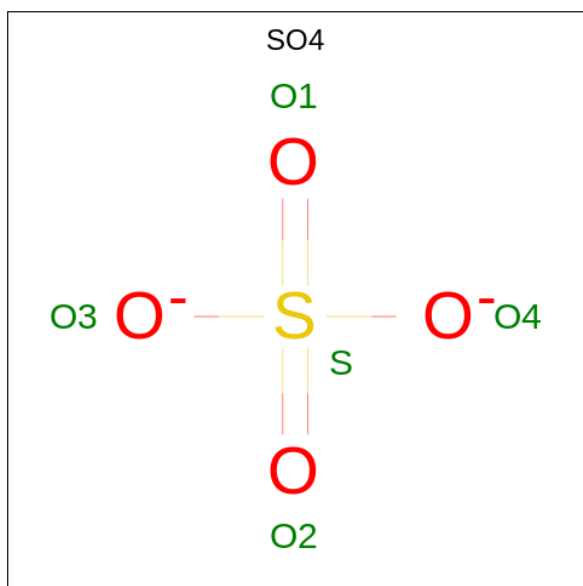
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



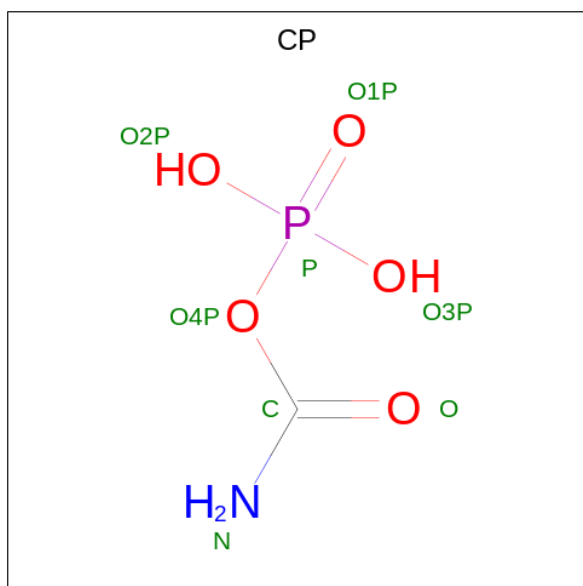
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

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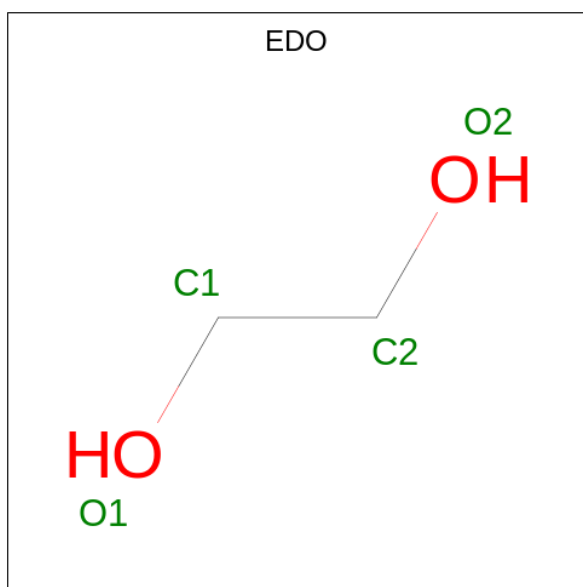
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is PHOSPHORIC ACID MONO(FORMAMIDE)ESTER (three-letter code: CP) (formula: $\text{CH}_4\text{NO}_5\text{P}$).



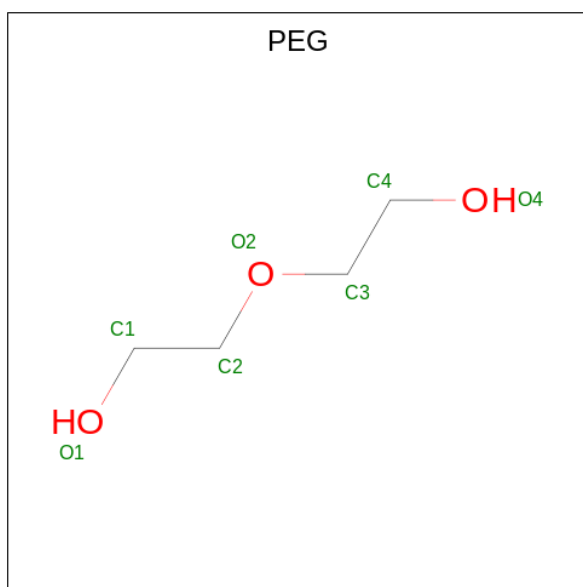
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			8	1	1	5	1		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



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

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).

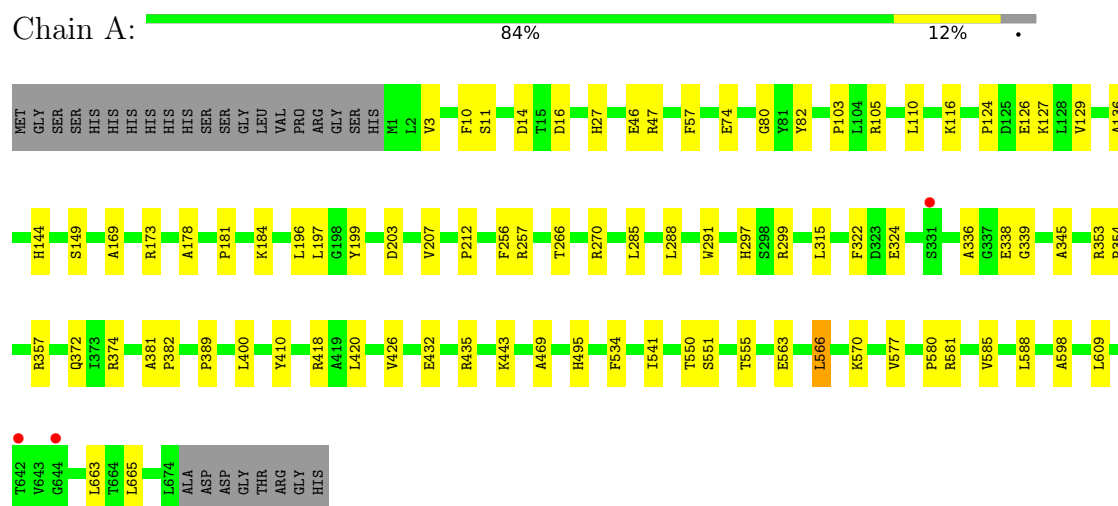


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		

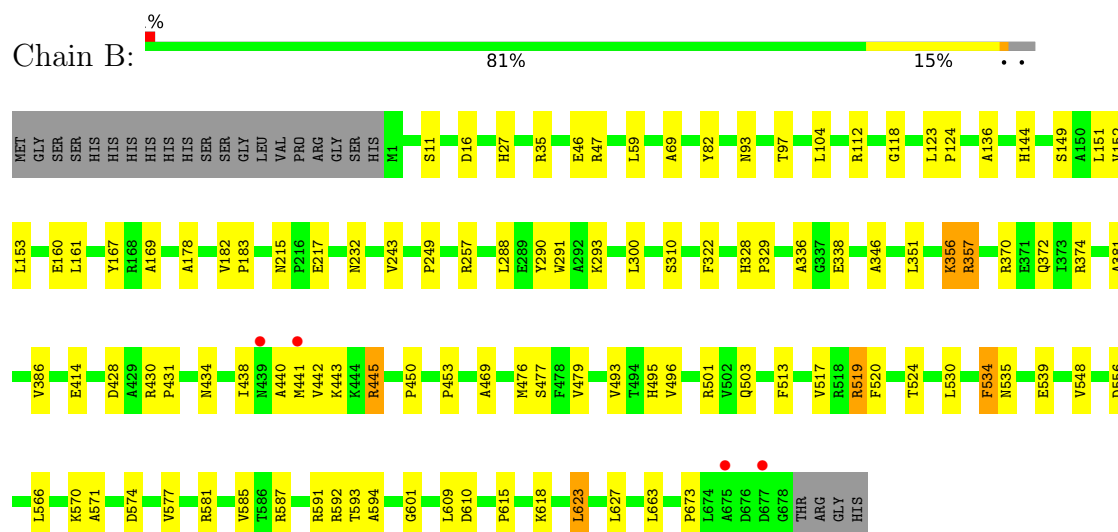
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: GdmN



• Molecule 1: GdmN



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.48Å 111.48Å 231.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.88 – 2.81 31.88 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.8 (31.88-2.81) 99.9 (31.88-2.81)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.13 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.171 , 0.220 0.169 , 0.217	Depositor DCC
R_{free} test set	2016 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10634	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 3.33% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, EDO, SO4, CP, 83Z, GOL, AMP, FE

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	0.49	0/5322	0.67	0/7238
1	B	0.47	0/5358	0.67	0/7286
All	All	0.48	0/10680	0.67	0/14524

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5201	0	5111	49	0
1	B	5237	0	5139	62	0
2	A	34	0	0	0	0
2	B	34	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	23	0	12	0	0
4	B	23	0	12	0	0
5	A	6	0	8	1	0
6	A	25	0	0	1	0
6	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	8	0	2	0	0
8	A	20	0	30	4	0
8	B	4	0	6	0	0
9	A	7	0	10	1	0
All	All	10634	0	10330	108	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 5.

All (108) 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:A:418:ARG:H	8:A:713:EDO:H11	1.15	1.10
1:B:434:ASN:O	1:B:438:ILE:HD12	1.98	0.64
1:A:418:ARG:N	8:A:713:EDO:H11	2.00	0.63
1:B:356:LYS:HD3	1:B:357:ARG:H	1.65	0.61
1:B:442:VAL:HA	1:B:556:ASP:HB2	1.82	0.61
1:B:623:LEU:HD22	1:B:627:LEU:HG	1.81	0.60
1:A:585:VAL:HG23	1:A:609:LEU:HD22	1.83	0.58
1:A:550:THR:HG21	9:A:716:PEG:H41	1.87	0.57
1:A:285:LEU:HD11	1:A:315:LEU:HD23	1.87	0.56
1:A:588:LEU:HB2	1:B:592[B]:ARG:HB2	1.86	0.56
1:A:257:ARG:HB3	1:B:104:LEU:CD1	2.37	0.55
1:B:438:ILE:HA	1:B:442:VAL:HG22	1.88	0.55
1:A:381:ALA:O	1:A:570:LYS:HE2	2.07	0.55
1:A:181:PRO:HD2	1:A:184:LYS:HD2	1.89	0.54
1:A:541:ILE:HG13	5:A:704:GOL:H11	1.89	0.54
1:B:152:VAL:HB	1:B:167:TYR:HB2	1.89	0.54
1:A:178:ALA:HB2	1:A:291:TRP:CZ2	2.44	0.53
1:B:585:VAL:HG23	1:B:609:LEU:HD22	1.91	0.53
1:B:609:LEU:HB2	1:B:615:PRO:HD2	1.91	0.53
1:B:450:PRO:HG2	1:B:495:HIS:CG	2.45	0.52
1:A:3:VAL:HG21	1:A:345:ALA:HB2	1.91	0.52
1:B:112:ARG:HG2	1:B:123:LEU:HB3	1.92	0.51
1:B:27:HIS:H	1:B:27:HIS:CD2	2.29	0.51
1:B:520:PHE:O	1:B:524:THR:OG1	2.22	0.51
1:B:430:ARG:NH1	1:B:524:THR:HB	2.25	0.51
1:A:11:SER:HB3	1:A:16:ASP:HA	1.93	0.51
1:A:124:PRO:HG2	1:A:127:LYS:HG3	1.93	0.50
1:B:381:ALA:O	1:B:570:LYS:HE2	2.11	0.50
1:B:215:ASN:OD1	1:B:217:GLU:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ARG:HE	1:A:110:LEU:HD21	1.77	0.50
1:B:445:ARG:HG2	1:B:445:ARG:HH11	1.77	0.50
1:A:266:THR:O	1:A:270:ARG:HG3	2.12	0.50
1:A:400:LEU:HD21	1:A:426:VAL:HG23	1.93	0.50
1:A:144:HIS:NE2	1:A:338:GLU:OE2	2.38	0.49
1:B:453:PRO:HD3	1:B:493:VAL:HB	1.94	0.49
1:B:136:ALA:HB1	1:B:336:ALA:O	2.12	0.48
1:B:356:LYS:HD3	1:B:357:ARG:N	2.27	0.48
1:B:519:ARG:HA	1:B:519:ARG:HD2	1.63	0.48
1:B:443:LYS:HE3	1:B:445:ARG:NE	2.29	0.48
1:A:149:SER:HA	1:A:169:ALA:O	2.14	0.48
1:B:151:LEU:O	1:B:300:LEU:HD12	2.14	0.48
1:B:178:ALA:HB2	1:B:291:TRP:CZ2	2.48	0.48
1:B:430:ARG:HH12	1:B:524:THR:HB	1.78	0.48
1:B:534:PHE:CE2	1:B:548:VAL:HG13	2.49	0.47
1:B:592[B]:ARG:NE	1:B:601:GLY:O	2.44	0.47
1:A:299:ARG:HG2	1:A:324:GLU:HB2	1.96	0.47
1:B:513:PHE:O	1:B:517:VAL:HG23	2.15	0.47
1:B:11:SER:HB3	1:B:16:ASP:HA	1.96	0.47
1:B:476:MET:HB3	1:B:501:ARG:HG2	1.96	0.47
1:A:432:GLU:HG3	1:A:435:ARG:NH2	2.29	0.47
1:A:598:ALA:HB1	1:B:581:ARG:HB3	1.95	0.46
1:A:196:LEU:HD23	1:A:256:PHE:CD2	2.50	0.46
1:B:232:ASN:HA	1:B:290:TYR:CE1	2.51	0.46
1:B:476:MET:HG2	1:B:503:GLN:HB2	1.98	0.46
1:A:382:PRO:HG2	1:A:577:VAL:HG21	1.96	0.46
1:B:414:GLU:OE1	1:B:414:GLU:N	2.42	0.45
1:B:574:ASP:O	1:B:577:VAL:HG22	2.17	0.45
1:B:535:ASN:HB2	1:B:539:GLU:HG3	1.98	0.45
1:B:346:ALA:HB2	1:B:351:LEU:HB2	1.99	0.45
1:A:372:GLN:HG2	8:A:715:EDO:O2	2.17	0.44
1:A:212:PRO:HG2	1:A:495:HIS:CD2	2.53	0.44
1:A:116:LYS:HE2	1:A:116:LYS:HB3	1.36	0.44
1:A:136:ALA:HB1	1:A:336:ALA:O	2.17	0.44
1:B:46:GLU:HG3	1:B:47:ARG:N	2.32	0.44
1:B:93:ASN:O	1:B:97:THR:HG23	2.17	0.44
1:A:103:PRO:HB2	1:A:105:ARG:HD3	2.00	0.44
1:B:310:SER:HB3	1:B:479:VAL:HG23	2.00	0.43
1:A:126:GLU:H	1:A:126:GLU:CD	2.21	0.43
1:A:389:PRO:HG3	1:A:566:LEU:HD13	2.01	0.43
1:B:243:VAL:HG22	1:B:249:PRO:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:SER:O	1:A:555:THR:HG23	2.18	0.42
1:B:144:HIS:NE2	1:B:338:GLU:OE2	2.42	0.42
1:B:428:ASP:OD2	1:B:431:PRO:HD3	2.18	0.42
1:A:288:LEU:HA	1:A:288:LEU:HD23	1.89	0.42
1:B:123:LEU:HD12	1:B:124:PRO:HD2	2.00	0.42
1:B:356:LYS:HA	1:B:356:LYS:HE2	2.02	0.42
1:B:386:VAL:HA	1:B:566:LEU:O	2.19	0.42
1:A:443:LYS:HE3	1:A:443:LYS:HB3	1.84	0.42
1:B:217:GLU:HG2	1:B:217:GLU:H	1.69	0.42
1:A:10:PHE:HA	1:A:57:PHE:HB2	2.02	0.42
1:B:495:HIS:ND1	1:B:496:VAL:HG12	2.35	0.42
1:A:297:HIS:ND1	6:A:708:SO4:O4	2.53	0.42
1:B:440:ALA:O	1:B:441:MET:C	2.58	0.42
1:A:580:PRO:HA	1:A:665:LEU:HD23	2.02	0.41
1:B:160:GLU:HG2	1:B:161:LEU:N	2.35	0.41
1:B:59:LEU:HD21	1:B:118:GLY:HA3	2.02	0.41
1:A:410:TYR:CE1	1:A:563:GLU:HA	2.55	0.41
1:A:74:GLU:H	1:A:74:GLU:CD	2.24	0.41
1:A:136:ALA:O	1:A:339:GLY:HA3	2.20	0.41
1:B:372:GLN:NE2	1:B:673:PRO:O	2.52	0.41
1:B:35:ARG:NH2	1:B:69:ALA:O	2.54	0.41
1:A:353:ARG:HG3	1:A:354:PRO:O	2.20	0.41
1:A:46:GLU:HG3	1:A:47:ARG:N	2.35	0.41
1:A:197:LEU:HD12	1:A:207:VAL:HG22	2.02	0.41
1:B:322:PHE:O	1:B:469:ALA:HB2	2.21	0.41
1:B:587:ARG:HG3	1:B:610:ASP:HB2	2.03	0.41
1:A:14:ASP:OD1	1:A:14:ASP:N	2.42	0.40
1:A:27:HIS:CD2	1:A:27:HIS:H	2.39	0.40
1:A:420:LEU:HD11	8:A:713:EDO:H22	2.03	0.40
1:B:623:LEU:HD23	1:B:623:LEU:HA	1.82	0.40
1:A:80:GLY:HA2	1:A:129:VAL:O	2.20	0.40
1:B:149:SER:HA	1:B:169:ALA:O	2.21	0.40
1:A:199:TYR:HB3	1:A:203:ASP:HB2	2.04	0.40
1:B:153:LEU:HD22	1:B:288:LEU:HD21	2.03	0.40
1:B:182:VAL:HB	1:B:183:PRO:HD3	2.03	0.40
1:A:322:PHE:O	1:A:469:ALA:HB2	2.21	0.40
1:B:328:HIS:CG	1:B:329:PRO:HD2	2.56	0.40
1:B:593:THR:HG23	1:B:594:ALA:O	2.22	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	673/702 (96%)	655 (97%)	18 (3%)	0	100	100
1	B	678/702 (97%)	644 (95%)	33 (5%)	1 (0%)	51	80
All	All	1351/1404 (96%)	1299 (96%)	51 (4%)	1 (0%)	51	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	571	ALA

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	538/559 (96%)	530 (98%)	8 (2%)	65	88
1	B	541/559 (97%)	525 (97%)	16 (3%)	41	73
All	All	1079/1118 (96%)	1055 (98%)	24 (2%)	52	81

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	TYR
1	A	173	ARG
1	A	357	ARG
1	A	374	ARG
1	A	534	PHE

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Mol	Chain	Res	Type
1	A	566	LEU
1	A	581	ARG
1	A	663	LEU
1	B	82	TYR
1	B	257	ARG
1	B	293	LYS
1	B	356	LYS
1	B	357	ARG
1	B	370	ARG
1	B	374	ARG
1	B	445	ARG
1	B	477	SER
1	B	519	ARG
1	B	530	LEU
1	B	534	PHE
1	B	591	ARG
1	B	618	LYS
1	B	623	LEU
1	B	663	LEU

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	232	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 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 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
6	SO4	A	709	-	4,4,4	0.30	0	6,6,6	0.34	0
4	AMP	A	703	3	22,25,25	1.08	1 (4%)	25,38,38	1.41	3 (12%)
6	SO4	A	705	-	4,4,4	0.28	0	6,6,6	0.45	0
5	GOL	A	704	-	5,5,5	1.91	1 (20%)	5,5,5	1.26	1 (20%)
4	AMP	B	703	3	22,25,25	0.98	2 (9%)	25,38,38	1.40	5 (20%)
9	PEG	A	716	-	6,6,6	1.30	0	5,5,5	1.49	1 (20%)
8	EDO	A	713	-	3,3,3	0.58	0	2,2,2	0.33	0
6	SO4	B	704	-	4,4,4	0.23	0	6,6,6	0.51	0
8	EDO	B	706	-	3,3,3	0.79	0	2,2,2	0.10	0
6	SO4	B	705	-	4,4,4	0.24	0	6,6,6	0.47	0
2	83Z	A	701	-	33,35,35	1.71	6 (18%)	39,48,48	2.07	16 (41%)
6	SO4	A	707	-	4,4,4	0.23	0	6,6,6	0.55	0
8	EDO	A	714	-	3,3,3	0.58	0	2,2,2	0.89	0
7	CP	A	710	-	6,7,7	3.84	2 (33%)	7,10,10	2.70	3 (42%)
2	83Z	B	701	-	33,35,35	1.69	5 (15%)	39,48,48	2.15	12 (30%)
8	EDO	A	712	-	3,3,3	0.64	0	2,2,2	0.19	0
6	SO4	A	706	-	4,4,4	0.24	0	6,6,6	0.49	0
8	EDO	A	715	-	3,3,3	0.88	0	2,2,2	0.23	0
6	SO4	A	708	-	4,4,4	0.37	0	6,6,6	0.39	0
8	EDO	A	711	-	3,3,3	0.76	0	2,2,2	0.33	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
8	EDO	B	706	-	-	0/1/1/1	-
4	AMP	A	703	3	-	1/6/26/26	0/3/3/3
2	83Z	A	701	-	-	9/42/42/42	0/1/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	A	715	-	-	0/1/1/1	-
8	EDO	A	711	-	-	1/1/1/1	-
8	EDO	A	714	-	-	1/1/1/1	-
5	GOL	A	704	-	-	2/4/4/4	-
8	EDO	A	712	-	-	0/1/1/1	-
4	AMP	B	703	3	-	0/6/26/26	0/3/3/3
7	CP	A	710	-	-	0/3/5/5	-
2	83Z	B	701	-	-	10/42/42/42	0/1/2/2
9	PEG	A	716	-	-	3/4/4/4	-
8	EDO	A	713	-	-	0/1/1/1	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	710	CP	C-N	7.03	1.46	1.33
7	A	710	CP	P-O4P	6.04	1.68	1.59
2	B	701	83Z	C13-N12	5.13	1.47	1.35
2	A	701	83Z	C13-N12	4.62	1.45	1.35
2	A	701	83Z	O07-C06	3.77	1.43	1.37
5	A	704	GOL	C3-C2	3.62	1.66	1.51
2	A	701	83Z	C32-C31	3.54	1.54	1.50
2	B	701	83Z	O07-C06	3.35	1.42	1.37
2	A	701	83Z	C30-C29	3.15	1.53	1.43
2	B	701	83Z	C30-C29	3.04	1.52	1.43
4	A	703	AMP	C5-C4	2.97	1.48	1.40
2	B	701	83Z	C32-C31	2.82	1.53	1.50
2	A	701	83Z	C09-CL1	2.78	1.78	1.72
2	B	701	83Z	C09-CL1	2.74	1.78	1.72
2	A	701	83Z	C11-N12	2.71	1.47	1.41
4	B	703	AMP	C2-N3	2.35	1.35	1.32
4	B	703	AMP	C5-C4	2.33	1.47	1.40

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	83Z	C14-C13-N12	7.18	124.35	114.50
7	A	710	CP	O-C-N	-5.12	117.06	125.51
2	A	701	83Z	C11-C09-CL1	-4.48	116.25	119.52
2	A	701	83Z	C24-C22-C20	-4.19	106.22	114.03
2	B	701	83Z	O16-C15-C14	4.10	120.12	110.05
2	A	701	83Z	O07-C06-C09	4.09	120.38	115.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	83Z	C04-C03-C02	-4.07	98.45	114.47
7	A	710	CP	O2P-P-O4P	4.06	117.62	105.25
2	A	701	83Z	C14-C13-N12	3.94	119.91	114.50
2	B	701	83Z	O27-C13-N12	-3.88	116.55	123.63
2	A	701	83Z	O16-C15-C14	3.63	118.95	110.05
2	B	701	83Z	C22-C20-C19	-3.53	103.30	110.64
2	B	701	83Z	O16-C15-C17	-3.26	103.01	110.81
2	B	701	83Z	O07-C06-C09	3.25	119.38	115.53
4	B	703	AMP	C4-C5-N7	-3.19	106.07	109.40
4	A	703	AMP	C4-C5-N7	-3.14	106.12	109.40
4	B	703	AMP	N3-C2-N1	-3.10	123.84	128.68
4	A	703	AMP	N3-C2-N1	-3.04	123.92	128.68
9	A	716	PEG	C3-O2-C2	2.57	124.44	113.29
2	A	701	83Z	C20-C19-C17	-2.52	121.11	127.73
2	A	701	83Z	C22-C20-C19	-2.51	105.42	110.64
2	A	701	83Z	C29-C30-C31	-2.50	118.47	124.53
2	A	701	83Z	O26-C25-C32	2.38	124.99	119.78
2	A	701	83Z	C01-C02-C03	2.31	119.75	114.88
4	B	703	AMP	O2P-P-O5'	-2.31	100.60	106.73
2	A	701	83Z	O27-C13-N12	-2.26	119.51	123.63
7	A	710	CP	O2P-P-O1P	-2.26	101.85	110.68
5	A	704	GOL	O2-C2-C3	2.23	118.96	109.12
4	B	703	AMP	O5'-P-O1P	-2.22	100.25	106.47
2	A	701	83Z	C05-C06-C09	-2.21	118.01	120.76
2	A	701	83Z	C14-C15-C17	-2.20	104.93	113.13
2	B	701	83Z	C28-C11-C09	2.17	120.58	118.26
2	B	701	83Z	C20-C19-C17	-2.16	122.04	127.73
4	A	703	AMP	C2-N1-C6	2.15	122.43	118.75
2	A	701	83Z	O26-C25-C24	-2.14	118.53	121.41
2	B	701	83Z	C01-C02-C03	2.13	119.38	114.88
2	A	701	83Z	C34-O33-C32	-2.12	110.03	112.93
4	B	703	AMP	O3P-P-O2P	2.06	115.52	107.64
2	B	701	83Z	C24-C22-C20	-2.05	110.21	114.03
2	B	701	83Z	C05-C06-C09	-2.03	118.22	120.76
2	A	701	83Z	C04-C03-C02	-2.01	106.54	114.47

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	83Z	O23-C22-C24-C25
2	A	701	83Z	C30-C31-C32-O33

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Mol	Chain	Res	Type	Atoms
2	B	701	83Z	C20-C22-C24-C25
2	B	701	83Z	O23-C22-C24-C25
5	A	704	GOL	O1-C1-C2-O2
2	A	701	83Z	O27-C13-N12-C11
2	B	701	83Z	O27-C13-N12-C11
2	A	701	83Z	C14-C13-N12-C11
2	B	701	83Z	C14-C13-N12-C11
2	A	701	83Z	C02-C29-C30-C31
2	A	701	83Z	C31-C32-O33-C34
5	A	704	GOL	O1-C1-C2-C3
9	A	716	PEG	O2-C3-C4-O4
2	A	701	83Z	C30-C31-C32-C25
8	A	711	EDO	O1-C1-C2-O2
2	B	701	83Z	C28-C11-N12-C13
2	B	701	83Z	C09-C11-N12-C13
9	A	716	PEG	C4-C3-O2-C2
4	A	703	AMP	C5'-O5'-P-O1P
2	B	701	83Z	C31-C32-O33-C34
2	B	701	83Z	C24-C25-C32-O33
2	B	701	83Z	O16-C15-C17-C19
2	B	701	83Z	O16-C15-C17-C18
8	A	714	EDO	O1-C1-C2-O2
9	A	716	PEG	C1-C2-O2-C3
2	A	701	83Z	C20-C22-C24-C25
2	A	701	83Z	C28-C11-N12-C13

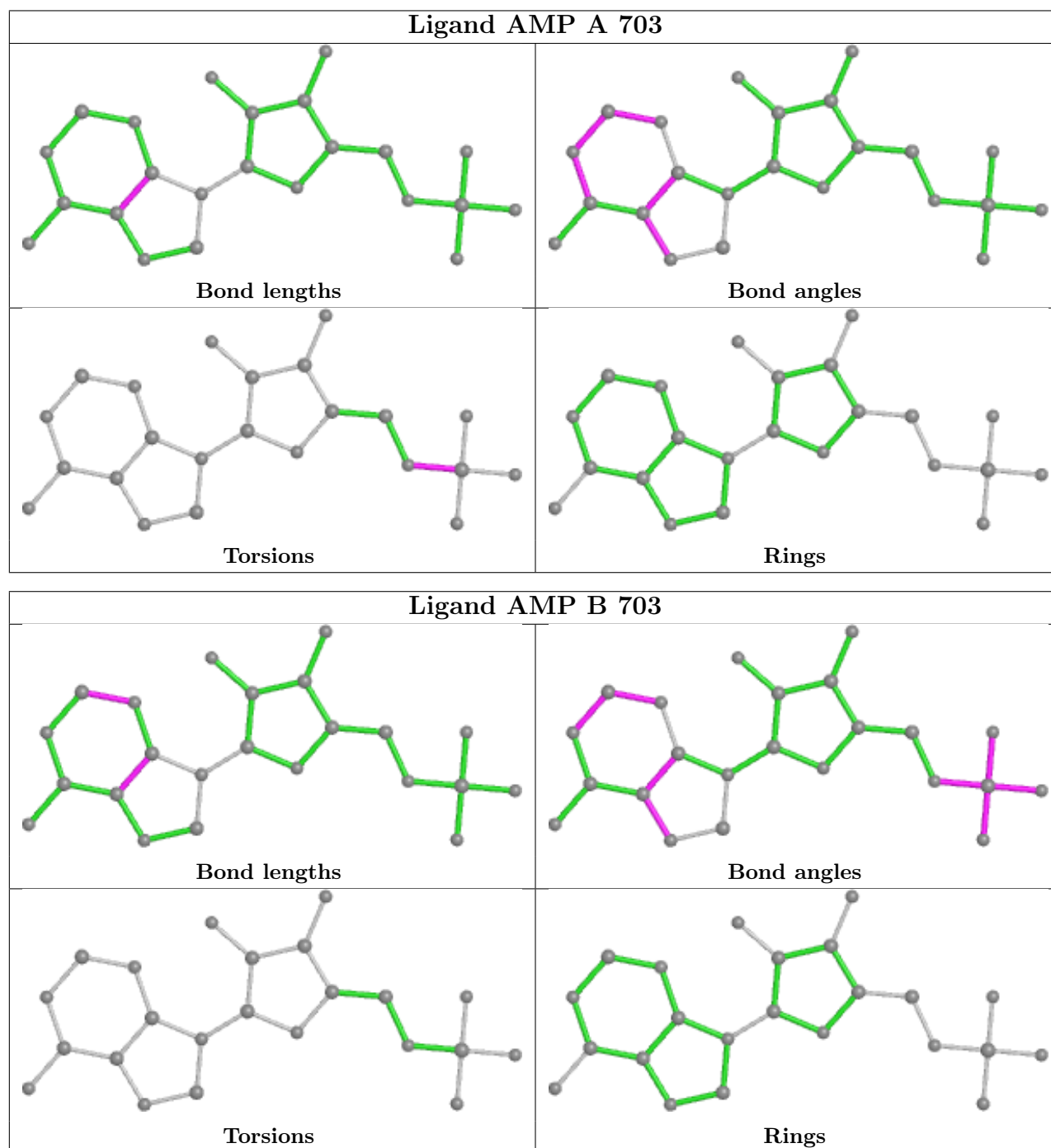
There are no ring outliers.

5 monomers are involved in 7 short contacts:

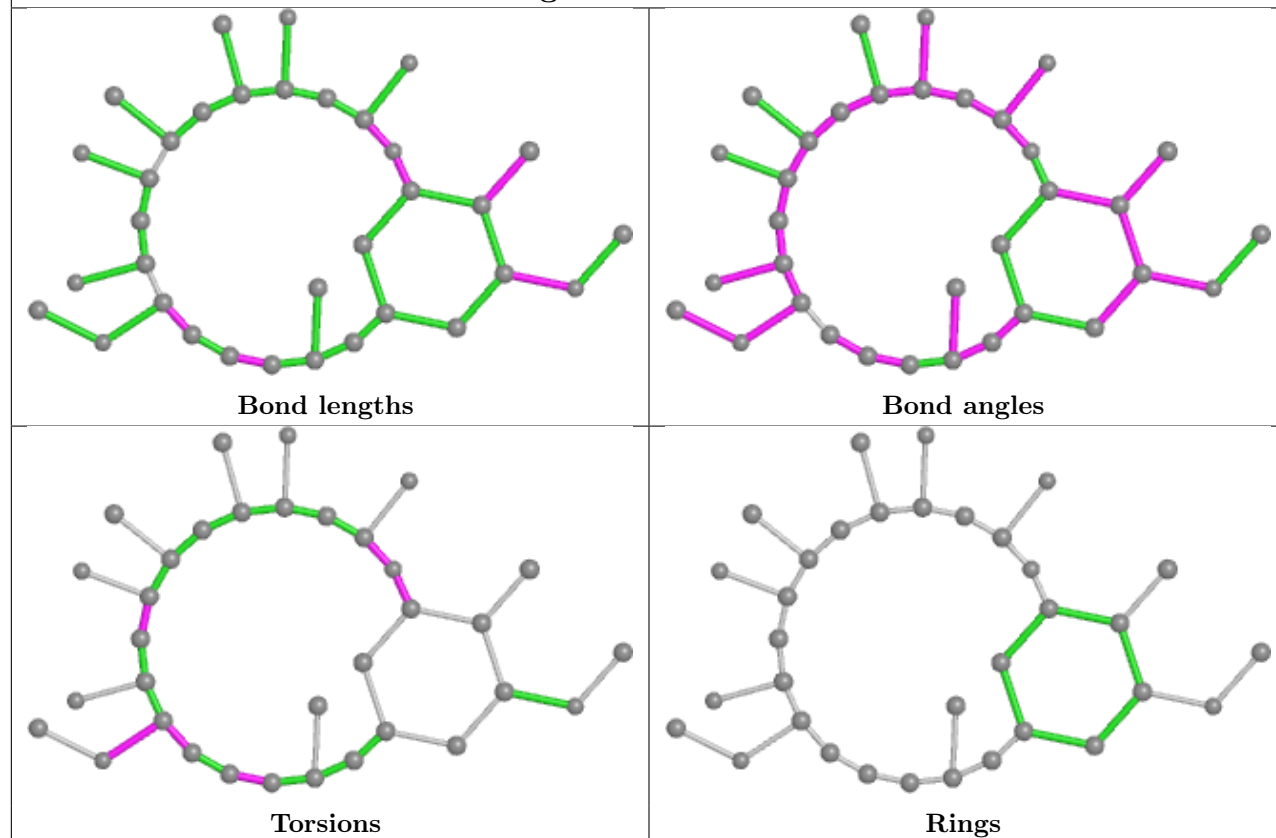
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	704	GOL	1	0
9	A	716	PEG	1	0
8	A	713	EDO	3	0
8	A	715	EDO	1	0
6	A	708	SO4	1	0

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

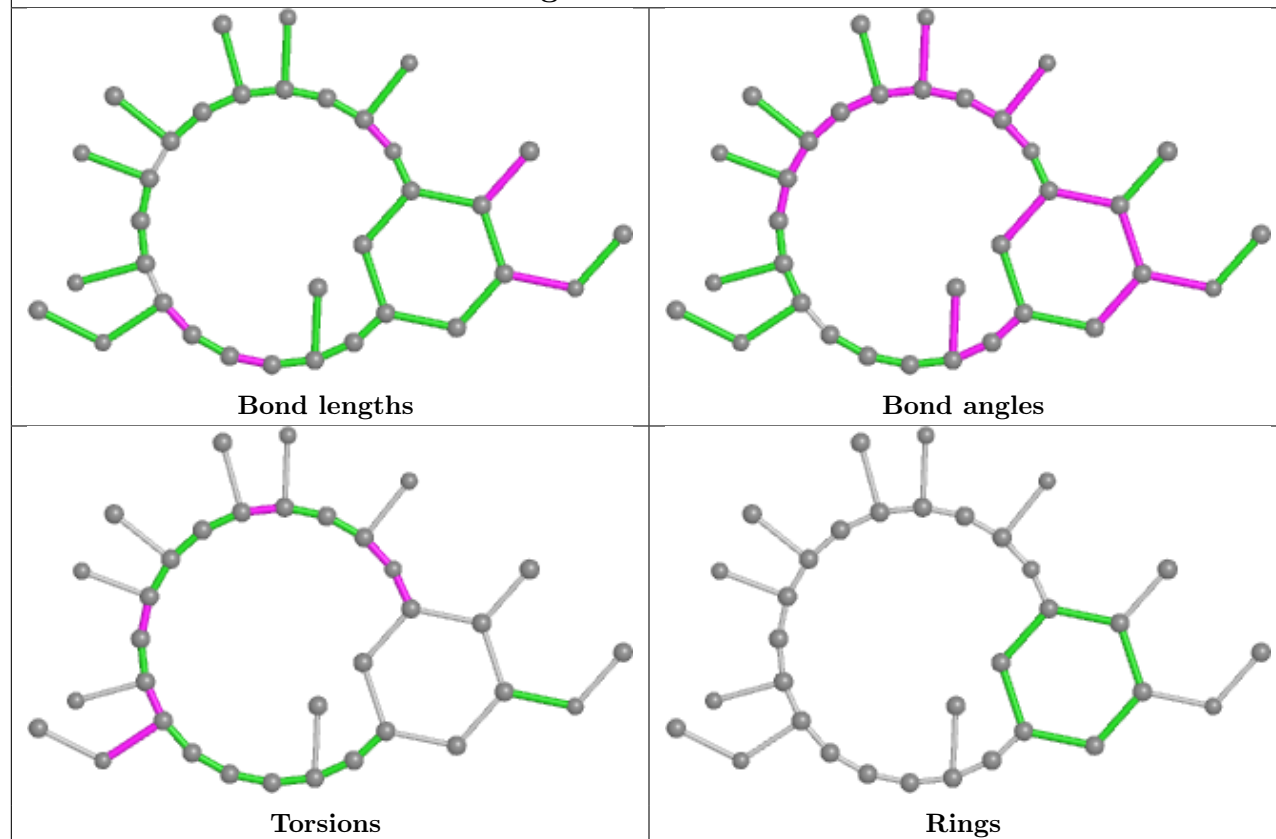
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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 83Z A 701



Ligand 83Z B 701



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%)	-0.43	3 (0%)	92 91	19, 31, 48, 65	0
1	B	678/702 (96%)	-0.34	4 (0%)	89 86	24, 39, 63, 77	0
All	All	1352/1404 (96%)	-0.39	7 (0%)	91 88	19, 34, 58, 77	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	677	ASP	3.7
1	A	644	GLY	2.9
1	B	441	MET	2.8
1	B	675	ALA	2.7
1	A	331	SER	2.4
1	B	439	ASN	2.1
1	A	642	THR	2.1

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](#)

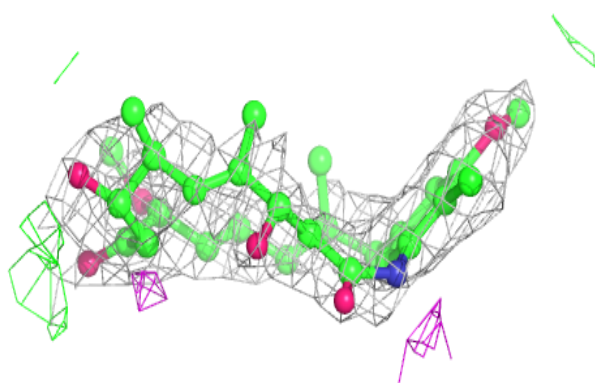
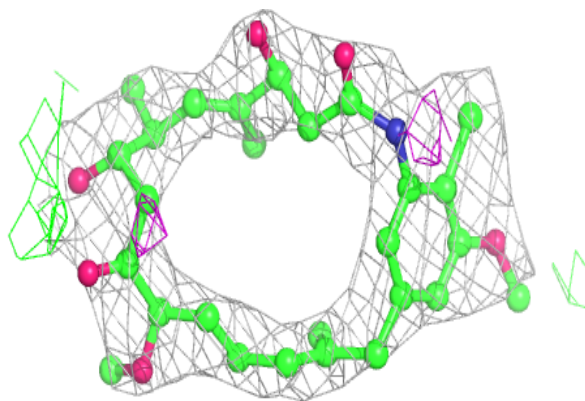
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	PEG	A	716	7/7	0.85	0.35	31,40,55,58	0
8	EDO	A	713	4/4	0.86	0.39	27,31,32,38	0
5	GOL	A	704	6/6	0.88	0.24	29,34,47,49	0
8	EDO	A	714	4/4	0.89	0.54	36,38,41,43	0
8	EDO	A	715	4/4	0.90	0.49	49,51,59,61	0
8	EDO	B	706	4/4	0.91	0.20	36,47,50,52	0
2	83Z	A	701	34/34	0.91	0.20	44,53,57,60	0
2	83Z	B	701	34/34	0.92	0.20	39,48,61,67	0
8	EDO	A	712	4/4	0.93	0.17	43,44,48,49	0
8	EDO	A	711	4/4	0.93	0.11	39,42,48,52	0
6	SO4	A	706	5/5	0.95	0.19	40,40,49,61	0
6	SO4	A	708	5/5	0.96	0.26	33,51,56,58	0
3	FE	B	702	1/1	0.96	0.17	30,30,30,30	0
6	SO4	A	709	5/5	0.97	0.17	49,54,72,74	0
7	CP	A	710	8/8	0.97	0.11	41,51,65,70	0
6	SO4	A	707	5/5	0.97	0.22	60,62,63,70	0
6	SO4	B	704	5/5	0.98	0.14	41,53,62,66	0
6	SO4	B	705	5/5	0.98	0.10	44,47,57,61	0
4	AMP	A	703	23/23	0.98	0.18	27,31,34,39	0
6	SO4	A	705	5/5	0.98	0.16	37,39,40,48	0
4	AMP	B	703	23/23	0.98	0.20	33,36,45,50	0
3	FE	A	702	1/1	0.99	0.20	31,31,31,31	0

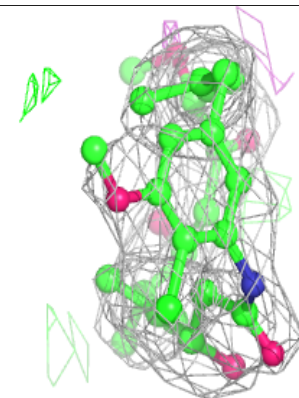
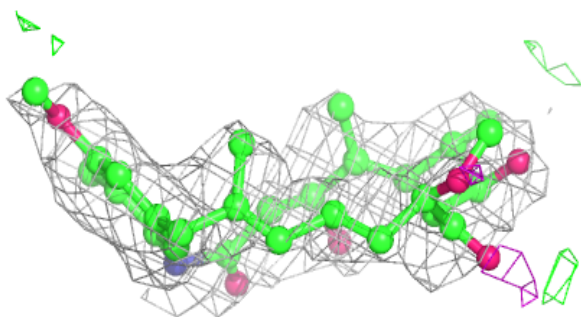
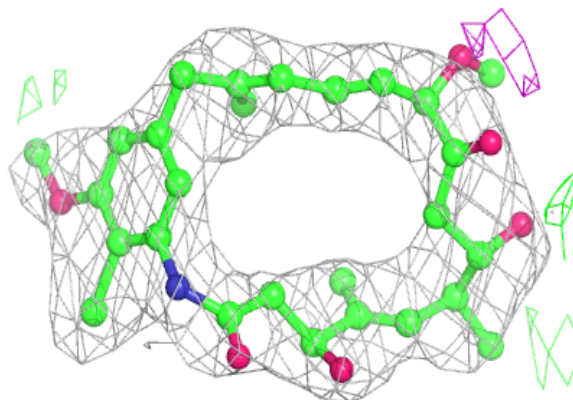
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 83Z A 701:

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

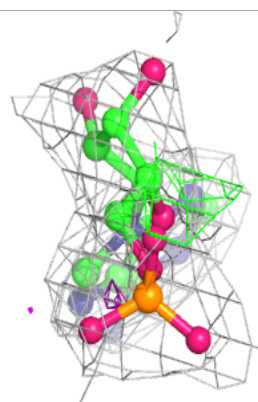
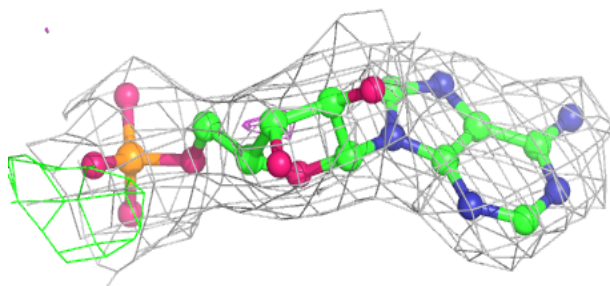
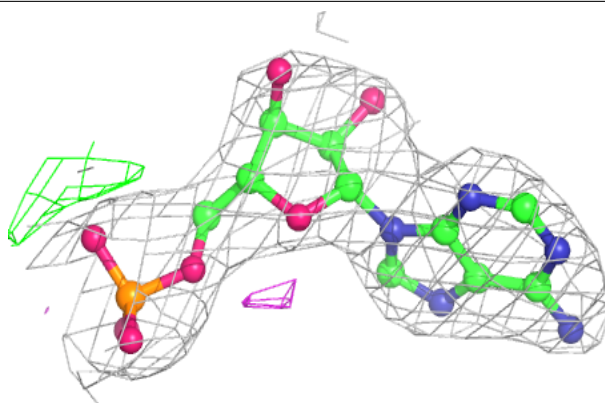
**Electron density around 83Z B 701:**

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

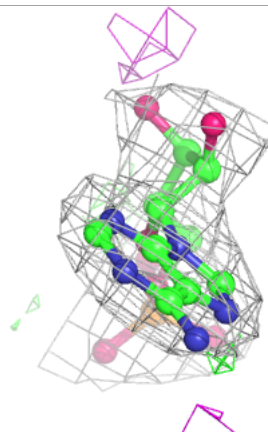
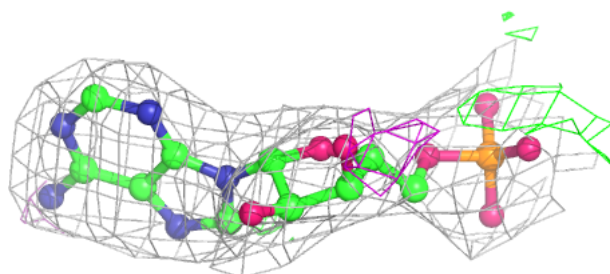
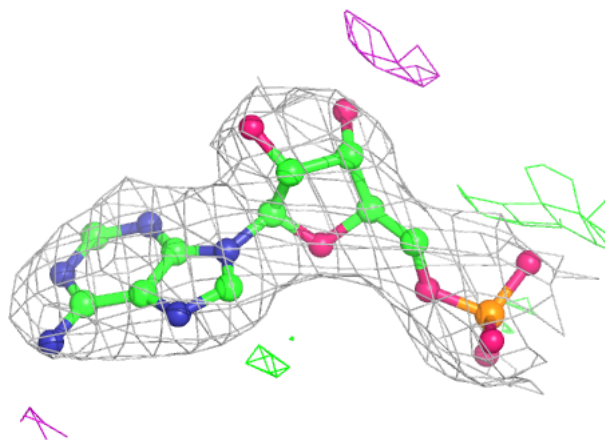


Electron density around AMP A 703:

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

**Electron density around AMP B 703:**

$2mF_o-DF_c$ (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.