



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:02 PM UTC

PDB ID : 7VYP / pdb_00007vyp
Title : The structure of GdmN complex with the natural tetrahedral intermediate, carbamoylated derivative, and AMP
Authors : Wei, J.; Zheng, J.; Zhou, J.; Kang, Q.; Bai, L.
Deposited on : 2021-11-15
Resolution : 2.88 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

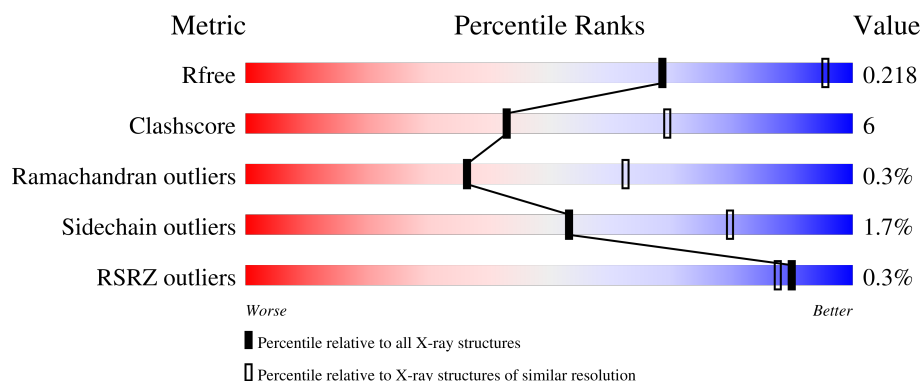
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	682	 87% 12% ..
1	B	682	 83% 16% .

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
5	EDO	B	706	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 10618 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
			5197	3295	914	979	9			
1	B	674	Total	C	N	O	S	0	1	0
			5141	3263	895	974	9			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

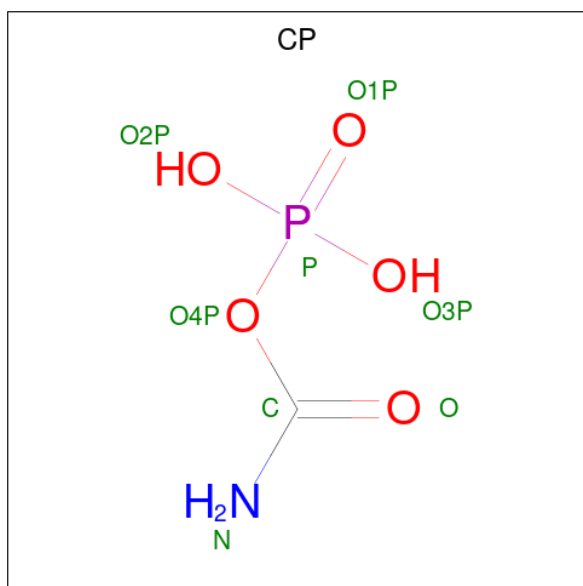
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is PHOSPHORIC ACID MONO(FORMAMIDE)ESTER (CCD ID: CP) (formula: $\text{CH}_4\text{NO}_5\text{P}$).



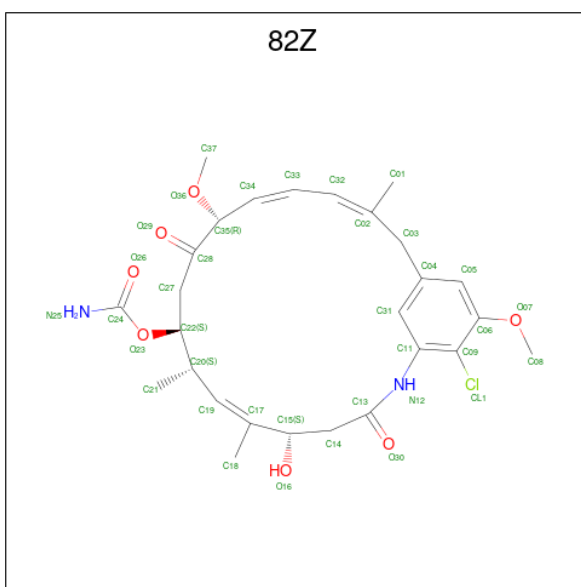
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 8 1 1 5 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



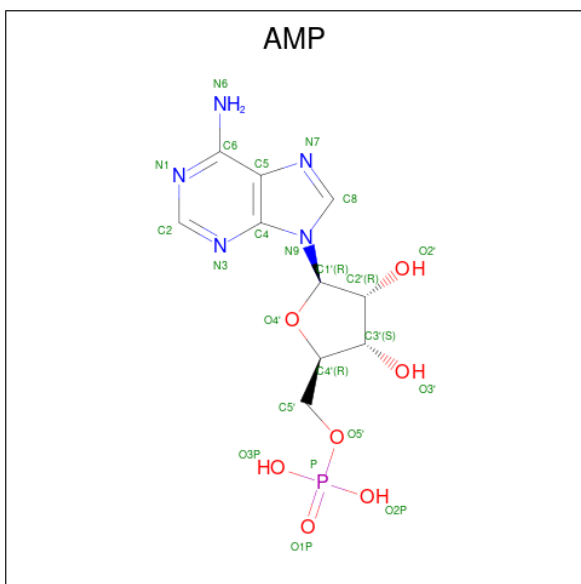
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is [(5S,6E,8S,9S,12R,13E,15E)-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] carbamate (CCD ID: 82Z) (formula: C₂₇H₃₅ClN₂O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Cl	N	O	0	0
			37	27	1	2	7		

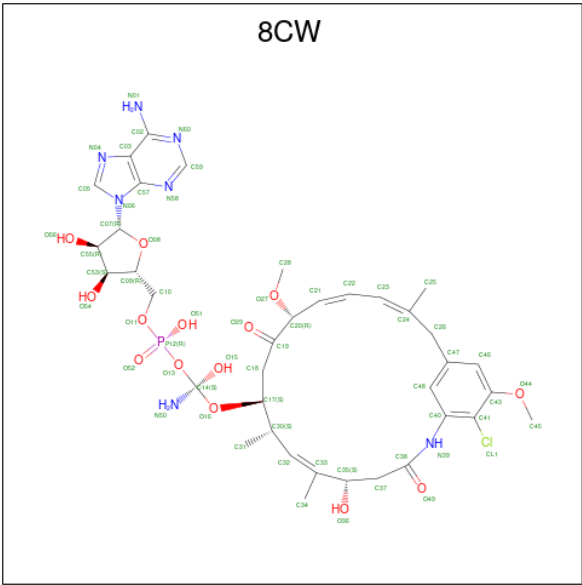
- Molecule 7 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 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-12,2

0-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 (CCD ID: 8CW) (formula: C₃₇H₄₉ClN₇O₁₄P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 9 is water.

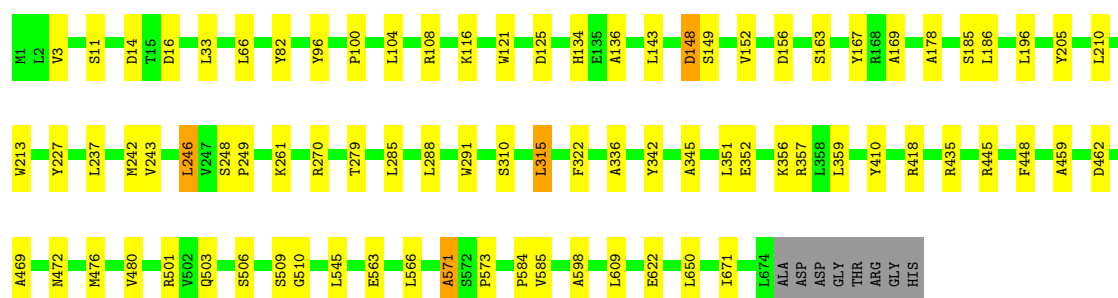
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	48	Total	0	0
			48 O		
9	B	22	Total	0	0
			22 O		

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.

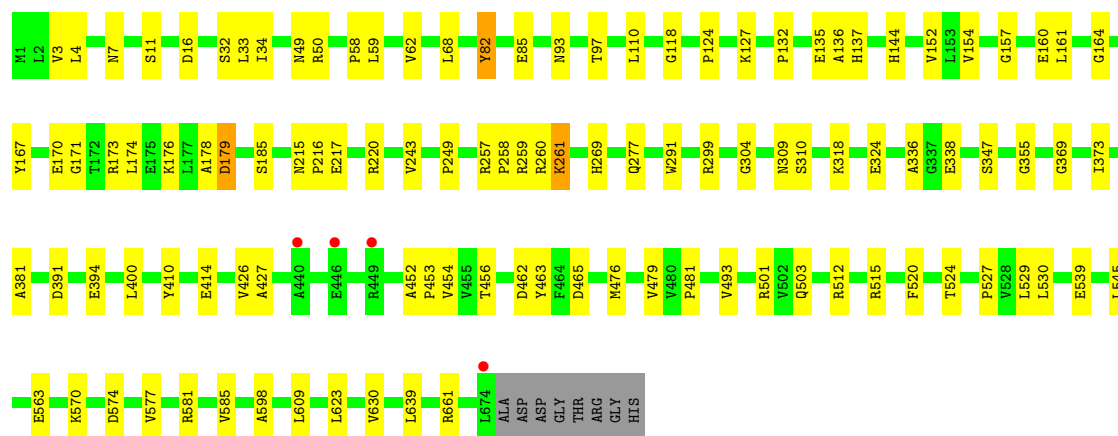
• Molecule 1: GdmN

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	111.03Å 111.03Å 231.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.76 – 2.88 27.76 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.8 (27.76-2.88) 99.7 (27.76-2.88)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.43 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.166 , 0.216 0.169 , 0.218	Depositor DCC
R_{free} test set	1846 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.2	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	10618	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: AMP, FE, EDO, 82Z, CP, SO4, 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	0.39	0/5318	0.57	0/7233
1	B	0.39	0/5262	0.59	0/7168
All	All	0.39	0/10580	0.58	0/14401

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	5197	0	5107	57	0
1	B	5141	0	4998	73	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	25	0	0	0	0
3	B	15	0	0	1	0
4	A	8	0	2	2	0
5	A	24	0	36	8	0
5	B	16	0	24	10	0
6	A	37	0	0	3	0
7	A	23	0	11	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	60	0	0	1	0
9	A	48	0	0	1	0
9	B	22	0	0	0	0
All	All	10618	0	10178	128	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 6.

All (128) 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)
7:A:715:AMP:C4'	7:A:715:AMP:O4'	1.68	1.17
1:B:176:LYS:NZ	1:B:179:ASP:OD2	2.22	0.73
1:B:152:VAL:HB	1:B:167:TYR:HB2	1.74	0.68
1:A:418:ARG:H	5:A:710:EDO:H11	1.59	0.68
1:B:539:GLU:CB	5:B:706:EDO:H21	2.25	0.67
1:A:3:VAL:HG21	1:A:345:ALA:HB2	1.76	0.66
1:B:85:GLU:H	5:B:708:EDO:H12	1.62	0.65
1:B:259:ARG:HB3	1:B:269:HIS:CE1	2.33	0.63
1:B:539:GLU:HB2	5:B:706:EDO:H21	1.80	0.62
1:B:452:ALA:HB1	1:B:476:MET:HE1	1.80	0.62
1:B:381:ALA:O	1:B:570:LYS:HE2	2.00	0.62
1:B:476:MET:HG2	1:B:503:GLN:HB2	1.81	0.62
1:B:50:ARG:HB3	5:B:706:EDO:H22	1.81	0.61
1:B:310:SER:HB3	1:B:479:VAL:HG23	1.84	0.60
1:A:418:ARG:HB2	5:A:710:EDO:H22	1.84	0.59
1:A:285:LEU:HD11	1:A:315:LEU:HD23	1.84	0.59
1:A:598:ALA:HB1	1:B:581:ARG:HB3	1.84	0.58
1:B:427:ALA:HB3	1:B:530:LEU:HD22	1.85	0.58
1:B:452:ALA:CB	1:B:476:MET:HE1	2.34	0.57
1:B:512:ARG:HH11	1:B:512:ARG:HB2	1.67	0.57
1:B:391:ASP:OD2	1:B:515:ARG:NH2	2.38	0.57
1:B:49:ASN:HB2	5:B:707:EDO:H12	1.87	0.56
1:A:14:ASP:OD1	1:A:14:ASP:N	2.39	0.56
1:A:445:ARG:NH1	4:A:707:CP:O3P	2.39	0.56
1:B:520:PHE:O	1:B:524:THR:HG23	2.06	0.55
1:A:476:MET:HG2	1:A:503:GLN:HB2	1.89	0.55
1:A:148:ASP:OD1	1:A:148:ASP:N	2.35	0.55
1:A:213:TRP:HZ2	1:A:435:ARG:HH22	1.53	0.55
6:A:714:82Z:N25	7:A:715:AMP:O3P	2.40	0.54
1:A:185:SER:HA	5:A:712:EDO:H21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:VAL:HB	1:A:167:TYR:HB2	1.88	0.54
1:A:149:SER:HA	1:A:169:ALA:O	2.08	0.53
1:A:11:SER:HB3	1:A:16:ASP:HA	1.90	0.53
1:A:163:SER:O	5:A:712:EDO:H12	2.09	0.52
1:B:124:PRO:HG2	1:B:127:LYS:HG3	1.91	0.52
1:A:116:LYS:HA	1:A:121:TRP:H	1.74	0.51
1:B:243:VAL:HG22	1:B:249:PRO:HG3	1.93	0.51
1:A:476:MET:HB3	1:A:501:ARG:HG2	1.92	0.51
1:B:574:ASP:O	1:B:577:VAL:HG22	2.11	0.51
1:B:414:GLU:OE1	1:B:414:GLU:N	2.38	0.50
1:A:418:ARG:H	5:A:710:EDO:C1	2.22	0.50
1:A:108:ARG:HD3	1:A:125:ASP:OD1	2.12	0.50
1:B:144:HIS:NE2	1:B:338:GLU:OE2	2.40	0.50
1:A:134:HIS:NE2	1:A:156:ASP:OD1	2.45	0.49
1:B:11:SER:HB3	1:B:16:ASP:HA	1.93	0.49
1:A:108:ARG:NH1	1:A:125:ASP:OD1	2.38	0.49
1:B:299:ARG:HD3	1:B:324:GLU:OE2	2.13	0.49
1:A:237:LEU:HB3	1:A:246:LEU:HD21	1.94	0.49
1:B:50:ARG:HB3	5:B:706:EDO:C2	2.42	0.49
1:A:585:VAL:HG23	1:A:609:LEU:HD22	1.94	0.49
1:B:3:VAL:HB	1:B:34[B]:ILE:CG1	2.44	0.48
1:A:622:GLU:H	1:A:622:GLU:CD	2.22	0.47
1:A:356:LYS:HE2	1:A:359:LEU:HD11	1.96	0.47
1:A:96:TYR:O	1:B:260:ARG:NH2	2.47	0.47
1:A:243:VAL:HG22	1:A:249:PRO:HG3	1.96	0.47
6:A:714:82Z:CL1	1:B:243:VAL:HG12	2.52	0.47
1:B:93:ASN:O	1:B:97:THR:HG23	2.15	0.47
1:B:215:ASN:OD1	1:B:217:GLU:HG3	2.15	0.47
1:A:196:LEU:HD11	1:A:248:SER:HB3	1.96	0.47
1:B:452:ALA:HB1	1:B:476:MET:CE	2.45	0.47
6:A:714:82Z:C24	7:A:715:AMP:O3P	2.63	0.46
1:A:356:LYS:HD3	1:A:357:ARG:O	2.16	0.46
1:B:58:PRO:O	1:B:62:VAL:HG23	2.15	0.46
1:B:585:VAL:HG23	1:B:609:LEU:HD22	1.98	0.46
1:B:630:VAL:HA	1:B:639:LEU:HD11	1.98	0.46
1:A:210:LEU:HD11	1:A:270:ARG:HG2	1.98	0.46
1:B:463:TYR:CE2	1:B:527:PRO:HD2	2.50	0.46
1:B:136:ALA:HB1	1:B:336:ALA:O	2.15	0.45
1:A:33:LEU:HD11	1:A:66:LEU:HD23	1.97	0.45
1:A:435:ARG:HD3	9:A:835:HOH:O	2.14	0.45
1:A:506:SER:H	1:A:509:SER:HB3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ARG:NE	1:B:173:ARG:HA	2.32	0.45
1:B:258:PRO:O	1:B:260:ARG:NH1	2.50	0.44
1:A:571:ALA:O	1:A:573:PRO:HD3	2.16	0.44
1:B:391:ASP:OD2	1:B:394:GLU:HB2	2.17	0.44
1:A:288:LEU:HD23	1:A:288:LEU:HA	1.67	0.44
1:A:186:LEU:N	5:A:712:EDO:O1	2.49	0.44
5:A:711:EDO:H12	1:B:598:ALA:HB2	2.00	0.44
1:A:459:ALA:O	1:A:462:ASP:HB2	2.18	0.44
1:A:178:ALA:HB2	1:A:291:TRP:CZ2	2.52	0.44
1:A:598:ALA:CB	1:B:581:ARG:HB3	2.48	0.43
1:A:116:LYS:HB3	1:A:116:LYS:NZ	2.33	0.43
1:B:259:ARG:NH2	3:B:703:SO4:O3	2.51	0.43
1:B:261:LYS:HD3	1:B:261:LYS:HA	1.76	0.43
1:B:178:ALA:HB2	1:B:291:TRP:CZ2	2.53	0.43
1:B:137:HIS:CE1	1:B:304:GLY:HA2	2.53	0.43
1:B:318:LYS:NZ	1:B:465:ASP:O	2.44	0.43
1:A:100:PRO:HA	1:B:260:ARG:NH2	2.34	0.43
1:B:277:GLN:HE22	1:B:309:ASN:HD21	1.66	0.43
1:B:476:MET:HE2	1:B:501:ARG:HE	1.84	0.43
1:A:342:TYR:HD1	1:A:351:LEU:HD11	1.83	0.43
1:B:132:PRO:HB2	1:B:135:GLU:HB2	2.00	0.43
1:A:143:LEU:HD11	1:A:351:LEU:HD21	2.00	0.42
1:B:110:LEU:HD23	1:B:110:LEU:HA	1.92	0.42
1:A:545:LEU:HD23	1:A:671:ILE:HD12	2.01	0.42
1:B:623:LEU:HD12	1:B:623:LEU:HA	1.87	0.42
1:B:400:LEU:HD21	1:B:426:VAL:HG23	2.01	0.42
1:B:465:ASP:HB3	1:B:481:PRO:HD2	2.00	0.42
1:B:4:LEU:HD12	1:B:32:SER:O	2.19	0.42
1:A:205:TYR:OH	4:A:707:CP:O2P	2.38	0.42
1:A:136:ALA:HB1	1:A:336:ALA:O	2.20	0.42
1:A:242:MET:HE2	1:A:242:MET:HB3	1.88	0.42
1:A:322:PHE:O	1:A:469:ALA:HB2	2.20	0.42
1:A:243:VAL:HG12	8:B:701:8CW:CL1	2.57	0.42
1:B:50:ARG:HB3	5:B:706:EDO:H11	2.01	0.42
1:B:369:GLY:O	1:B:373:ILE:HG13	2.20	0.42
1:A:410:TYR:CE1	1:A:563:GLU:HA	2.55	0.41
1:A:448:PHE:CD1	1:A:448:PHE:C	2.97	0.41
1:B:154:VAL:O	1:B:164:GLY:HA2	2.20	0.41
1:B:216:PRO:O	1:B:220:ARG:HB2	2.19	0.41
1:A:261:LYS:HD3	1:A:261:LYS:HA	1.69	0.41
1:B:50:ARG:HB3	5:B:706:EDO:C1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:TYR:CE1	1:B:563:GLU:HA	2.55	0.41
1:B:453:PRO:HB3	1:B:493:VAL:HG21	2.03	0.41
1:A:104:LEU:CD1	1:B:257:ARG:HB3	2.51	0.41
1:A:357:ARG:HH11	1:A:472:ASN:HB3	1.85	0.41
1:B:157:GLY:O	1:B:185:SER:OG	2.38	0.41
1:B:174:LEU:HA	1:B:174:LEU:HD23	1.74	0.41
1:B:529:LEU:HD23	1:B:529:LEU:HA	1.92	0.41
1:B:661:ARG:HB3	5:B:706:EDO:H12	2.03	0.41
1:B:661:ARG:HD2	5:B:706:EDO:H12	2.03	0.41
1:A:227:TYR:CE1	1:A:279:THR:HG23	2.57	0.40
1:A:650:LEU:HD23	1:A:650:LEU:HA	1.80	0.40
1:B:59:LEU:HD21	1:B:118:GLY:HA3	2.03	0.40
1:B:33:LEU:HD23	1:B:33:LEU:HA	1.92	0.40
1:B:160:GLU:HG2	1:B:161:LEU:N	2.35	0.40
1:A:584:PRO:HD3	5:A:711:EDO:H11	2.03	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 [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	673/682 (99%)	651 (97%)	20 (3%)	2 (0%)	36	62
1	B	673/682 (99%)	630 (94%)	41 (6%)	2 (0%)	36	62
All	All	1346/1364 (99%)	1281 (95%)	61 (4%)	4 (0%)	36	62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	355	GLY
1	A	571	ALA

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Mol	Chain	Res	Type
1	A	510	GLY
1	B	171	GLY

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	537/542 (99%)	529 (98%)	8 (2%)	57	82
1	B	525/542 (97%)	515 (98%)	10 (2%)	50	77
All	All	1062/1084 (98%)	1044 (98%)	18 (2%)	53	80

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	TYR
1	A	148	ASP
1	A	246	LEU
1	A	310	SER
1	A	315	LEU
1	A	352	GLU
1	A	480	VAL
1	A	566	LEU
1	B	68	LEU
1	B	82	TYR
1	B	170	GLU
1	B	179	ASP
1	B	261	LYS
1	B	347	SER
1	B	454	VAL
1	B	456	THR
1	B	462	ASP
1	B	545	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	137	HIS
1	A	267	GLN
1	A	473	HIS
1	A	660	GLN
1	B	94	HIS
1	B	232	ASN
1	B	608	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 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	EDO	A	709	-	3,3,3	0.59	0	2,2,2	0.11	0
5	EDO	A	711	-	3,3,3	0.63	0	2,2,2	0.30	0
3	SO4	B	705	-	4,4,4	0.28	0	6,6,6	0.29	0
3	SO4	B	703	-	4,4,4	0.31	0	6,6,6	0.35	0
5	EDO	B	706	-	3,3,3	0.45	0	2,2,2	0.23	0
5	EDO	A	708	-	3,3,3	0.71	0	2,2,2	0.02	0
5	EDO	B	708	-	3,3,3	0.64	0	2,2,2	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	702	-	4,4,4	0.26	0	6,6,6	0.23	0
3	SO4	A	705	-	4,4,4	0.20	0	6,6,6	0.21	0
5	EDO	B	709	-	3,3,3	0.59	0	2,2,2	0.25	0
3	SO4	A	704	-	4,4,4	0.32	0	6,6,6	0.31	0
5	EDO	A	713	-	3,3,3	0.54	0	2,2,2	0.34	0
3	SO4	A	703	-	4,4,4	0.21	0	6,6,6	0.32	0
7	AMP	A	715	2	25,25,25	3.34	9 (36%)	37,38,38	2.06	10 (27%)
6	82Z	A	714	-	37,38,38	2.00	7 (18%)	42,52,52	2.78	15 (35%)
3	SO4	A	706	-	4,4,4	0.34	0	6,6,6	0.33	0
5	EDO	A	712	-	3,3,3	0.56	0	2,2,2	0.15	0
3	SO4	B	704	-	4,4,4	0.24	0	6,6,6	0.47	0
4	CP	A	707	-	6,7,7	3.54	2 (33%)	7,10,10	1.62	2 (28%)
5	EDO	A	710	-	3,3,3	0.46	0	2,2,2	0.38	0
8	8CW	B	701	2	60,64,64	2.87	22 (36%)	75,94,94	2.48	23 (30%)
5	EDO	B	707	-	3,3,3	0.59	0	2,2,2	0.09	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
4	CP	A	707	-	-	0/3/5/5	-
5	EDO	B	708	-	-	1/1/1/1	-
5	EDO	A	713	-	-	1/1/1/1	-
5	EDO	A	709	-	-	1/1/1/1	-
5	EDO	A	710	-	-	1/1/1/1	-
8	8CW	B	701	2	-	10/53/79/79	0/4/5/5
7	AMP	A	715	2	-	1/10/26/26	0/3/3/3
5	EDO	A	711	-	-	0/1/1/1	-
5	EDO	B	707	-	-	1/1/1/1	-
6	82Z	A	714	-	-	16/46/46/46	0/1/2/2
5	EDO	B	706	-	-	0/1/1/1	-
5	EDO	A	708	-	-	0/1/1/1	-
5	EDO	A	712	-	-	1/1/1/1	-
5	EDO	B	709	-	-	1/1/1/1	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	715	AMP	O4'-C4'	10.34	1.68	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	701	8CW	C53-C09	-8.97	1.30	1.53
7	A	715	AMP	C3'-C4'	-8.77	1.30	1.53
6	A	714	82Z	C24-N25	7.68	1.47	1.33
4	A	707	CP	C-N	7.58	1.47	1.33
8	B	701	8CW	C55-C07	-7.36	1.30	1.53
8	B	701	8CW	C02-N01	7.01	1.52	1.34
8	B	701	8CW	C26-C47	5.45	1.60	1.51
8	B	701	8CW	O08-C07	5.34	1.54	1.42
8	B	701	8CW	O08-C09	5.14	1.56	1.45
7	A	715	AMP	O4'-C1'	-5.11	1.30	1.42
8	B	701	8CW	C38-N39	5.00	1.46	1.35
7	A	715	AMP	C6-N6	4.69	1.46	1.34
8	B	701	8CW	C22-C23	4.37	1.56	1.43
8	B	701	8CW	C55-C53	4.28	1.65	1.53
8	B	701	8CW	C20-C21	4.11	1.54	1.50
6	A	714	82Z	C13-N12	4.06	1.44	1.35
8	B	701	8CW	P12-O13	3.80	1.70	1.59
7	A	715	AMP	O2'-C2'	-3.79	1.33	1.43
8	B	701	8CW	C05-N06	-3.78	1.31	1.37
6	A	714	82Z	O23-C22	-3.77	1.39	1.46
4	A	707	CP	P-O4P	3.56	1.66	1.59
8	B	701	8CW	C34-C33	3.39	1.56	1.50
8	B	701	8CW	C25-C24	3.30	1.58	1.50
8	B	701	8CW	C41-CL1	3.29	1.79	1.72
6	A	714	82Z	O23-C24	3.17	1.41	1.35
8	B	701	8CW	C03-N04	-2.83	1.33	1.39
6	A	714	82Z	C33-C32	2.81	1.51	1.43
7	A	715	AMP	C8-N9	-2.76	1.32	1.37
8	B	701	8CW	O49-C38	-2.68	1.18	1.23
8	B	701	8CW	C26-C24	2.65	1.54	1.52
8	B	701	8CW	O44-C43	2.62	1.41	1.37
8	B	701	8CW	C30-C32	2.45	1.56	1.51
6	A	714	82Z	O30-C13	-2.39	1.18	1.23
7	A	715	AMP	O3'-C3'	2.33	1.48	1.43
6	A	714	82Z	O29-C28	-2.32	1.17	1.21
8	B	701	8CW	C57-N06	-2.26	1.33	1.37
7	A	715	AMP	C5-N7	-2.05	1.35	1.39
7	A	715	AMP	C2'-C3'	2.01	1.58	1.53
8	B	701	8CW	C18-C19	2.01	1.56	1.51

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	714	82Z	C33-C32-C02	-10.25	113.27	127.69
8	B	701	8CW	C22-C23-C24	-6.98	117.88	127.69
8	B	701	8CW	C37-C38-N39	6.76	122.97	114.62
8	B	701	8CW	C03-C57-N58	-5.49	119.15	126.72
8	B	701	8CW	N58-C57-N06	5.49	136.50	127.17
8	B	701	8CW	C23-C22-C21	-5.30	112.14	124.43
6	A	714	82Z	O23-C24-N25	5.25	119.06	110.92
6	A	714	82Z	C14-C13-N12	5.18	121.03	114.62
6	A	714	82Z	C01-C02-C03	5.12	119.82	115.53
7	A	715	AMP	C5-C4-N3	-5.07	119.73	126.72
8	B	701	8CW	N60-C59-N58	-5.03	120.96	128.58
8	B	701	8CW	C25-C24-C26	4.81	119.56	115.53
8	B	701	8CW	C57-N06-C05	4.60	110.56	105.74
7	A	715	AMP	N3-C2-N1	-4.47	121.82	128.58
7	A	715	AMP	N3-C4-N9	4.32	134.51	127.17
8	B	701	8CW	O44-C43-C41	4.14	119.97	115.44
6	A	714	82Z	C14-C15-C17	-4.11	107.19	111.78
6	A	714	82Z	O26-C24-N25	-4.02	119.24	125.58
8	B	701	8CW	C59-N58-C57	3.88	121.32	111.83
7	A	715	AMP	C4-N9-C8	3.66	109.58	105.74
6	A	714	82Z	C21-C20-C22	3.64	117.11	111.78
6	A	714	82Z	O07-C06-C09	3.62	119.41	115.44
8	B	701	8CW	C18-C17-C30	-3.62	106.11	115.05
8	B	701	8CW	C37-C35-C33	-3.59	107.78	111.78
8	B	701	8CW	O49-C38-N39	-3.56	117.25	123.64
7	A	715	AMP	C2-N3-C4	3.46	120.28	111.83
7	A	715	AMP	N9-C8-N7	-3.44	109.05	113.94
8	B	701	8CW	N06-C05-N04	-3.44	109.06	113.94
4	A	707	CP	O-C-N	-3.42	120.19	125.58
8	B	701	8CW	C17-C30-C32	-3.25	104.45	110.33
8	B	701	8CW	C09-O08-C07	-3.22	102.37	109.47
6	A	714	82Z	C20-C19-C17	-3.16	120.68	128.00
8	B	701	8CW	C55-C07-N06	-3.11	105.57	113.30
6	A	714	82Z	O30-C13-N12	-3.02	118.22	123.64
6	A	714	82Z	C27-C22-C20	-2.96	107.74	115.05
7	A	715	AMP	C5-N7-C8	2.96	108.10	103.45
6	A	714	82Z	O16-C15-C14	2.93	117.00	109.96
7	A	715	AMP	C4-C5-N7	-2.69	107.50	110.58
7	A	715	AMP	C2'-C1'-N9	-2.53	107.02	113.30
6	A	714	82Z	C18-C17-C15	2.49	119.96	115.33
7	A	715	AMP	O5'-P-O1P	2.42	112.98	106.44
8	B	701	8CW	O36-C35-C33	-2.23	105.49	111.08
8	B	701	8CW	O08-C09-C10	-2.20	102.28	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	707	CP	O2P-P-O4P	2.20	111.72	105.32
6	A	714	82Z	O16-C15-C17	-2.17	105.64	111.08
6	A	714	82Z	C22-C20-C19	-2.14	106.45	110.33
8	B	701	8CW	C03-N04-C05	2.05	106.67	103.45
8	B	701	8CW	C34-C33-C35	2.04	119.13	115.33
8	B	701	8CW	C53-C55-C07	2.04	105.32	101.46
8	B	701	8CW	O13-P12-O52	2.01	115.86	109.64

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	714	82Z	C21-C20-C22-C27
6	A	714	82Z	C21-C20-C22-O23
6	A	714	82Z	C19-C20-C22-C27
6	A	714	82Z	C19-C20-C22-O23
6	A	714	82Z	N25-C24-O23-C22
6	A	714	82Z	O26-C24-O23-C22
6	A	714	82Z	C27-C28-C35-O36
8	B	701	8CW	C30-C17-C18-C19
8	B	701	8CW	O16-C17-C18-C19
8	B	701	8CW	C10-O11-P12-O13
6	A	714	82Z	O30-C13-N12-C11
8	B	701	8CW	O49-C38-N39-C40
6	A	714	82Z	C14-C13-N12-C11
8	B	701	8CW	C37-C38-N39-C40
8	B	701	8CW	C21-C22-C23-C24
8	B	701	8CW	C19-C20-C21-C22
5	A	712	EDO	O1-C1-C2-O2
5	A	709	EDO	O1-C1-C2-O2
5	B	709	EDO	O1-C1-C2-O2
6	A	714	82Z	C34-C35-O36-C37
8	B	701	8CW	C21-C20-O27-C28
6	A	714	82Z	C31-C11-N12-C13
7	A	715	AMP	C5'-O5'-P-O2P
6	A	714	82Z	C09-C11-N12-C13
6	A	714	82Z	O30-C13-C14-C15
6	A	714	82Z	C33-C34-C35-C28
6	A	714	82Z	N12-C13-C14-C15
5	B	708	EDO	O1-C1-C2-O2
6	A	714	82Z	O29-C28-C35-O36
8	B	701	8CW	C48-C40-N39-C38

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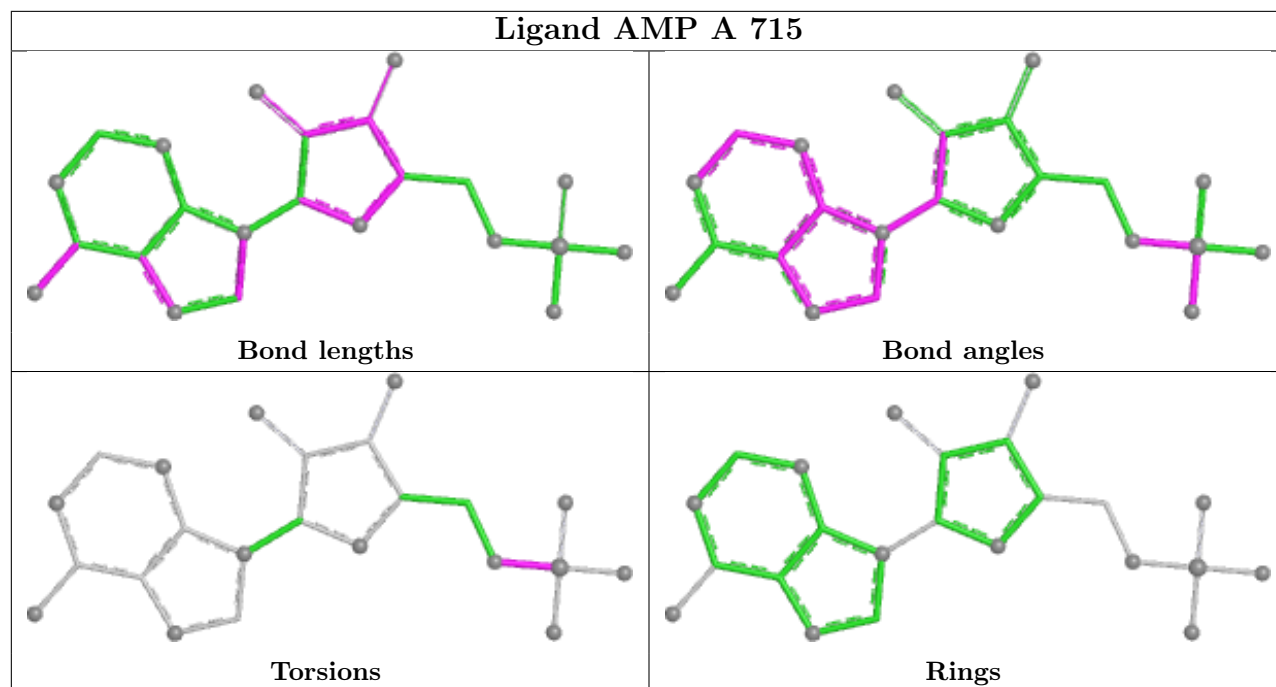
Mol	Chain	Res	Type	Atoms
5	B	707	EDO	O1-C1-C2-O2
5	A	713	EDO	O1-C1-C2-O2
8	B	701	8CW	O27-C20-C21-C22
5	A	710	EDO	O1-C1-C2-O2

There are no ring outliers.

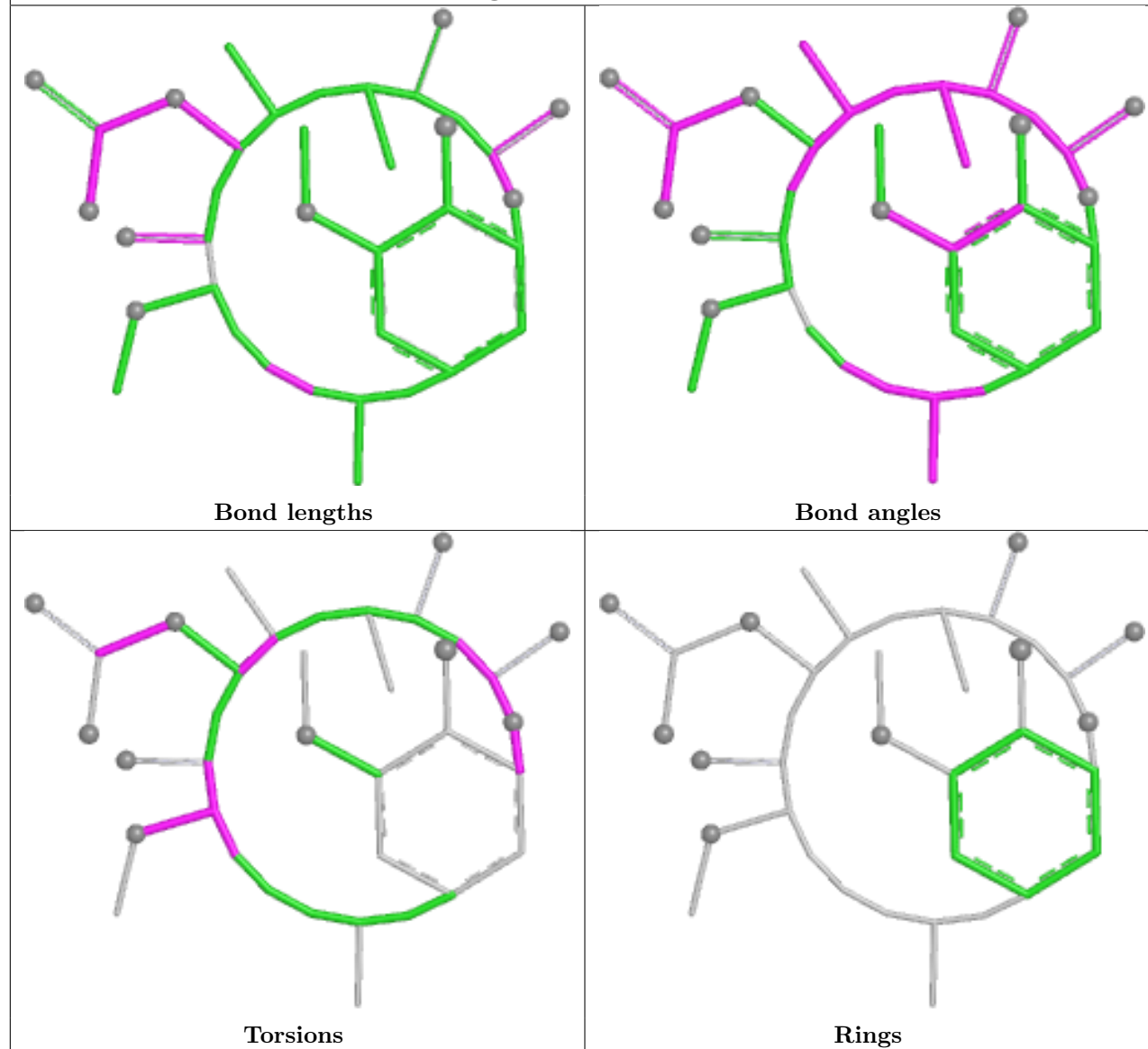
11 monomers are involved in 26 short contacts:

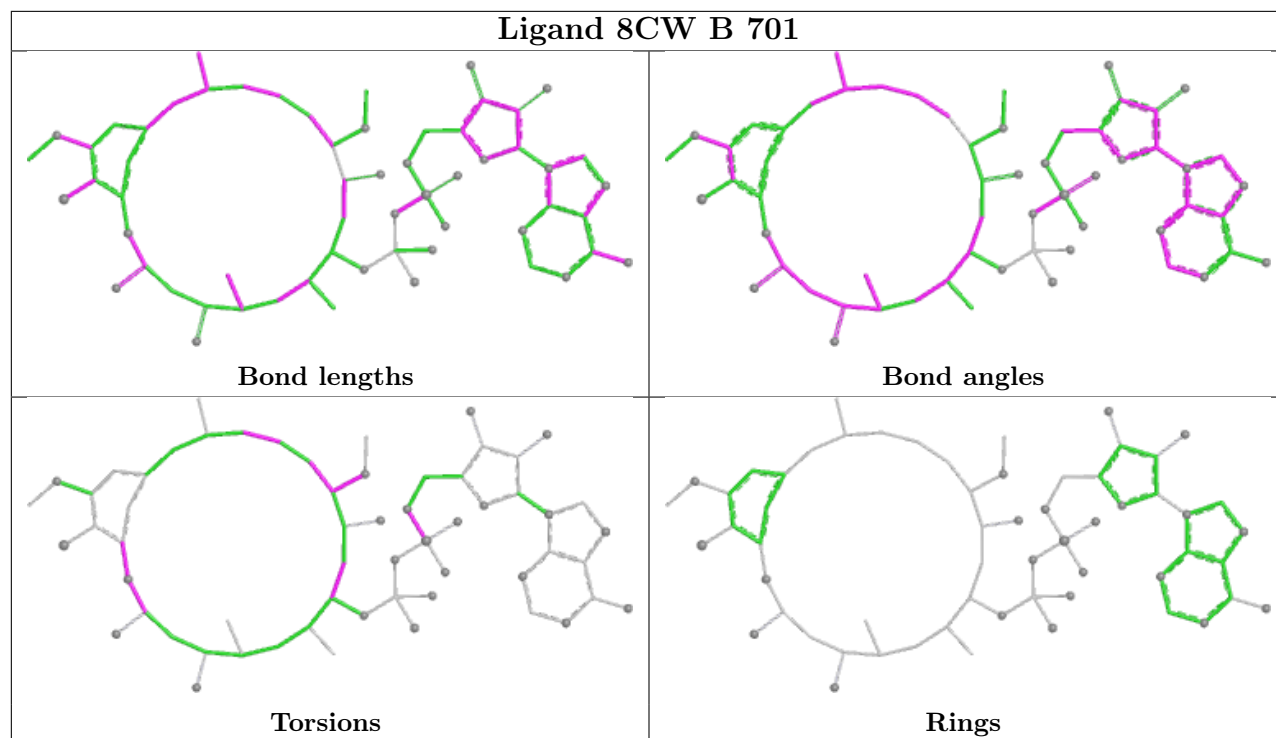
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	711	EDO	2	0
3	B	703	SO4	1	0
5	B	706	EDO	8	0
5	B	708	EDO	1	0
7	A	715	AMP	3	0
6	A	714	82Z	3	0
5	A	712	EDO	3	0
4	A	707	CP	2	0
5	A	710	EDO	3	0
8	B	701	8CW	1	0
5	B	707	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand 82Z A 714





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	674/682 (98%)	-0.71	0 100 100	18, 37, 55, 69	1 (0%)
1	B	674/682 (98%)	-0.39	4 (0%) 85 81	24, 46, 69, 84	1 (0%)
All	All	1348/1364 (98%)	-0.55	4 (0%) 90 87	18, 41, 63, 84	2 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	440	ALA	4.8
1	B	446	GLU	2.7
1	B	674	LEU	2.5
1	B	449	ARG	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 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
5	EDO	A	708	4/4	0.68	0.17	47,48,49,54	0

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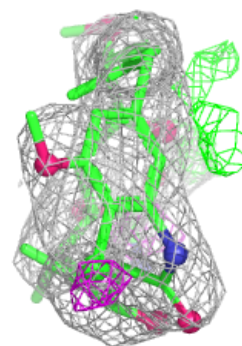
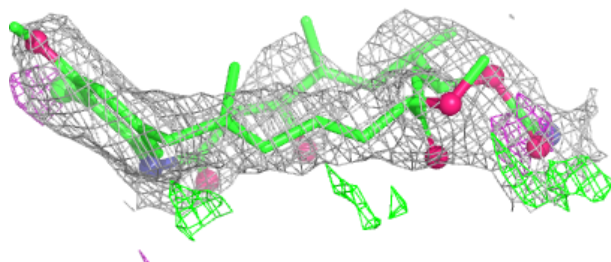
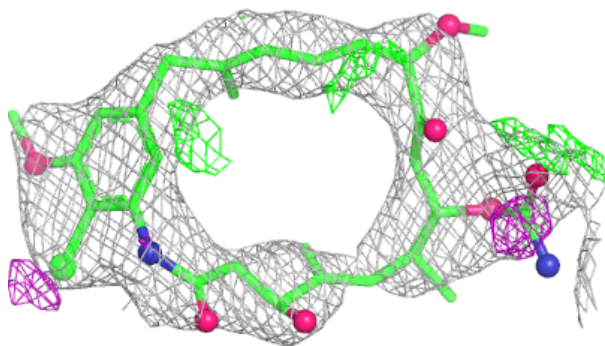
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	B	708	4/4	0.77	0.20	46,49,50,51	0
5	EDO	B	707	4/4	0.80	0.18	44,51,56,59	0
5	EDO	A	711	4/4	0.81	0.17	48,50,53,55	0
5	EDO	A	709	4/4	0.83	0.15	45,50,59,59	0
4	CP	A	707	8/8	0.86	0.16	63,69,72,74	0
5	EDO	B	709	4/4	0.86	0.13	52,55,56,59	0
5	EDO	B	706	4/4	0.87	0.20	39,45,45,48	0
6	82Z	A	714	37/37	0.87	0.17	40,51,58,63	37
5	EDO	A	713	4/4	0.89	0.16	42,49,49,54	0
8	8CW	B	701	60/60	0.89	0.14	30,41,52,63	60
3	SO4	B	703	5/5	0.90	0.10	61,62,72,76	0
3	SO4	A	706	5/5	0.92	0.09	57,58,73,75	0
5	EDO	A	712	4/4	0.92	0.27	39,40,41,41	0
5	EDO	A	710	4/4	0.92	0.33	38,39,42,43	0
3	SO4	B	705	5/5	0.93	0.10	56,67,68,69	0
3	SO4	A	704	5/5	0.94	0.12	38,52,61,68	0
3	SO4	A	705	5/5	0.94	0.11	63,63,73,78	0
7	AMP	A	715	23/23	0.96	0.07	32,37,42,46	0
3	SO4	B	704	5/5	0.96	0.09	48,56,64,66	0
3	SO4	A	702	5/5	0.97	0.09	40,43,54,61	0
3	SO4	A	703	5/5	0.97	0.06	41,45,47,52	0
2	FE	A	701	1/1	0.99	0.02	32,32,32,32	0
2	FE	B	702	1/1	1.00	0.04	40,40,40,40	0

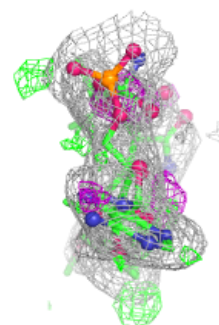
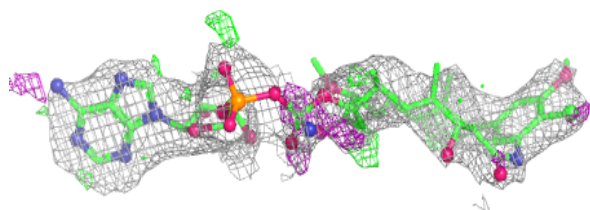
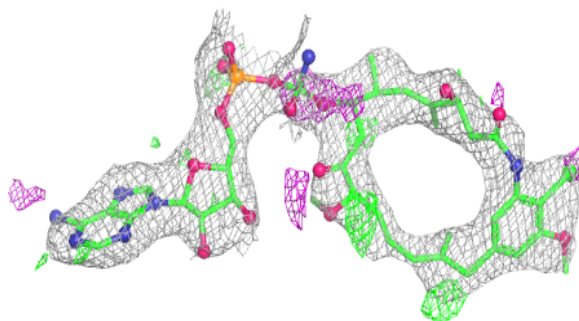
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

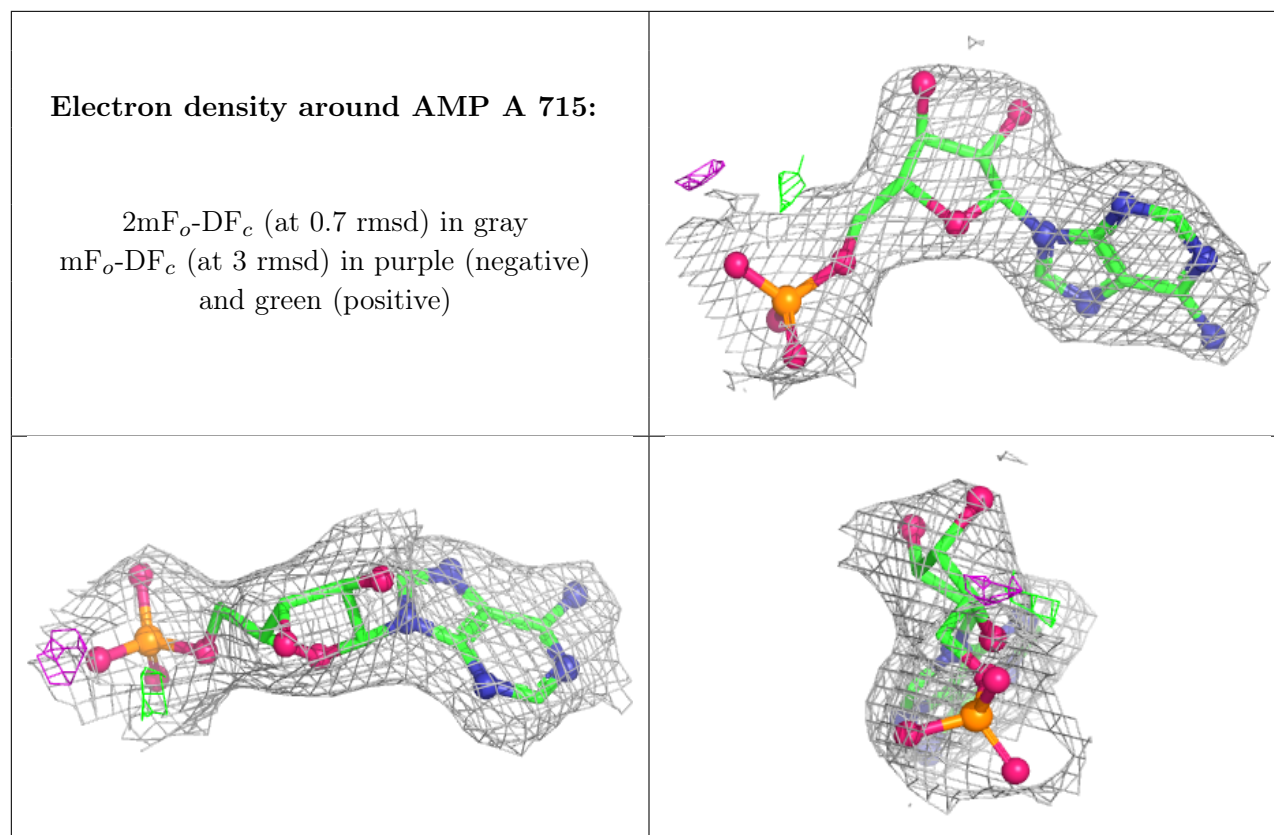
Electron density around 82Z A 714:

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

**Electron density around 8CW 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.