



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:54 AM UTC

PDB ID : 1JGT / pdb_00001jgt
Title : CRYSTAL STRUCTURE OF BETA-LACTAM SYNTHETASE
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Deposited on : 2001-06-26
Resolution : 1.95 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

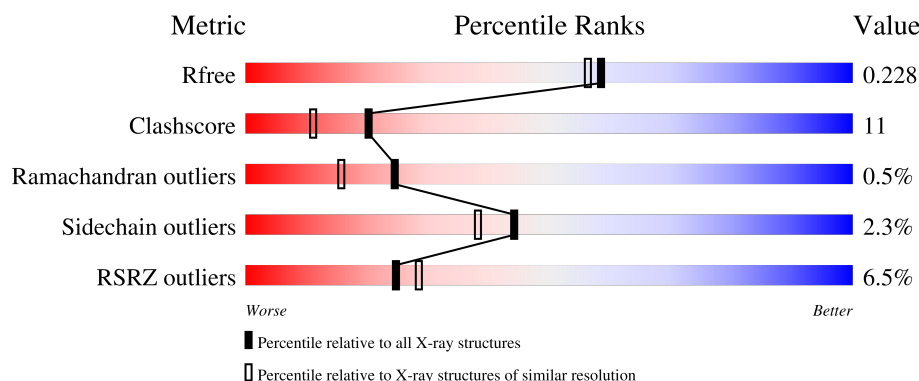
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	513	9% 74% 19% • •
1	B	513	4% 78% 18% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CMA	A	803	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8189 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

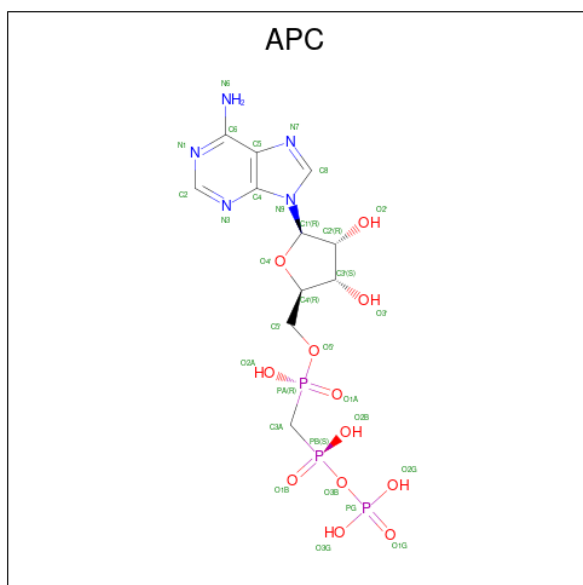
- Molecule 1 is a protein called BETA-LACTAM SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3690	2306	678	698	8			
1	B	500	Total	C	N	O	S	0	0	0
			3749	2337	691	713	8			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

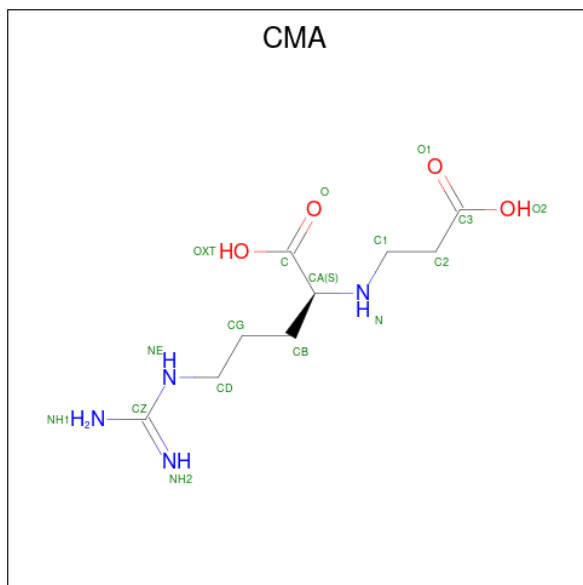
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



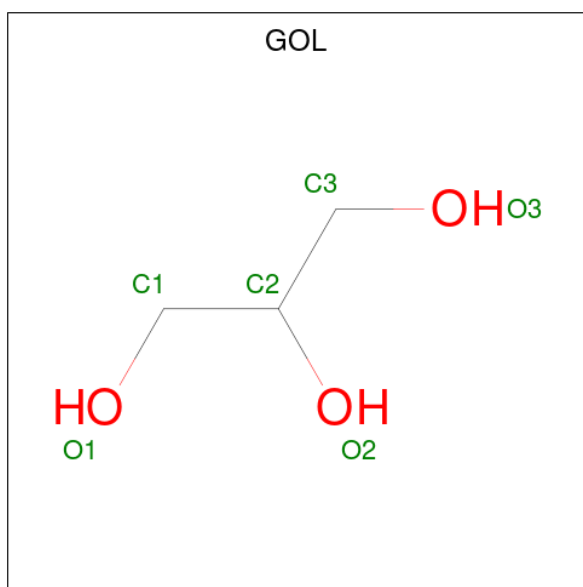
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 4 is N2-(CARBOXYETHYL)-L-ARGININE (CCD ID: CMA) (formula: $C_9H_{18}N_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	9	4	4		
4	B	1	Total	C	N	O	0	0
			17	9	4	4		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

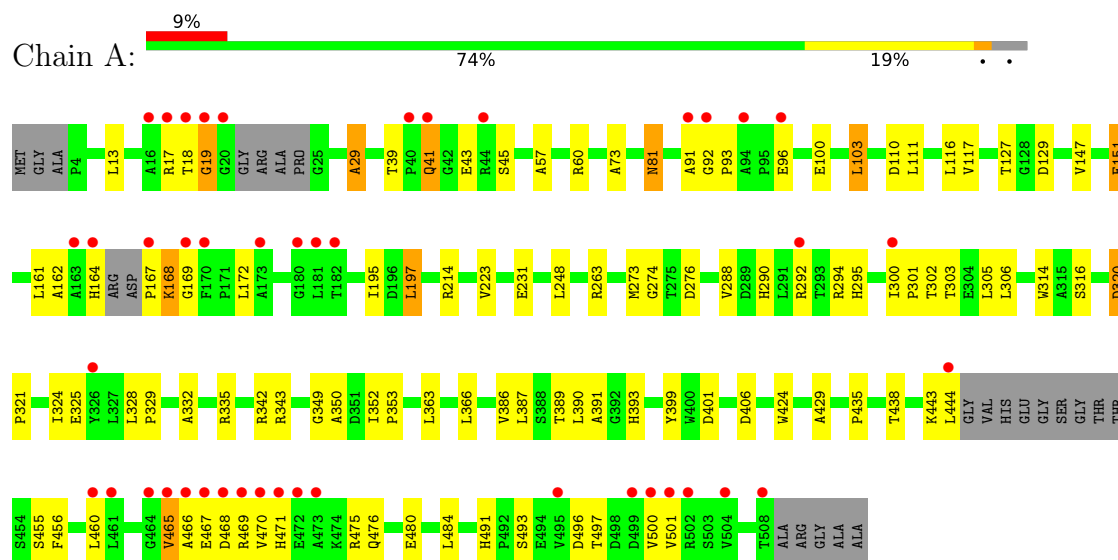
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	289	Total	O	0	0
			289	289		
6	B	333	Total	O	0	0
			333	333		

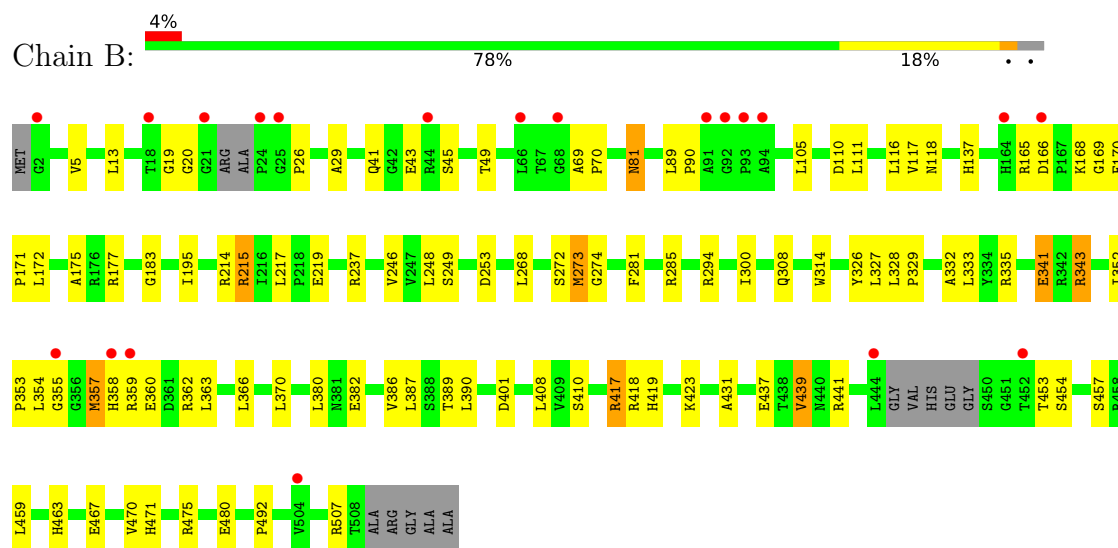
3 Residue-property plots [i](#)

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: BETA-LACTAM SYNTHETASE



• Molecule 1: BETA-LACTAM SYNTHETASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.35Å 97.87Å 80.97Å 90.00° 90.78° 90.00°	Depositor
Resolution (Å)	19.89 – 1.95 19.89 – 1.95	Depositor EDS
% Data completeness (in resolution range)	95.0 (19.89-1.95) 94.9 (19.89-1.95)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 1.94Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.195 , 0.228 0.195 , 0.228	Depositor DCC
R_{free} test set	5838 reflections (8.38%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8189	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: APC, MG, GOL, CMA

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	0.38	0/3763	0.94	13/5131 (0.3%)
1	B	0.38	0/3824	0.93	10/5216 (0.2%)
All	All	0.38	0/7587	0.93	23/10347 (0.2%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	VAL	N-CA-C	7.65	119.59	108.58
1	B	117	VAL	N-CA-C	7.43	118.70	108.89
1	A	29	ALA	N-CA-C	-7.42	102.89	112.23
1	B	29	ALA	N-CA-C	-6.91	103.85	112.90
1	B	401	ASP	N-CA-C	-6.62	100.63	110.23
1	B	195	ILE	N-CA-C	6.48	117.25	108.17
1	A	343	ARG	N-CA-C	-6.42	98.27	108.73
1	A	401	ASP	N-CA-C	-6.39	100.83	110.28
1	A	39	THR	CA-C-N	6.25	125.47	118.97
1	A	39	THR	C-N-CA	6.25	125.47	118.97
1	B	13	LEU	N-CA-C	-5.83	97.72	107.80
1	A	248	LEU	N-CA-C	5.82	118.45	109.07
1	B	248	LEU	N-CA-C	5.78	118.90	109.59
1	A	57	ALA	N-CA-C	-5.74	102.55	109.72
1	A	363	LEU	N-CA-C	5.72	122.46	109.81
1	A	195	ILE	N-CA-C	5.58	115.98	108.17
1	B	390	LEU	N-CA-C	-5.51	105.82	112.54
1	B	439	VAL	N-CA-C	5.50	115.70	110.42
1	B	343	ARG	N-CA-C	-5.47	98.84	108.20
1	A	424	TRP	N-CA-C	5.35	117.55	111.02
1	A	320	ASP	CA-C-N	5.25	125.30	119.32
1	A	320	ASP	C-N-CA	5.25	125.30	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	363	LEU	N-CA-C	5.24	121.39	109.81

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	3690	0	3686	89	0
1	B	3749	0	3733	74	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	6	0
3	B	31	0	12	2	0
4	A	17	0	15	7	0
4	B	17	0	15	1	0
5	B	30	0	40	6	0
6	A	289	0	0	5	0
6	B	333	0	0	4	0
All	All	8189	0	7513	168	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 11.

All (168) 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)
3:A:801:APC:PA	4:A:803:CMA:O2	2.26	0.94
1:A:41:GLN:HB2	1:A:45:SER:HB3	1.48	0.92
1:A:17:ARG:HB3	1:A:151:GLU:HG2	1.54	0.88
1:B:358:HIS:HB2	1:B:366:LEU:HD13	1.57	0.85
4:A:803:CMA:O1	6:A:955:HOH:O	1.95	0.84
1:A:342:ARG:H	1:A:393:HIS:HD2	1.24	0.81
1:B:341:GLU:HG3	6:B:1233:HOH:O	1.80	0.80
1:B:215:ARG:HG3	5:B:712:GOL:H31	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:801:APC:H5'1	4:A:803:CMA:O2	1.84	0.78
1:B:81:ASN:HD22	1:B:81:ASN:H	1.32	0.77
1:A:41:GLN:HE21	1:A:45:SER:HB3	1.49	0.76
1:B:355:GLY:HA3	1:B:366:LEU:HD11	1.66	0.75
1:A:306:LEU:HD21	1:A:455:SER:HB3	1.69	0.74
1:B:41:GLN:OE1	1:B:45:SER:HB3	1.87	0.74
1:A:92:GLY:H	1:A:93:PRO:CD	2.01	0.74
1:A:167:PRO:HG2	1:A:168:LYS:HD3	1.72	0.71
1:A:92:GLY:H	1:A:93:PRO:HD2	1.55	0.71
1:A:294:ARG:HD2	1:A:294:ARG:C	2.15	0.71
1:A:41:GLN:HE21	1:A:45:SER:CB	2.07	0.68
3:A:801:APC:O2A	4:A:803:CMA:O2	2.12	0.68
1:A:17:ARG:CB	1:A:151:GLU:HG2	2.25	0.66
1:A:466:ALA:O	1:A:469:ARG:HB2	1.97	0.65
1:B:453:THR:HG23	1:B:457:SER:HB2	1.78	0.64
1:B:308:GLN:HE22	1:B:335:ARG:HH21	1.44	0.64
1:A:476:GLN:O	1:A:480:GLU:HG2	1.98	0.64
1:B:328:LEU:HB2	1:B:329:PRO:HD3	1.80	0.63
1:A:168:LYS:HD3	1:A:168:LYS:H	1.64	0.63
1:B:357:MET:HA	1:B:357:MET:HE3	1.79	0.63
1:B:358:HIS:CB	1:B:366:LEU:HD13	2.27	0.62
1:A:467:GLU:C	1:A:469:ARG:H	2.05	0.62
1:A:491:HIS:HD2	1:A:493:SER:H	1.47	0.62
1:A:17:ARG:HG3	1:A:18:THR:H	1.66	0.61
1:A:92:GLY:N	1:A:93:PRO:HD2	2.15	0.61
1:B:69:ALA:HB1	1:B:70:PRO:HD2	1.82	0.61
1:A:460:LEU:HB3	1:A:465:VAL:HG11	1.82	0.60
1:A:466:ALA:HB3	1:A:469:ARG:HD2	1.83	0.60
1:A:321:PRO:HG3	1:A:475:ARG:HA	1.83	0.60
1:A:116:LEU:HD23	1:B:214:ARG:HB2	1.84	0.60
1:B:89:LEU:HD21	1:B:105:LEU:HD23	1.84	0.59
1:B:26:PRO:HG3	1:B:49:THR:HG21	1.85	0.58
1:B:110:ASP:CG	1:B:111:LEU:H	2.11	0.58
1:B:170:PHE:HB3	1:B:171:PRO:HD2	1.85	0.58
1:B:410:SER:OG	5:B:713:GOL:H31	2.04	0.58
1:B:453:THR:HG22	1:B:454:SER:O	2.04	0.58
1:A:168:LYS:HD3	1:A:168:LYS:N	2.18	0.58
1:A:73:ALA:HB2	1:A:103:LEU:HD13	1.87	0.57
1:A:92:GLY:N	1:A:93:PRO:CD	2.68	0.57
1:A:60:ARG:HH21	1:A:60:ARG:HG3	1.69	0.57
1:A:342:ARG:N	1:A:393:HIS:HD2	2.01	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:VAL:HA	1:B:389:THR:OG1	2.05	0.56
3:A:801:APC:H5'1	4:A:803:CMA:C3	2.35	0.56
1:A:13:LEU:C	1:A:13:LEU:HD13	2.31	0.56
1:A:491:HIS:CD2	1:A:493:SER:H	2.24	0.56
1:B:471:HIS:HE1	1:B:475:ARG:NH1	2.04	0.55
3:A:801:APC:O2A	4:A:803:CMA:C3	2.55	0.55
1:A:167:PRO:HG2	1:A:168:LYS:CD	2.35	0.55
1:A:214:ARG:HB2	1:B:116:LEU:HD23	1.89	0.54
1:A:390:LEU:HD12	1:A:390:LEU:C	2.32	0.54
1:B:418:ARG:HG2	1:B:419:HIS:CD2	2.42	0.54
1:B:467:GLU:HA	1:B:470:VAL:HG23	1.89	0.54
1:A:497:THR:O	1:A:501:VAL:HG23	2.08	0.54
1:B:300:ILE:HG13	1:B:300:ILE:O	2.08	0.54
1:A:162:ALA:C	1:A:164:HIS:H	2.15	0.53
1:A:480:GLU:O	1:A:484:LEU:HG	2.08	0.53
1:B:437:GLU:O	1:B:441:ARG:HB2	2.08	0.53
1:A:467:GLU:C	1:A:469:ARG:N	2.67	0.53
1:A:467:GLU:O	1:A:468:ASP:HB3	2.07	0.53
1:A:19:GLY:HA2	1:A:43:GLU:HB3	1.91	0.53
1:B:453:THR:CG2	1:B:457:SER:HB2	2.39	0.52
1:A:300:ILE:HD13	1:A:332:ALA:HB1	1.91	0.52
1:A:321:PRO:CG	1:A:475:ARG:HA	2.40	0.52
1:B:169:GLY:HA3	1:B:183:GLY:O	2.10	0.52
1:B:333:LEU:C	1:B:333:LEU:HD23	2.34	0.52
1:B:354:LEU:HD21	1:B:408:LEU:HD22	1.92	0.51
1:A:460:LEU:HD13	1:A:501:VAL:HG13	1.93	0.51
1:B:417:ARG:HH21	1:B:417:ARG:HB2	1.76	0.51
1:A:29:ALA:HA	1:A:314:TRP:CZ2	2.46	0.51
1:A:292:ARG:HH11	1:A:292:ARG:HG2	1.76	0.51
1:B:353:PRO:HA	1:B:370:LEU:HD13	1.91	0.51
1:B:215:ARG:HB3	5:B:713:GOL:O3	2.10	0.51
1:A:127:THR:HG23	1:A:127:THR:O	2.10	0.51
1:A:390:LEU:HD12	1:A:391:ALA:N	2.25	0.50
1:A:81:ASN:H	1:A:81:ASN:HD22	1.58	0.50
1:A:366:LEU:C	1:A:366:LEU:HD23	2.37	0.50
1:B:81:ASN:HD22	1:B:81:ASN:N	2.00	0.50
1:B:172:LEU:HB2	1:B:175:ALA:HB3	1.93	0.50
1:B:326:TYR:CE1	4:B:804:CMA:HG1	2.47	0.50
1:B:353:PRO:HA	1:B:370:LEU:CD1	2.42	0.49
1:A:342:ARG:H	1:A:393:HIS:CD2	2.16	0.49
1:B:358:HIS:CE1	1:B:360:GLU:O	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:801:APC:H5'2	4:A:803:CMA:O2	2.07	0.49
1:B:358:HIS:CE1	1:B:362:ARG:O	2.66	0.48
1:B:314:TRP:CE3	1:B:492:PRO:HG2	2.49	0.48
1:B:418:ARG:HG2	1:B:419:HIS:CG	2.48	0.48
1:A:288:VAL:HG21	1:A:295:HIS:CG	2.48	0.48
1:A:443:LYS:O	1:A:444:LEU:HB3	2.13	0.48
1:B:137:HIS:HD2	6:B:1044:HOH:O	1.97	0.48
1:A:325:GLU:OE2	1:A:456:PHE:HB3	2.14	0.48
1:A:302:THR:O	1:A:306:LEU:HD23	2.14	0.47
1:B:357:MET:HA	1:B:357:MET:CE	2.43	0.47
1:A:147:VAL:HB	1:A:172:LEU:HD21	1.96	0.47
1:A:386:VAL:HA	1:A:389:THR:OG1	2.14	0.47
1:A:81:ASN:HD22	1:A:81:ASN:N	2.11	0.47
1:A:335:ARG:NH1	6:A:1185:HOH:O	2.47	0.47
1:B:281:PHE:O	1:B:285:ARG:HG3	2.14	0.47
1:B:217:LEU:HG	5:B:713:GOL:O3	2.14	0.47
1:B:382:GLU:HG2	6:B:1078:HOH:O	2.14	0.47
1:B:294:ARG:HG2	5:B:709:GOL:O1	2.15	0.46
1:A:73:ALA:CB	1:A:103:LEU:HD13	2.46	0.46
1:A:273:MET:HG2	1:A:274:GLY:N	2.31	0.46
1:A:73:ALA:HB2	1:A:103:LEU:CD1	2.45	0.46
1:A:231:GLU:CD	1:A:263:ARG:HE	2.24	0.46
1:A:475:ARG:HG2	1:A:475:ARG:HH11	1.81	0.46
1:B:81:ASN:ND2	1:B:118:ASN:H	2.14	0.46
1:B:246:VAL:HG23	1:B:268:LEU:HD11	1.97	0.46
1:B:418:ARG:HG2	1:B:419:HIS:N	2.30	0.46
1:B:110:ASP:CG	1:B:111:LEU:N	2.75	0.45
1:A:335:ARG:NH2	6:A:1186:HOH:O	2.48	0.45
1:A:349:GLY:O	1:A:353:PRO:HD2	2.17	0.45
1:A:17:ARG:HD3	1:A:151:GLU:OE2	2.17	0.45
1:A:60:ARG:HG3	1:A:60:ARG:NH2	2.31	0.45
1:A:290:HIS:CG	1:A:435:PRO:HD3	2.52	0.45
1:A:335:ARG:NE	6:A:1186:HOH:O	2.48	0.45
1:B:165:ARG:HG3	1:B:166:ASP:OD2	2.16	0.45
1:B:177:ARG:NH1	1:B:177:ARG:HB3	2.32	0.44
1:A:301:PRO:HB2	1:A:303:THR:HG22	1.99	0.44
1:B:19:GLY:HA2	1:B:43:GLU:HG2	1.99	0.44
1:A:110:ASP:CG	1:A:111:LEU:H	2.25	0.44
1:A:350:ALA:HB2	1:A:399:TYR:CD1	2.52	0.44
1:A:292:ARG:HG2	1:A:292:ARG:NH1	2.32	0.44
1:A:320:ASP:O	1:A:324:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:PRO:HG2	1:A:438:THR:OG1	2.17	0.44
1:A:496:ASP:O	1:A:500:VAL:HG23	2.18	0.44
1:A:406:ASP:OD1	5:B:712:GOL:H32	2.18	0.43
1:B:431:ALA:HA	1:B:439:VAL:HG21	2.00	0.43
1:A:223:VAL:HG13	1:A:429:ALA:HA	2.00	0.43
1:A:456:PHE:O	1:A:460:LEU:HD23	2.17	0.43
1:B:177:ARG:HB3	1:B:177:ARG:HH11	1.82	0.43
1:A:19:GLY:CA	1:A:43:GLU:HB3	2.48	0.43
1:B:237:ARG:O	1:B:343:ARG:HD3	2.18	0.43
1:B:272:SER:HA	3:B:802:APC:H2	2.01	0.43
1:B:359:ARG:HA	1:B:417:ARG:NH1	2.34	0.43
1:A:305:LEU:HD11	1:A:329:PRO:HA	2.00	0.43
1:A:29:ALA:HA	1:A:314:TRP:CH2	2.54	0.42
1:B:169:GLY:O	1:B:183:GLY:HA2	2.19	0.42
1:B:308:GLN:HG3	1:B:332:ALA:HB2	2.01	0.42
1:A:470:VAL:HG23	1:A:471:HIS:N	2.34	0.42
1:B:41:GLN:HG2	1:B:70:PRO:HB3	2.01	0.42
1:B:249:SER:HB3	3:B:802:APC:O1B	2.20	0.42
1:B:253:ASP:CG	1:B:423:LYS:HZ2	2.27	0.42
1:B:333:LEU:HD23	1:B:333:LEU:O	2.19	0.42
1:B:20:GLY:N	1:B:43:GLU:OE2	2.53	0.41
1:A:129:ASP:O	1:A:197:LEU:HB2	2.20	0.41
1:A:352:ILE:HB	1:A:353:PRO:CD	2.49	0.41
1:B:480:GLU:OE2	1:B:507:ARG:NH1	2.52	0.41
1:A:335:ARG:HG2	1:A:335:ARG:HH11	1.85	0.41
1:A:393:HIS:HE1	6:A:1055:HOH:O	2.02	0.41
1:B:352:ILE:HB	1:B:353:PRO:CD	2.49	0.41
1:B:358:HIS:HD2	6:B:981:HOH:O	2.03	0.41
1:B:273:MET:HE2	1:B:274:GLY:CA	2.50	0.41
1:B:308:GLN:HE22	1:B:335:ARG:HD3	1.84	0.41
1:A:316:SER:HB3	1:A:387:LEU:HD21	2.02	0.41
1:A:328:LEU:N	1:A:329:PRO:HD2	2.35	0.41
1:B:453:THR:HG23	1:B:457:SER:CB	2.48	0.41
1:B:327:LEU:HD13	1:B:387:LEU:HD21	2.02	0.41
1:A:96:GLU:HG3	1:A:100:GLU:OE2	2.21	0.40
1:A:294:ARG:HD2	1:A:294:ARG:O	2.20	0.40
1:B:459:LEU:O	1:B:463:HIS:HD2	2.04	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	482/513 (94%)	458 (95%)	20 (4%)	4 (1%)	16	8
1	B	494/513 (96%)	482 (98%)	11 (2%)	1 (0%)	43	36
All	All	976/1026 (95%)	940 (96%)	31 (3%)	5 (0%)	24	16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	90	PRO
1	A	19	GLY
1	A	91	ALA
1	A	465	VAL
1	A	169	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	383/395 (97%)	375 (98%)	8 (2%)	47	41
1	B	388/395 (98%)	378 (97%)	10 (3%)	40	33
All	All	771/790 (98%)	753 (98%)	18 (2%)	44	38

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

Mol	Chain	Res	Type
1	A	41	GLN

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Mol	Chain	Res	Type
1	A	81	ASN
1	A	103	LEU
1	A	151	GLU
1	A	161	LEU
1	A	168	LYS
1	A	197	LEU
1	A	276	ASP
1	B	5	VAL
1	B	81	ASN
1	B	168	LYS
1	B	215	ARG
1	B	219	GLU
1	B	273	MET
1	B	341	GLU
1	B	357	MET
1	B	380	LEU
1	B	417	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	81	ASN
1	A	118	ASN
1	A	186	GLN
1	A	236	GLN
1	A	290	HIS
1	A	381	ASN
1	A	393	HIS
1	A	440	ASN
1	A	491	HIS
1	B	81	ASN
1	B	137	HIS
1	B	186	GLN
1	B	236	GLN
1	B	308	GLN
1	B	358	HIS
1	B	372	HIS
1	B	381	ASN
1	B	463	HIS
1	B	471	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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$
3	APC	A	801	4,2	29,33,33	2.20	6 (20%)	44,52,52	1.56	6 (13%)
3	APC	B	802	2	29,33,33	2.24	7 (24%)	44,52,52	1.56	5 (11%)
5	GOL	B	711	-	5,5,5	0.98	0	5,5,5	0.38	0
5	GOL	B	712	-	5,5,5	0.95	0	5,5,5	0.38	0
5	GOL	B	710	-	5,5,5	0.99	0	5,5,5	0.39	0
5	GOL	B	713	-	5,5,5	0.88	0	5,5,5	0.40	0
5	GOL	B	709	-	5,5,5	0.90	0	5,5,5	0.43	0
4	CMA	A	803	3	16,16,16	0.87	0	15,19,19	1.60	1 (6%)
4	CMA	B	804	-	16,16,16	0.80	0	15,19,19	1.58	1 (6%)

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
3	APC	A	801	4,2	-	8/19/38/38	0/3/3/3
3	APC	B	802	2	-	9/19/38/38	0/3/3/3
5	GOL	B	711	-	-	0/4/4/4	-
5	GOL	B	712	-	-	0/4/4/4	-
5	GOL	B	710	-	-	0/4/4/4	-
5	GOL	B	713	-	-	0/4/4/4	-
5	GOL	B	709	-	-	0/4/4/4	-
4	CMA	A	803	3	-	9/17/17/17	-
4	CMA	B	804	-	-	10/17/17/17	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	APC	O5'-C5'	-7.44	1.16	1.44
3	A	801	APC	O5'-C5'	-7.20	1.17	1.44
3	A	801	APC	C6-N6	-4.46	1.22	1.34
3	B	802	APC	C6-N6	-4.37	1.23	1.34
3	B	802	APC	C2-N1	3.75	1.40	1.33
3	A	801	APC	C2-N1	3.70	1.40	1.33
3	A	801	APC	PB-O2B	-3.38	1.48	1.56
3	B	802	APC	C4-N3	3.34	1.40	1.34
3	A	801	APC	C4-N3	3.05	1.40	1.34
3	B	802	APC	PB-O2B	-3.04	1.49	1.56
3	A	801	APC	PA-O2A	-2.19	1.51	1.56
3	B	802	APC	C4-N9	2.07	1.42	1.37
3	B	802	APC	PA-O2A	-2.03	1.51	1.56

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	804	CMA	C1-N-CA	5.32	123.30	113.76
4	A	803	CMA	C1-N-CA	5.31	123.28	113.76
3	B	802	APC	C2-N1-C6	5.22	127.30	118.73
3	A	801	APC	C2-N1-C6	5.18	127.24	118.73
3	A	801	APC	N3-C2-N1	-4.40	121.92	128.58
3	B	802	APC	N3-C2-N1	-4.39	121.93	128.58
3	A	801	APC	C3'-C2'-C1'	3.89	108.81	101.46
3	B	802	APC	C3'-C2'-C1'	3.63	108.33	101.46
3	B	802	APC	O1B-PB-C3A	-2.79	101.72	109.05
3	A	801	APC	O1B-PB-C3A	-2.62	102.14	109.05
3	A	801	APC	C5-C6-N1	-2.31	111.65	117.51
3	B	802	APC	C5-C6-N1	-2.25	111.80	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	APC	N6-C6-N1	2.03	122.90	118.38

There are no chirality outliers.

All (36) torsion outliers are listed below:

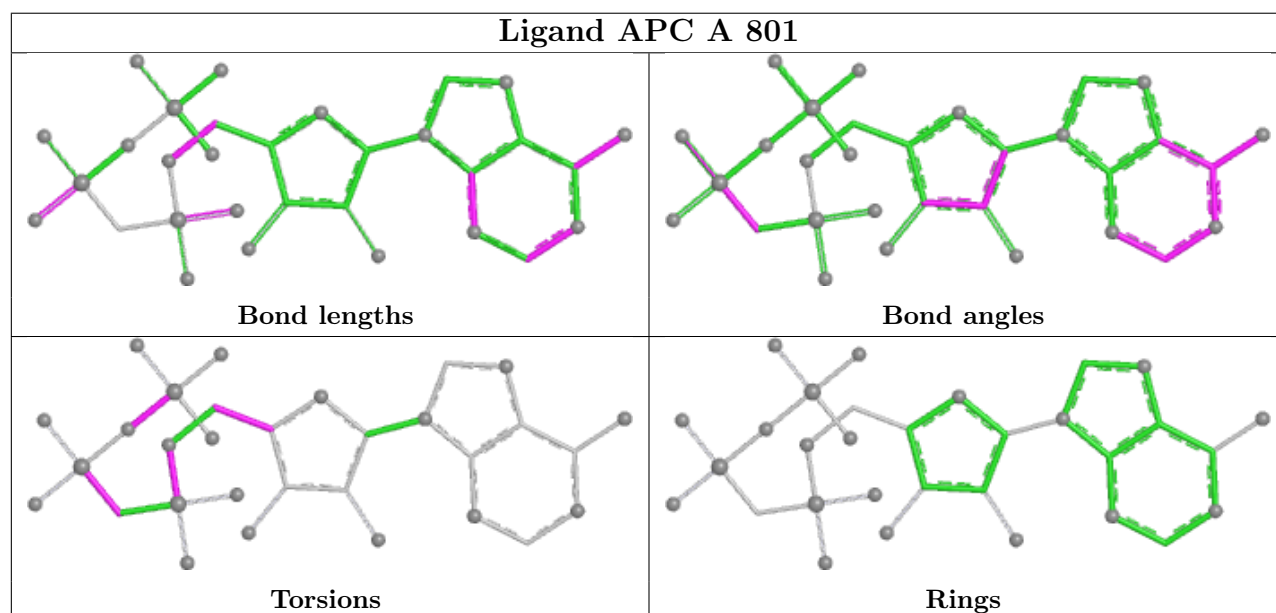
Mol	Chain	Res	Type	Atoms
3	A	801	APC	PB-O3B-PG-O2G
3	A	801	APC	PA-C3A-PB-O1B
3	A	801	APC	PA-C3A-PB-O2B
3	A	801	APC	PA-C3A-PB-O3B
3	A	801	APC	C5'-O5'-PA-O1A
3	A	801	APC	O4'-C4'-C5'-O5'
3	B	802	APC	PB-O3B-PG-O2G
3	B	802	APC	PB-O3B-PG-O3G
3	B	802	APC	PA-C3A-PB-O1B
3	B	802	APC	PA-C3A-PB-O2B
3	B	802	APC	PA-C3A-PB-O3B
3	B	802	APC	C5'-O5'-PA-O1A
3	B	802	APC	O4'-C4'-C5'-O5'
4	B	804	CMA	C-CA-CB-CG
4	B	804	CMA	CB-CA-N-C1
4	B	804	CMA	C-CA-N-C1
4	A	803	CMA	N-CA-CB-CG
4	B	804	CMA	N-CA-CB-CG
3	A	801	APC	C3'-C4'-C5'-O5'
3	B	802	APC	C3'-C4'-C5'-O5'
4	A	803	CMA	C-CA-CB-CG
4	B	804	CMA	N-C1-C2-C3
4	A	803	CMA	CA-CB-CG-CD
4	B	804	CMA	CA-CB-CG-CD
4	A	803	CMA	NE-CD-CG-CB
4	B	804	CMA	NE-CD-CG-CB
4	B	804	CMA	C1-C2-C3-O1
4	B	804	CMA	C1-C2-C3-O2
4	A	803	CMA	C2-C1-N-CA
4	B	804	CMA	C2-C1-N-CA
4	A	803	CMA	CB-CA-N-C1
4	A	803	CMA	C-CA-N-C1
3	A	801	APC	C5'-O5'-PA-O2A
3	B	802	APC	C5'-O5'-PA-O2A
4	A	803	CMA	C1-C2-C3-O1
4	A	803	CMA	C1-C2-C3-O2

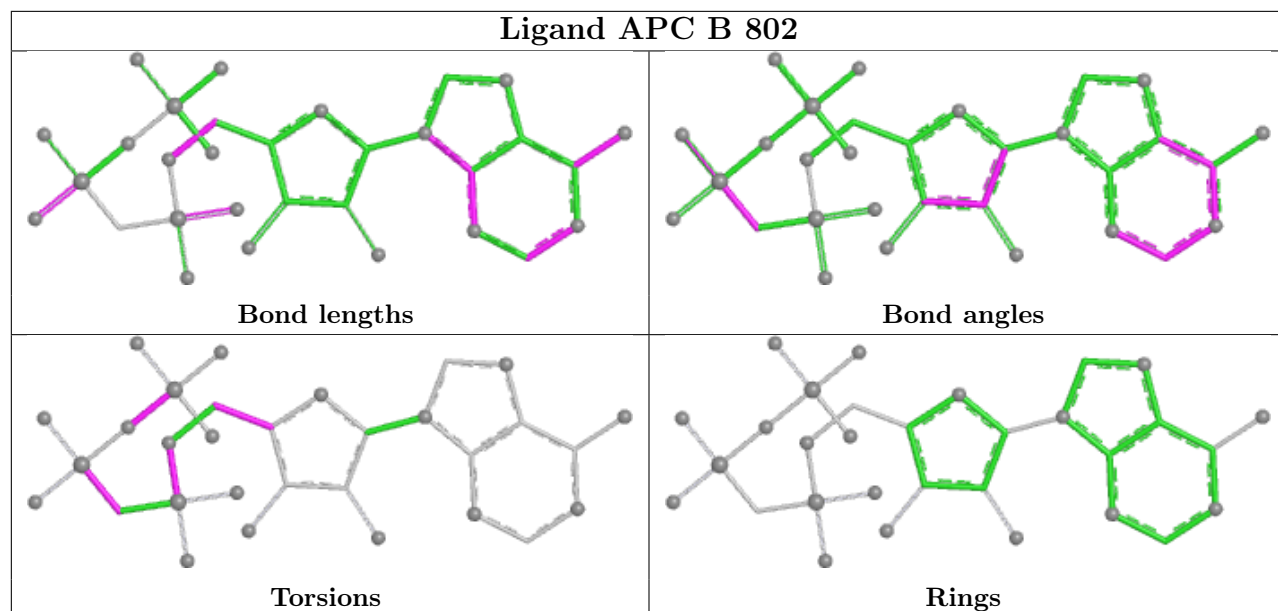
There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	APC	6	0
3	B	802	APC	2	0
5	B	712	GOL	2	0
5	B	713	GOL	3	0
5	B	709	GOL	1	0
4	A	803	CMA	7	0
4	B	804	CMA	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	490/513 (95%)	0.31	44 (8%) 15 17	16, 27, 63, 76	0
1	B	500/513 (97%)	0.17	20 (4%) 42 49	15, 25, 47, 68	0
All	All	990/1026 (96%)	0.24	64 (6%) 25 28	15, 26, 55, 76	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	91	ALA	4.6
1	A	20	GLY	4.5
1	B	21	GLY	4.4
1	B	18	THR	4.4
1	A	19	GLY	4.1
1	A	508	THR	3.9
1	A	326	TYR	3.8
1	A	167	PRO	3.7
1	B	164	HIS	3.7
1	A	470	VAL	3.7
1	B	25	GLY	3.5
1	B	93	PRO	3.3
1	A	40	PRO	3.2
1	A	18	THR	3.1
1	A	181	LEU	3.1
1	A	173	ALA	3.1
1	A	444	LEU	3.1
1	A	182	THR	3.1
1	B	94	ALA	3.1
1	B	166	ASP	3.0
1	A	461	LEU	3.0
1	A	464	GLY	3.0
1	A	163	ALA	3.0
1	B	452	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	91	ALA	3.0
1	A	500	VAL	2.9
1	A	504	VAL	2.9
1	A	169	GLY	2.9
1	B	66	LEU	2.8
1	A	170	PHE	2.8
1	B	24	PRO	2.8
1	A	460	LEU	2.7
1	A	164	HIS	2.7
1	A	468	ASP	2.7
1	A	465	VAL	2.6
1	B	359	ARG	2.6
1	B	444	LEU	2.6
1	B	68	GLY	2.5
1	A	473	ALA	2.5
1	A	472	GLU	2.5
1	A	180	GLY	2.5
1	A	94	ALA	2.4
1	A	501	VAL	2.4
1	A	92	GLY	2.4
1	A	16	ALA	2.3
1	B	358	HIS	2.3
1	B	92	GLY	2.3
1	A	469	ARG	2.3
1	A	499	ASP	2.3
1	B	504	VAL	2.2
1	B	355	GLY	2.2
1	A	292	ARG	2.2
1	A	300	ILE	2.1
1	A	17	ARG	2.1
1	A	467	GLU	2.1
1	A	466	ALA	2.1
1	B	2	GLY	2.1
1	A	96	GLU	2.1
1	A	41	GLN	2.1
1	A	502	ARG	2.1
1	A	471	HIS	2.0
1	A	44	ARG	2.0
1	A	495	VAL	2.0
1	B	44	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

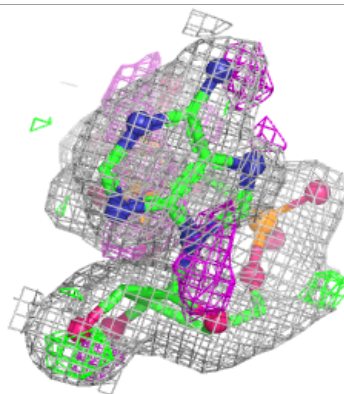
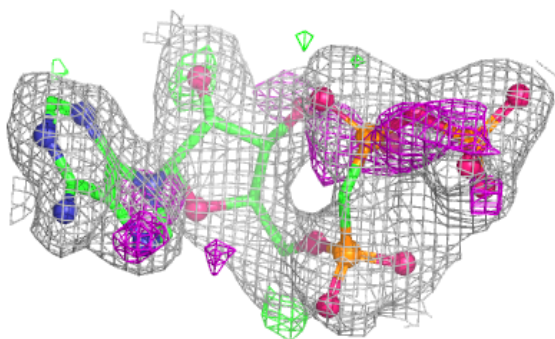
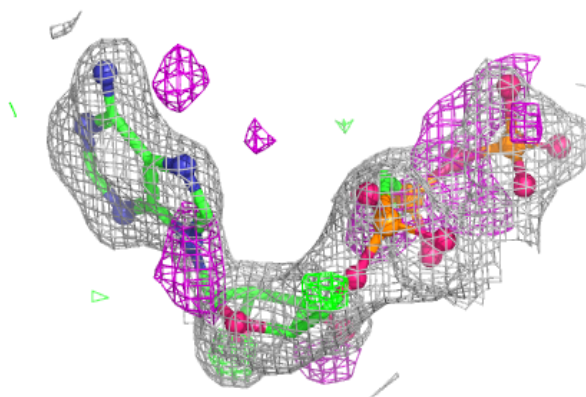
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	B	713	6/6	0.60	0.21	59,60,61,63	0
5	GOL	B	711	6/6	0.65	0.14	64,64,65,65	0
5	GOL	B	712	6/6	0.74	0.16	61,62,62,62	0
5	GOL	B	710	6/6	0.78	0.14	60,61,62,62	0
4	CMA	A	803	17/17	0.79	0.13	46,50,61,62	0
4	CMA	B	804	17/17	0.82	0.13	28,36,47,48	0
5	GOL	B	709	6/6	0.83	0.14	55,56,57,57	0
3	APC	B	802	31/31	0.84	0.12	30,40,45,45	0
3	APC	A	801	31/31	0.90	0.10	27,37,40,41	0
2	MG	A	902	1/1	0.93	0.07	42,42,42,42	0
2	MG	B	901	1/1	0.96	0.06	39,39,39,39	0

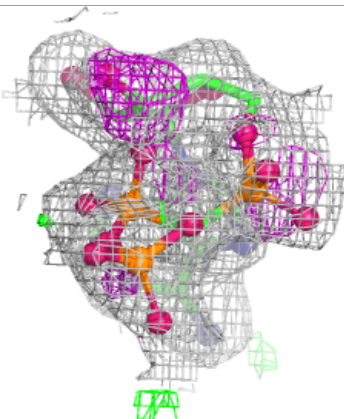
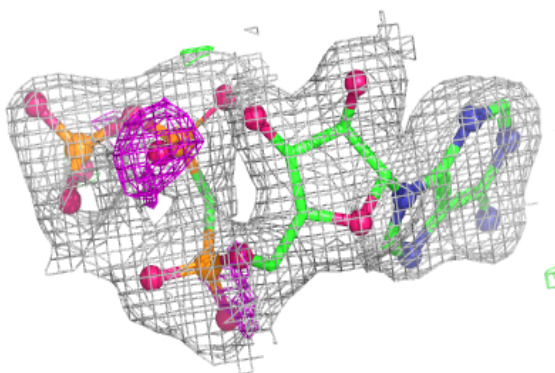
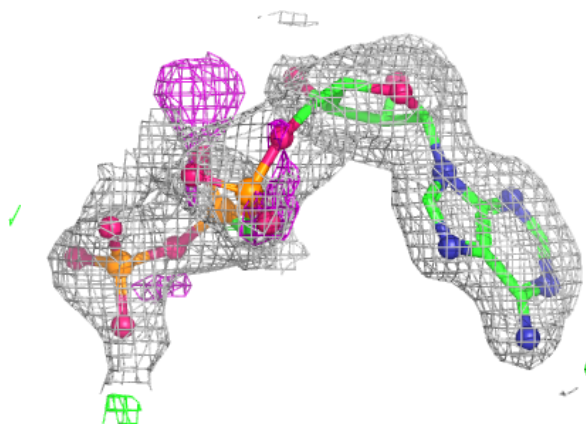
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around APC B 802:

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

**Electron density around APC A 801:**

$2mF_o-DF_c$ (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.