



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2026 – 03:50 PM JST

PDB ID : 44SL / pdb_000044sl
Title : Crystal structure of the complex of erythrose-4-phosphate dehydrogenase from *Acinetobacter baumannii* with Adenosine monophosphate at 2.40 Angstrom resolution.
Authors : Ahmad, N.; Viswanathan, V.; Kumari, A.; Singh, A.; Kumar, A.; Sharma, P.; Chopra, S.; Jeyakanthan, J.; Sharma, S.; Raje, C.I.; Singh, T.P.
Deposited on : 2026-08-11
Resolution : 2.40 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

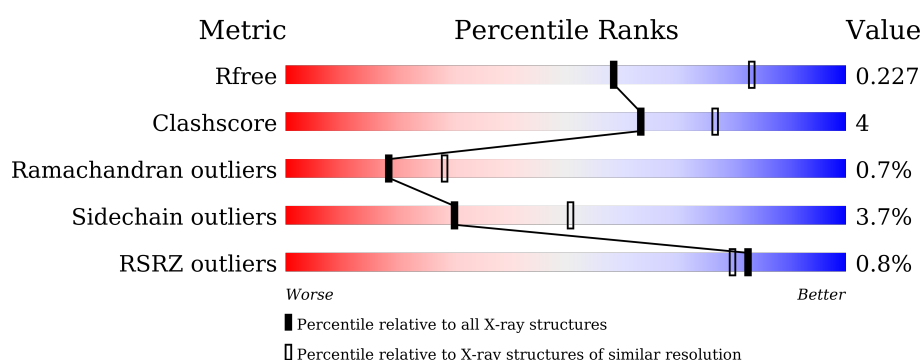
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	341	% 87% 11%
1	B	341	2% 83% 15%
1	C	341	89% 9%
1	D	341	86% 12%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11553 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.

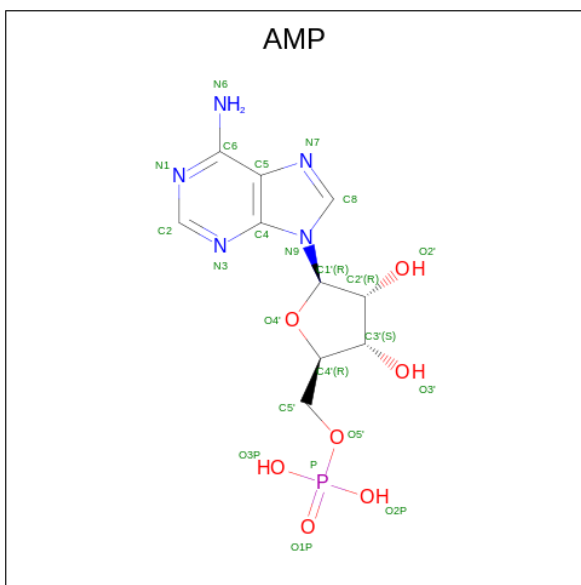
- Molecule 1 is a protein called Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	1	0
			2676	1700	469	498	9			
1	C	340	Total	C	N	O	S	0	1	0
			2684	1704	473	498	9			
1	B	340	Total	C	N	O	S	0	1	0
			2681	1703	472	497	9			
1	D	340	Total	C	N	O	S	0	1	0
			2681	1703	472	497	9			

There are 12 discrepancies between the modelled and reference sequences:

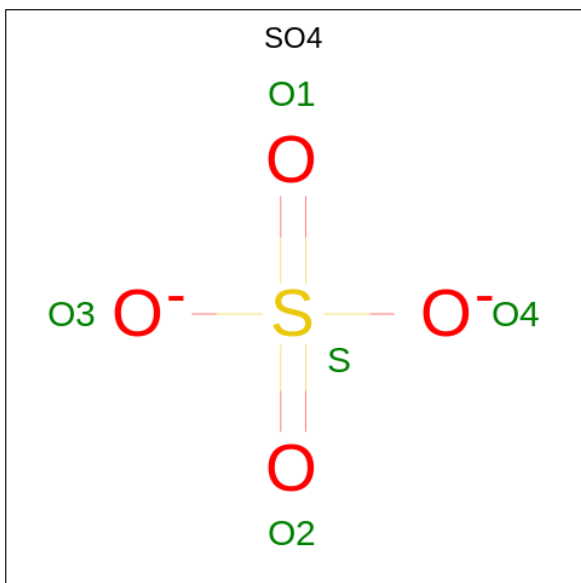
Chain	Residue	Modelled	Actual	Comment	Reference
A	89	GLN	LYS	conflict	UNP A0A0D5YKI8
A	235	ASP	ASN	conflict	UNP A0A0D5YKI8
A	306	LEU	SER	conflict	UNP A0A0D5YKI8
C	89	GLN	LYS	conflict	UNP A0A0D5YKI8
C	235	ASP	ASN	conflict	UNP A0A0D5YKI8
C	306	LEU	SER	conflict	UNP A0A0D5YKI8
B	89	GLN	LYS	conflict	UNP A0A0D5YKI8
B	235	ASP	ASN	conflict	UNP A0A0D5YKI8
B	306	LEU	SER	conflict	UNP A0A0D5YKI8
D	89	GLN	LYS	conflict	UNP A0A0D5YKI8
D	235	ASP	ASN	conflict	UNP A0A0D5YKI8
D	306	LEU	SER	conflict	UNP A0A0D5YKI8

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P) (labeled as "Ligand of Interest" by depositor).



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

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

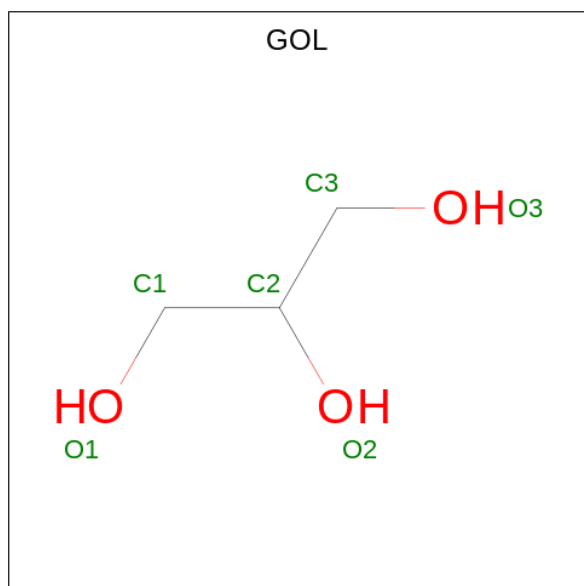


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



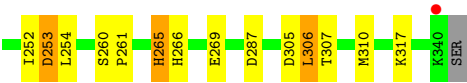
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	179	Total 179	O 179	0	0
6	C	194	Total 194	O 194	0	0
6	B	136	Total 136	O 136	0	0
6	D	198	Total 198	O 198	0	0

- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	147.58Å 167.01Å 155.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.51 – 2.40 83.51 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (83.51-2.40) 99.9 (83.51-2.40)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.172 , 0.221 0.179 , 0.227	Depositor DCC
R_{free} test set	1111 reflections (1.48%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11553	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: SO4, GOL, MG, AMP

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	0.56	0/2733	1.06	3/3716 (0.1%)
1	B	0.55	0/2738	1.09	14/3722 (0.4%)
1	C	0.57	0/2738	1.08	8/3722 (0.2%)
1	D	0.55	0/2738	1.07	12/3722 (0.3%)
All	All	0.56	0/10947	1.08	37/14882 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	1
1	D	0	3
All	All	0	6

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	149	ASP	CA-CB-CG	7.26	119.86	112.60
1	B	219	THR	CA-CB-OG1	-6.56	99.76	109.60
1	B	2	GLN	CB-CA-C	6.50	120.51	109.53
1	D	202	HIS	CA-CB-CG	6.24	120.04	113.80
1	C	65	GLU	CB-CA-C	-6.21	103.29	111.42
1	A	202	HIS	CA-CB-CG	6.17	119.97	113.80
1	D	135	ASP	CA-CB-CG	6.14	118.74	112.60
1	C	278	ASP	CA-CB-CG	6.06	118.66	112.60
1	D	94	PRO	N-CA-CB	-6.02	98.77	102.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	253	ASP	CA-CB-CG	6.00	118.60	112.60
1	B	94	PRO	N-CA-CB	-5.95	97.01	103.25
1	B	202	HIS	CA-CB-CG	5.93	119.73	113.80
1	C	94	PRO	N-CA-CB	-5.68	99.01	102.81
1	B	2	GLN	N-CA-CB	-5.58	101.63	110.06
1	B	149	ASP	CA-CB-CG	5.58	118.18	112.60
1	B	154	ASP	CA-CB-CG	5.51	118.11	112.60
1	D	253	ASP	CA-CB-CG	5.50	118.09	112.60
1	B	204	ASP	CA-CB-CG	5.44	118.04	112.60
1	D	219	THR	CA-CB-OG1	-5.38	101.53	109.60
1	C	287	ASP	CA-CB-CG	5.33	117.93	112.60
1	D	199	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	39	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	253	ASP	CA-CB-CG	5.24	117.84	112.60
1	D	61	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	194	ASP	CA-CB-CG	5.21	117.81	112.60
1	D	154	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	135	ASP	CA-CB-CG	5.17	117.77	112.60
1	D	235	ASP	CB-CA-C	-5.11	102.73	111.26
1	B	305	ASP	CA-CB-CG	5.10	117.70	112.60
1	C	135	ASP	CA-CB-CG	5.09	117.69	112.60
1	D	265	HIS	CA-CB-CG	5.08	118.88	113.80
1	B	199	ASP	CA-CB-CG	5.07	117.67	112.60
1	D	305	ASP	CA-CB-CG	5.04	117.64	112.60
1	B	334	ASP	CB-CA-C	5.03	119.09	110.74
1	C	228	ARG	CB-CG-CD	5.02	122.84	111.30
1	A	204	ASP	CA-CB-CG	5.01	117.61	112.60
1	C	199	ASP	CA-CB-CG	5.00	117.61	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	3	ARG	Sidechain
1	B	78	ARG	Sidechain
1	C	18	ARG	Sidechain
1	D	206[A]	ARG	Sidechain
1	D	206[B]	ARG	Sidechain
1	D	236	ARG	Sidechain

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	2676	0	2684	22	0
1	B	2681	0	2692	25	0
1	C	2684	0	2691	19	0
1	D	2681	0	2692	22	0
2	A	23	0	12	1	0
2	B	23	0	12	0	0
2	C	23	0	12	1	0
2	D	23	0	12	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
3	D	5	0	0	0	0
4	A	1	0	0	0	0
5	C	6	0	8	0	0
6	A	179	0	0	4	0
6	B	136	0	0	5	0
6	C	194	0	0	4	0
6	D	198	0	0	5	0
All	All	11553	0	10815	86	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (86) 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:136:HIS:HB2	6:A:562:HOH:O	1.73	0.88
1:C:287:ASP:HB3	1:C:306:LEU:HD21	1.61	0.83
1:B:232:LYS:HG2	6:B:572:HOH:O	1.90	0.71
1:D:287:ASP:HB3	1:D:306:LEU:HD21	1.73	0.71
1:C:305:ASP:OD2	1:D:206[B]:ARG:NH2	2.25	0.70
1:B:103:VAL:HG11	1:B:119:HIS:ND1	2.08	0.67
1:C:200:HIS:O	1:C:208:ALA:HB1	1.96	0.65
1:B:87:GLN:HG3	1:B:89:GLN:O	1.98	0.62
1:D:265:HIS:CE1	1:D:269:GLU:OE2	2.55	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ASP:HB3	1:B:306:LEU:HD21	1.84	0.58
1:B:2:GLN:HA	1:B:101:ASP:OD2	2.06	0.56
1:C:240:TYR:OH	1:D:253:ASP:OD2	2.18	0.55
1:C:226:LEU:C	1:C:226:LEU:HD23	2.31	0.55
1:B:90:PRO:HA	1:B:93:LEU:HD12	1.89	0.55
1:B:9:PHE:O	1:B:14[A]:ARG:NH1	2.41	0.54
1:B:14[B]:ARG:NH1	6:B:504:HOH:O	2.40	0.54
1:B:27:PHE:HB3	1:B:29:PHE:CE1	2.42	0.54
1:D:234:GLU:O	1:D:235:ASP:HB2	2.08	0.54
1:A:200:HIS:O	1:A:208:ALA:HB1	2.08	0.54
2:A:401:AMP:H5'1	6:A:596:HOH:O	2.09	0.53
1:A:4:ILE:HD13	1:A:29:PHE:CD2	2.44	0.52
1:D:265:HIS:HB2	6:D:606:HOH:O	2.10	0.51
1:B:76:ASN:HA	6:B:543:HOH:O	2.10	0.51
1:C:312:VAL:HG22	1:D:184:LEU:HD21	1.92	0.51
1:D:287:ASP:HB3	1:D:306:LEU:CD2	2.38	0.50
1:C:287:ASP:HB3	1:C:306:LEU:CD2	2.38	0.50
1:D:226:LEU:C	1:D:226:LEU:HD23	2.37	0.50
1:B:187:GLU:OE2	1:B:322:TYR:OH	2.28	0.50
1:B:4:ILE:HD13	1:B:29:PHE:CD2	2.46	0.50
1:C:306:LEU:C	1:C:306:LEU:HD12	2.37	0.49
2:C:401:AMP:H5'1	6:C:576:HOH:O	2.12	0.49
1:A:104:LEU:HD22	1:A:332:LEU:HD22	1.95	0.49
1:A:289:PRO:HA	1:B:206:ARG:CZ	2.43	0.48
1:D:93:LEU:HD13	1:D:95:TRP:CZ2	2.48	0.48
1:D:200:HIS:O	1:D:208:ALA:HB1	2.13	0.47
1:C:187:GLU:OE2	1:C:322:TYR:OH	2.32	0.47
1:A:159:SER:O	1:A:160:VAL:HG22	2.16	0.46
1:B:168:VAL:HB	1:B:169:PRO:HD3	1.97	0.46
1:A:314:HIS:HD2	6:A:588:HOH:O	1.99	0.46
1:A:306:LEU:HD12	1:A:306:LEU:C	2.41	0.45
1:B:243:ARG:NH2	6:B:508:HOH:O	2.48	0.45
1:B:40:VAL:O	1:B:44:VAL:HG23	2.17	0.45
2:D:401:AMP:H5'1	6:D:579:HOH:O	2.16	0.45
1:C:168:VAL:HB	1:C:169:PRO:HD3	1.99	0.45
1:D:306:LEU:C	1:D:306:LEU:HD12	2.41	0.45
1:D:168:VAL:HB	1:D:169:PRO:HD3	1.98	0.45
1:A:95:TRP:HA	1:A:95:TRP:CE3	2.51	0.44
1:C:136:HIS:HB3	6:C:594:HOH:O	2.16	0.44
1:B:2:GLN:HG3	6:B:530:HOH:O	2.17	0.44
1:B:226:LEU:C	1:B:226:LEU:HD23	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLU:HG2	1:A:92:LEU:HD13	2.00	0.44
1:C:18:ARG:HG3	1:C:47:PHE:CE1	2.52	0.44
1:B:117:THR:HG22	1:B:120:LEU:HD12	1.99	0.44
1:B:39:ASP:OD1	1:B:40:VAL:N	2.50	0.44
1:B:306:LEU:C	1:B:306:LEU:HD12	2.43	0.43
1:A:34:ILE:HG23	1:A:82:VAL:HG11	2.00	0.43
1:B:21:PHE:CD1	1:B:75:SER:HB3	2.54	0.43
1:A:95:TRP:HA	1:A:95:TRP:HE3	1.84	0.43
1:D:260:SER:HB2	1:D:261:PRO:CD	2.48	0.43
1:A:202:HIS:CD2	6:A:649:HOH:O	2.71	0.43
1:C:228:ARG:NH2	6:C:506:HOH:O	2.51	0.43
1:D:248:ASN:O	1:D:249:VAL:HB	2.19	0.42
1:D:213:GLN:NE2	6:D:508:HOH:O	2.53	0.42
1:B:4:ILE:HD13	1:B:29:PHE:HD2	1.84	0.42
1:D:254:LEU:O	1:D:317:LYS:HA	2.20	0.42
1:C:285:VAL:HG22	1:C:304:VAL:HB	2.02	0.42
1:C:36:ASP:O	1:C:86:GLN:HA	2.19	0.42
1:D:266:HIS:HD2	6:D:596:HOH:O	2.02	0.42
1:A:153:THR:O	1:A:155:GLN:HG3	2.20	0.42
1:A:215:ILE:HB	1:B:292:SER:HB3	2.02	0.42
1:A:187:GLU:OE2	1:A:322:TYR:OH	2.35	0.41
1:D:310:MET:HE2	1:D:317:LYS:HD2	2.01	0.41
1:A:226:LEU:C	1:A:226:LEU:HD23	2.44	0.41
1:D:4:ILE:HG13	1:D:102:VAL:HB	2.01	0.41
1:A:340:LYS:HA	1:A:340:LYS:HD2	1.84	0.41
1:B:148:ALA:C	1:B:150:VAL:H	2.27	0.41
1:A:287:ASP:HB3	1:A:306:LEU:HD21	2.02	0.41
1:C:155:GLN:HA	6:C:563:HOH:O	2.20	0.41
1:D:4:ILE:HD13	1:D:29:PHE:CD1	2.56	0.41
1:D:232:LYS:HG2	6:D:647:HOH:O	2.20	0.41
1:A:253:ASP:OD2	1:A:317:LYS:HD3	2.21	0.41
1:C:287:ASP:HA	1:C:306:LEU:HG	2.03	0.41
1:C:202:HIS:HB3	1:C:208:ALA:HB2	2.02	0.40
1:A:65:GLU:O	1:A:66:ASN:HB3	2.21	0.40
1:A:183:ALA:O	1:A:237:ILE:HA	2.21	0.40
1:C:93:LEU:HD13	1:C:95:TRP:CZ2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	339/341 (99%)	318 (94%)	19 (6%)	2 (1%)	21	32
1	B	339/341 (99%)	317 (94%)	18 (5%)	4 (1%)	10	16
1	C	339/341 (99%)	324 (96%)	13 (4%)	2 (1%)	21	32
1	D	339/341 (99%)	320 (94%)	17 (5%)	2 (1%)	21	32
All	All	1356/1364 (99%)	1279 (94%)	67 (5%)	10 (1%)	18	28

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	VAL
1	A	249	VAL
1	C	160	VAL
1	C	249	VAL
1	B	160	VAL
1	B	249	VAL
1	D	249	VAL
1	B	94	PRO
1	D	160	VAL
1	B	149	ASP

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	292/292 (100%)	281 (96%)	11 (4%)	29	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	292/292 (100%)	280 (96%)	12 (4%)	27	46
1	C	292/292 (100%)	283 (97%)	9 (3%)	35	57
1	D	292/292 (100%)	281 (96%)	11 (4%)	29	49
All	All	1168/1168 (100%)	1125 (96%)	43 (4%)	30	51

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	92	LEU
1	A	95	TRP
1	A	203	ARG
1	A	228	ARG
1	A	232	LYS
1	A	234	GLU
1	A	252	ILE
1	A	253	ASP
1	A	269	GLU
1	A	306	LEU
1	C	12	ILE
1	C	79	LEU
1	C	95	TRP
1	C	203	ARG
1	C	228	ARG
1	C	229	VAL
1	C	253	ASP
1	C	306	LEU
1	C	307	THR
1	B	74	GLN
1	B	80	LEU
1	B	92	LEU
1	B	94	PRO
1	B	97	SER
1	B	98	LEU
1	B	117	THR
1	B	196	SER
1	B	203	ARG
1	B	297	HIS
1	B	306	LEU
1	B	307	THR
1	D	43	LEU

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Mol	Chain	Res	Type
1	D	94	PRO
1	D	95	TRP
1	D	98	LEU
1	D	105	GLU
1	D	153	THR
1	D	196	SER
1	D	203	ARG
1	D	252	ILE
1	D	306	LEU
1	D	307	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	74	GLN
1	A	113	HIS
1	A	136	HIS
1	A	165	GLN
1	A	213	GLN
1	A	315	GLN
1	C	41	HIS
1	C	89	GLN
1	C	213	GLN
1	C	315	GLN
1	B	28	HIS
1	B	72	ASN
1	B	165	GLN
1	B	213	GLN
1	B	248	ASN
1	B	265	HIS
1	B	315	GLN
1	D	248	ASN
1	D	266	HIS
1	D	296	ASN

5.3.3 RNA ⓘ

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 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	AMP	B	401	-	25,25,25	0.39	0	38,38,38	0.60	0
3	SO4	B	402	-	4,4,4	0.34	0	6,6,6	0.14	0
2	AMP	D	401	-	25,25,25	0.49	0	38,38,38	0.69	0
3	SO4	D	402	-	4,4,4	0.35	0	6,6,6	0.12	0
3	SO4	C	404	-	4,4,4	0.39	0	6,6,6	0.11	0
2	AMP	C	401	-	25,25,25	0.52	0	38,38,38	0.48	0
2	AMP	A	401	-	25,25,25	0.37	0	38,38,38	0.55	0
3	SO4	C	402	-	4,4,4	0.33	0	6,6,6	0.23	0
5	GOL	C	403	-	5,5,5	0.17	0	5,5,5	0.32	0
3	SO4	A	402	-	4,4,4	0.35	0	6,6,6	0.19	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AMP	B	401	-	-	4/10/26/26	0/3/3/3
2	AMP	D	401	-	-	5/10/26/26	0/3/3/3
2	AMP	C	401	-	-	3/10/26/26	0/3/3/3
5	GOL	C	403	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AMP	A	401	-	-	3/10/26/26	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	AMP	C5'-O5'-P-O1P
2	B	401	AMP	C5'-O5'-P-O2P
2	B	401	AMP	C5'-O5'-P-O3P
2	D	401	AMP	C5'-O5'-P-O2P
2	D	401	AMP	C5'-O5'-P-O3P
2	D	401	AMP	O4'-C4'-C5'-O5'
5	C	403	GOL	C1-C2-C3-O3
2	A	401	AMP	O4'-C4'-C5'-O5'
2	C	401	AMP	O4'-C4'-C5'-O5'
2	C	401	AMP	C3'-C4'-C5'-O5'
2	A	401	AMP	C3'-C4'-C5'-O5'
2	B	401	AMP	O4'-C4'-C5'-O5'
2	D	401	AMP	C3'-C4'-C5'-O5'
5	C	403	GOL	O2-C2-C3-O3
2	D	401	AMP	C5'-O5'-P-O1P
2	C	401	AMP	C4'-C5'-O5'-P
2	A	401	AMP	C2'-C1'-N9-C8

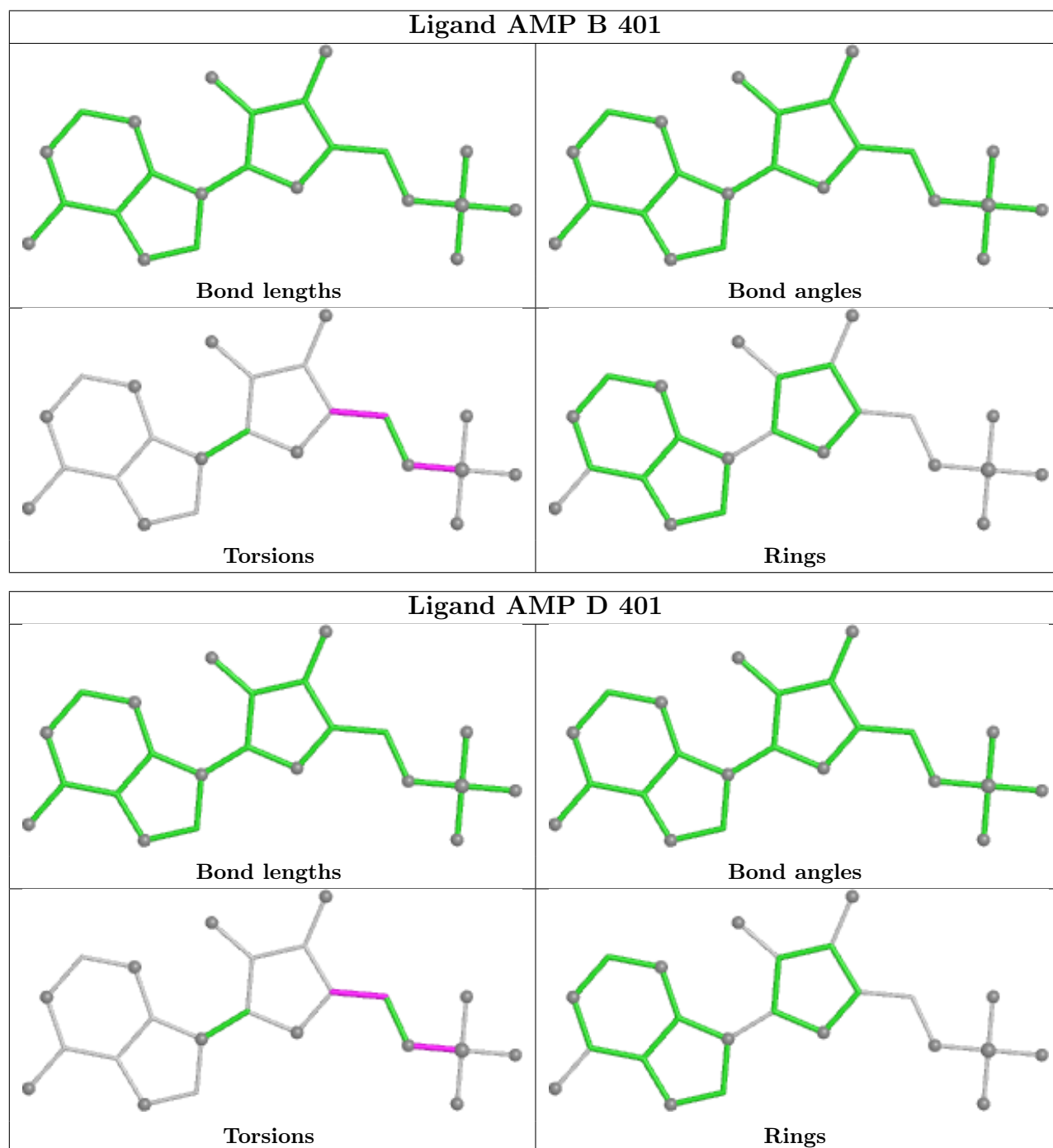
There are no ring outliers.

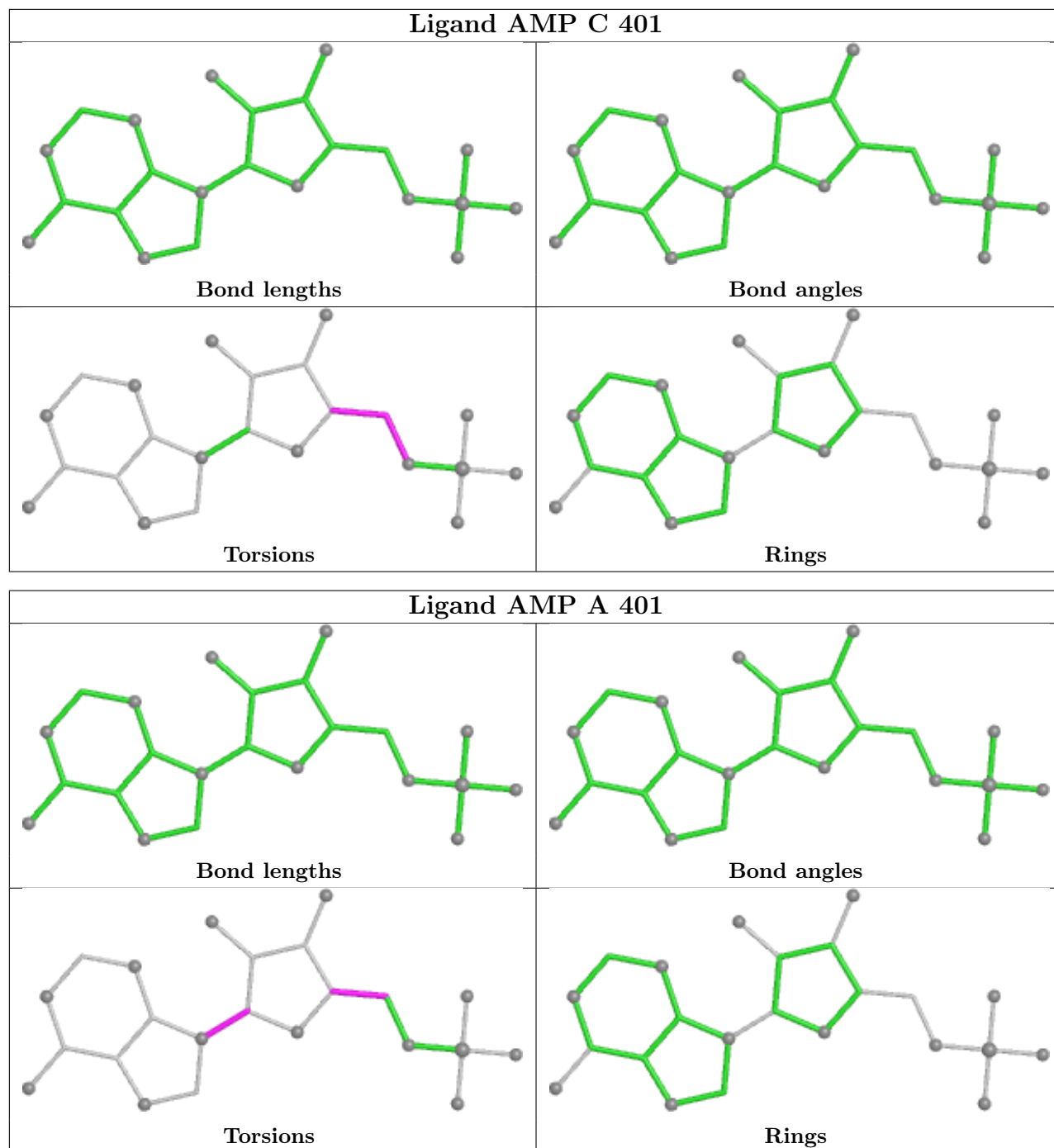
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	AMP	1	0
2	C	401	AMP	1	0
2	A	401	AMP	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 [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	340/341 (99%)	-0.39	3 (0%) 81 78	21, 47, 78, 121	1 (0%)
1	B	340/341 (99%)	0.01	7 (2%) 63 59	24, 52, 106, 131	1 (0%)
1	C	340/341 (99%)	-0.49	0 100 100	19, 45, 68, 119	1 (0%)
1	D	340/341 (99%)	-0.39	1 (0%) 90 88	26, 47, 71, 115	1 (0%)
All	All	1360/1364 (99%)	-0.32	11 (0%) 82 80	19, 47, 88, 131	4 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	3.4
1	B	98	LEU	3.4
1	A	340	LYS	2.9
1	B	203	ARG	2.8
1	B	2	GLN	2.7
1	B	64	ILE	2.6
1	B	1	MET	2.4
1	B	100	ILE	2.3
1	D	340	LYS	2.2
1	A	203	ARG	2.2
1	B	70	TYR	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](#)

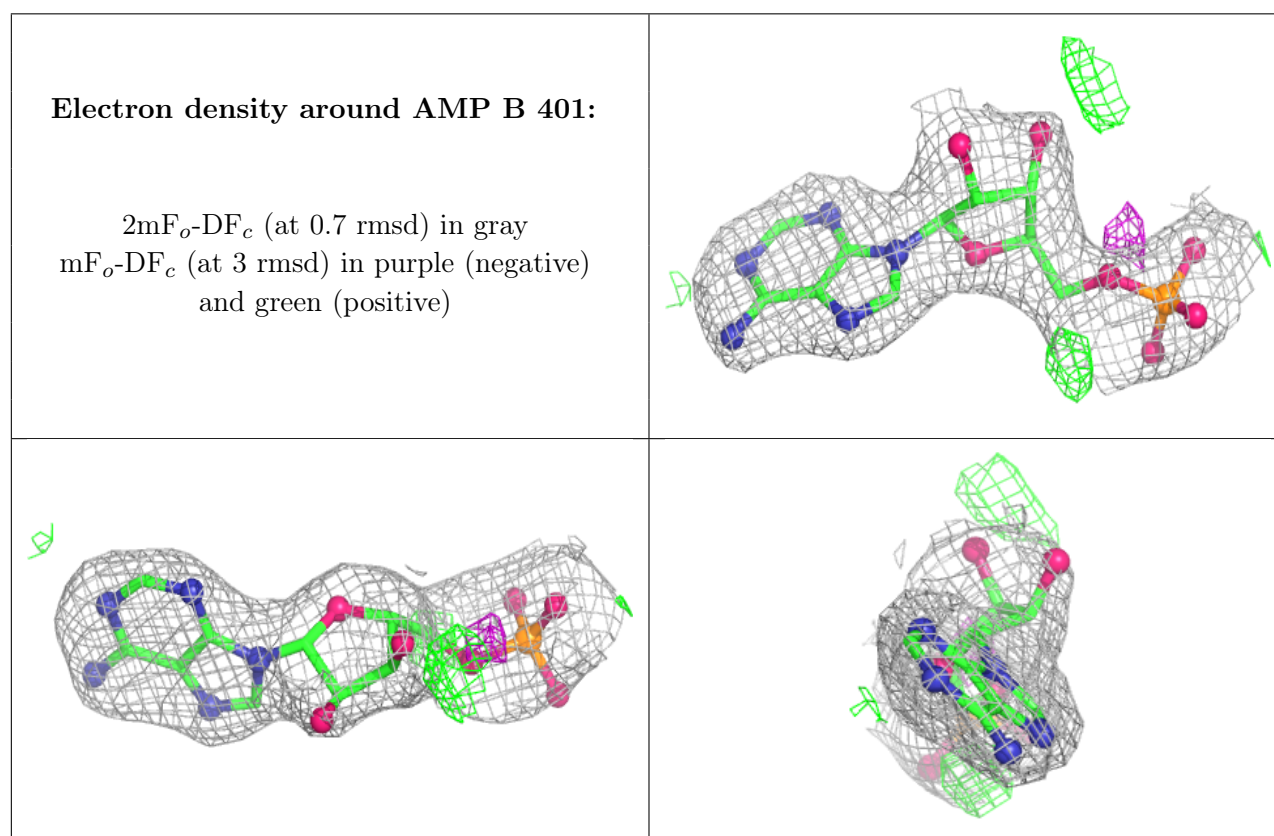
There are no oligosaccharides in this entry.

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.

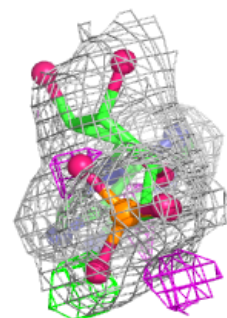
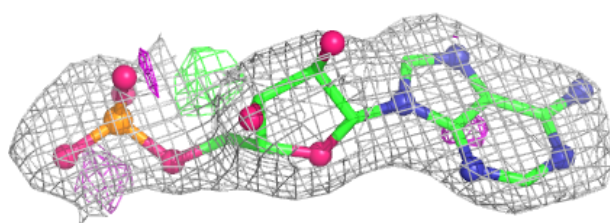
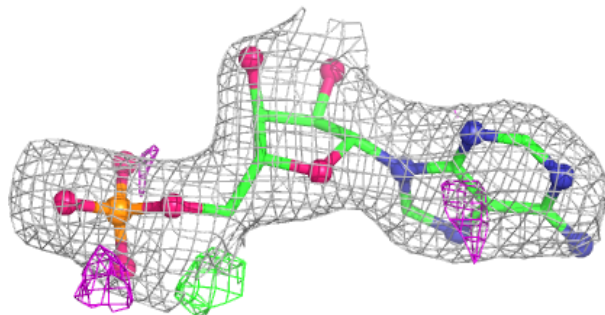
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	402	5/5	0.83	0.10	69,81,87,91	0
3	SO4	C	404	5/5	0.83	0.14	54,56,63,65	5
5	GOL	C	403	6/6	0.83	0.15	72,79,82,84	0
2	AMP	B	401	23/23	0.85	0.12	63,85,110,119	0
3	SO4	B	402	5/5	0.89	0.08	82,86,96,100	0
3	SO4	D	402	5/5	0.89	0.09	87,88,93,95	0
3	SO4	C	402	5/5	0.89	0.09	64,79,83,83	0
2	AMP	A	401	23/23	0.91	0.10	52,71,108,133	0
2	AMP	D	401	23/23	0.92	0.10	46,54,87,95	0
2	AMP	C	401	23/23	0.93	0.10	55,61,110,129	0
4	MG	A	403	1/1	0.97	0.06	66,66,66,66	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.

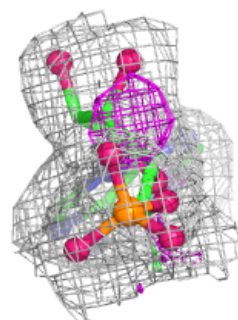
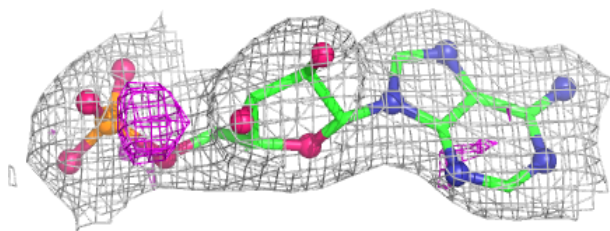
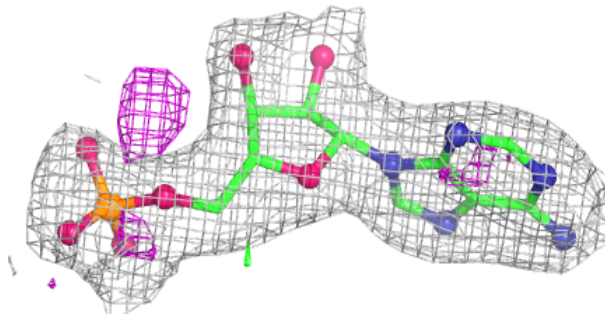


Electron density around AMP A 401:

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

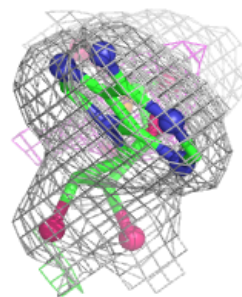
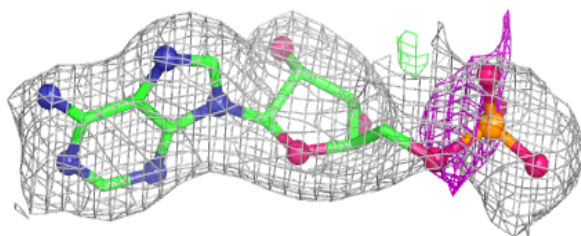
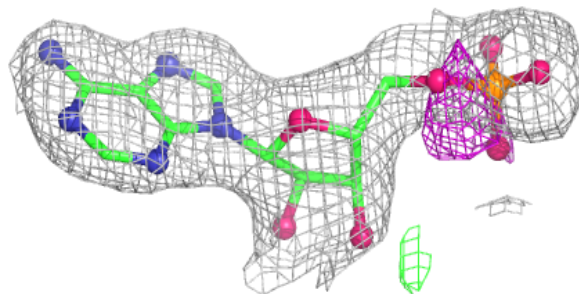
**Electron density around AMP D 401:**

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



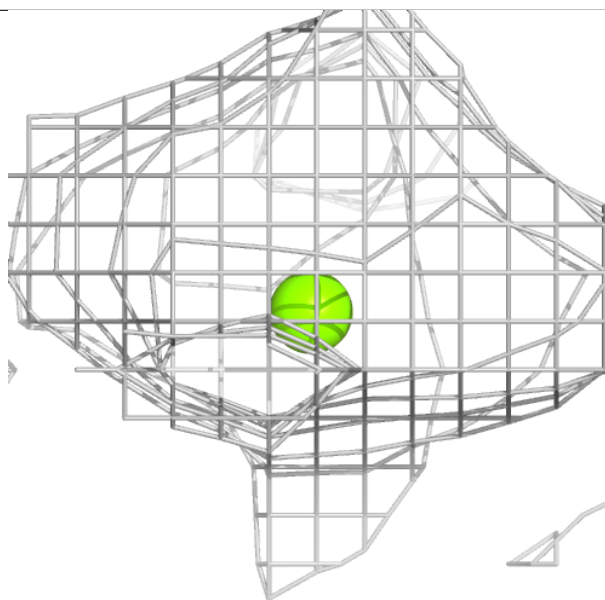
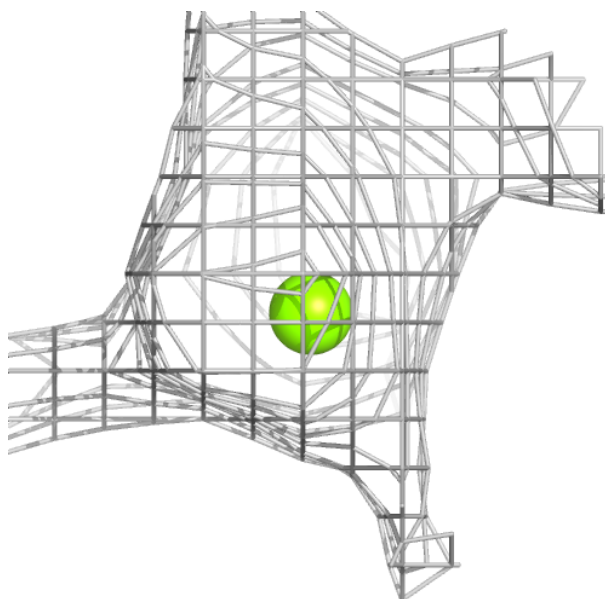
Electron density around AMP C 401:

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



Electron density around MG A 403:

$2mF_o-DF_c$ (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.