



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 01:21 PM UTC

PDB ID : 2X3K / pdb_00002x3k
Title : CO-COMPLEX STRUCTURE OF ACHROMOBACTIN SYNTHETASE
PROTEIN D (ACSD) WITH AMP AND SULFATE FROM PECTOBAC-
TERIUM CHRYSANTHEMI
Authors : Schmelz, S.; Naismith, J.H.
Deposited on : 2010-01-25
Resolution : 2.50 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

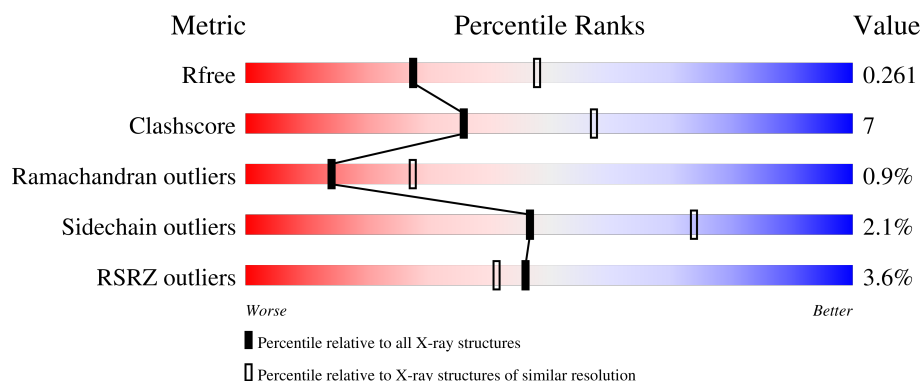
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

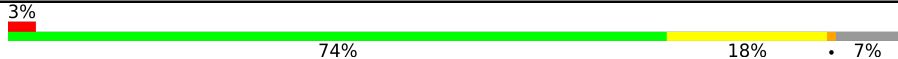
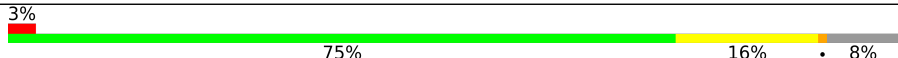
The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	620	
1	B	620	

2 Entry composition [i](#)

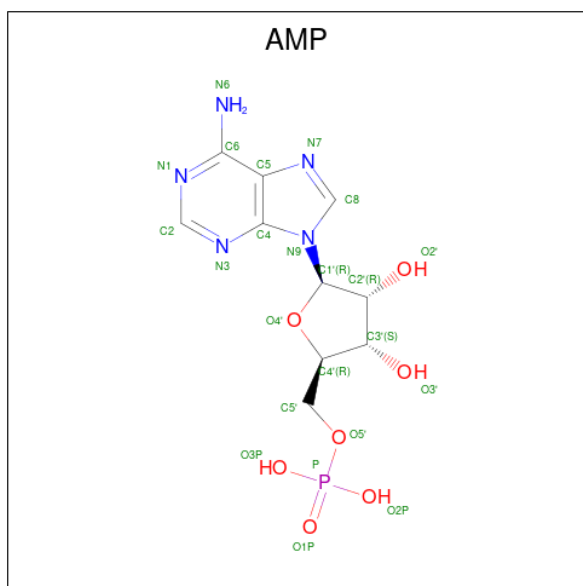
There are 4 unique types of molecules in this entry. The entry contains 9417 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACSD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	575	Total	C	N	O	S	0	2	0
			4623	2940	840	823	20			
1	B	570	Total	C	N	O	S	0	0	0
			4569	2908	830	811	20			

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	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		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

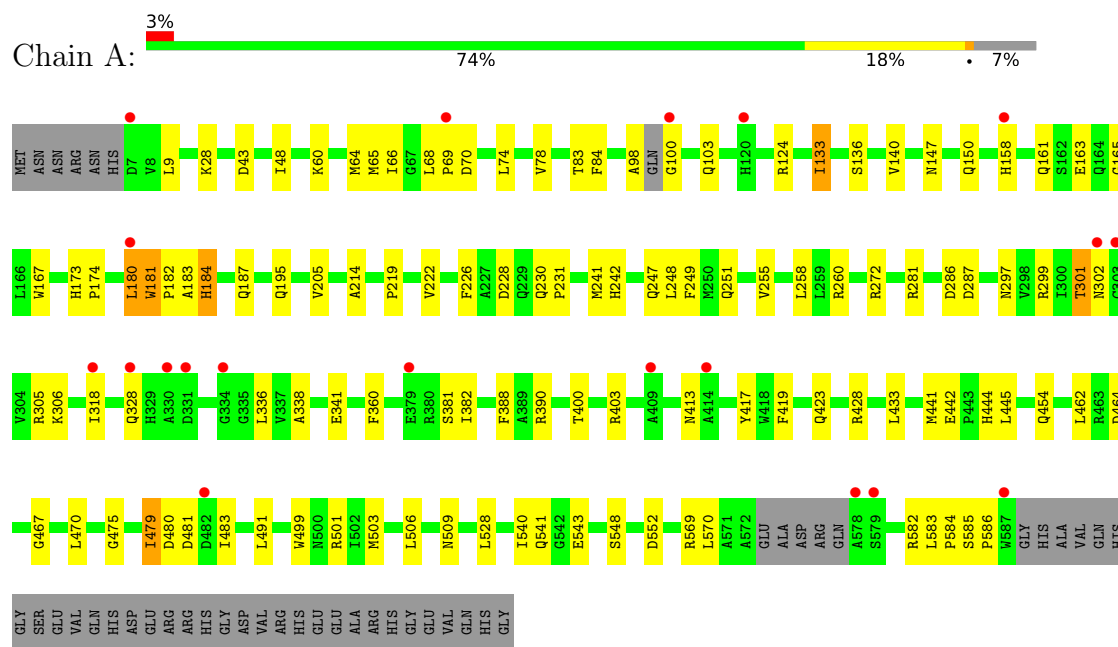
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total	O	0	0
			87	87		
4	B	82	Total	O	0	0
			82	82		

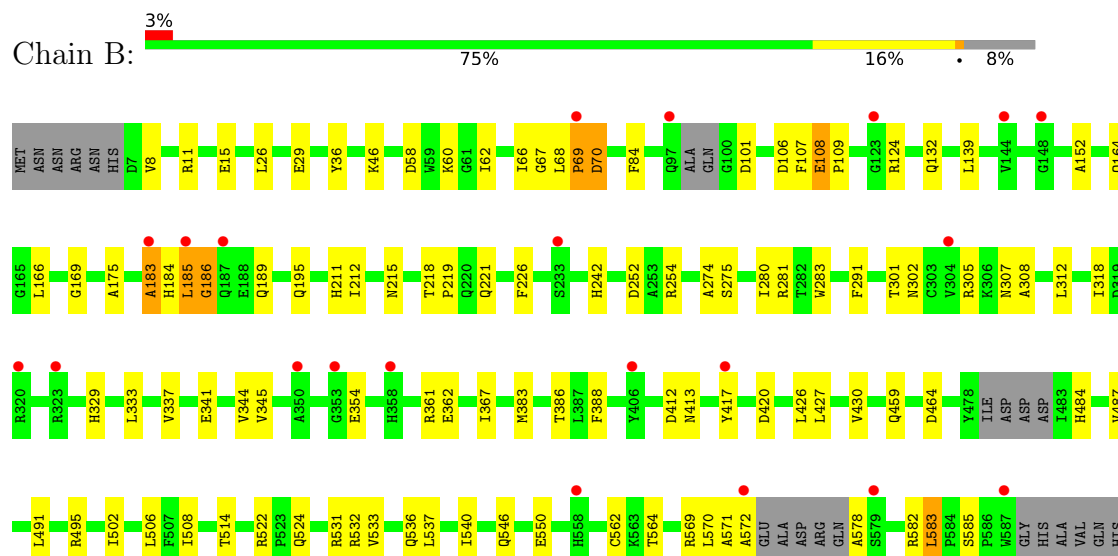
3 Residue-property plots [i](#)

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: ACSD



• Molecule 1: ACSD



GLY
SER
GLU
VAL
GLN
HIS
ASP
GLU
ARG
ARG
HIS
GLY
ASP
VAL
HIS
HIS
GLU
GLU
ALA
ARG
HIS
GLY
GLU
VAL
GLN
HIS
GLY

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.70Å 70.00Å 96.00Å 95.00° 101.90° 94.70°	Depositor
Resolution (Å)	39.66 – 2.50 39.66 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.6 (39.66-2.50) 96.6 (39.66-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.205 , 0.261 0.207 , 0.261	Depositor DCC
R_{free} test set	2469 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9417	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.39% 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, 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	0.91	5/4748 (0.1%)	1.04	13/6452 (0.2%)
1	B	0.90	1/4688 (0.0%)	1.06	18/6368 (0.3%)
All	All	0.91	6/9436 (0.1%)	1.05	31/12820 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	454	GLN	CD-OE1	6.18	1.35	1.23
1	A	195	GLN	CD-OE1	6.13	1.35	1.23
1	B	189	GLN	CD-OE1	5.64	1.34	1.23
1	A	328	GLN	CD-OE1	5.51	1.34	1.23
1	A	147	ASN	CG-ND2	-5.17	1.22	1.33
1	A	147	ASN	CG-OD1	5.00	1.33	1.23

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	445	LEU	N-CA-C	6.58	120.18	111.75
1	B	484	HIS	CA-C-N	6.11	126.28	119.32
1	B	484	HIS	C-N-CA	6.11	126.28	119.32
1	B	62	ILE	CB-CA-C	-6.08	104.23	110.13
1	B	8	VAL	N-CA-C	-6.08	104.58	110.72
1	A	48	ILE	CA-C-N	6.03	124.00	119.66
1	A	48	ILE	C-N-CA	6.03	124.00	119.66
1	B	108	GLU	CA-C-N	5.95	127.27	119.84
1	B	108	GLU	C-N-CA	5.95	127.27	119.84
1	B	291	PHE	N-CA-C	-5.88	102.61	110.55
1	B	341	GLU	CA-C-N	5.68	125.38	119.64
1	B	341	GLU	C-N-CA	5.68	125.38	119.64
1	A	341	GLU	CA-C-N	5.66	125.35	119.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	GLU	C-N-CA	5.66	125.35	119.64
1	B	583	LEU	CA-C-N	5.52	125.49	120.03
1	B	583	LEU	C-N-CA	5.52	125.49	120.03
1	A	241	MET	N-CA-C	5.44	116.67	108.46
1	B	275	SER	CA-C-N	-5.43	114.66	120.03
1	B	275	SER	C-N-CA	-5.43	114.66	120.03
1	A	205	VAL	N-CA-C	5.35	113.58	109.19
1	A	301	THR	CB-CA-C	-5.30	110.48	116.63
1	B	186	GLY	N-CA-C	5.24	119.46	112.65
1	A	133	ILE	N-CA-C	5.23	115.44	110.42
1	B	175	ALA	CA-C-N	5.20	124.82	119.05
1	B	175	ALA	C-N-CA	5.20	124.82	119.05
1	B	152	ALA	N-CA-C	5.20	117.68	111.71
1	B	487	VAL	N-CA-C	-5.17	105.67	110.53
1	A	43	ASP	N-CA-C	-5.08	106.86	113.16
1	A	548	SER	CA-C-N	-5.07	114.85	119.82
1	A	548	SER	C-N-CA	-5.07	114.85	119.82
1	A	28	LYS	N-CA-C	5.02	116.83	111.36

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	4623	0	4537	65	0
1	B	4569	0	4495	69	0
2	A	23	0	12	0	0
2	B	23	0	12	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	87	0	0	3	0
4	B	82	0	0	5	0
All	All	9417	0	9056	133	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 7.

All (133) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:HIS:CG	1:B:185:LEU:H	1.56	1.21
1:B:413:ASN:O	1:B:417:TYR:HD1	1.37	1.03
1:B:184:HIS:CD2	1:B:185:LEU:H	1.80	0.99
1:B:184:HIS:CG	1:B:185:LEU:N	2.29	0.94
1:B:301:THR:HG22	1:B:301:THR:O	1.73	0.88
1:B:124:ARG:HH11	1:B:572:ALA:HB2	1.38	0.87
1:B:413:ASN:O	1:B:417:TYR:CD1	2.29	0.83
1:A:467:GLY:O	1:A:501:ARG:NH1	2.17	0.78
1:B:184:HIS:CD2	1:B:185:LEU:N	2.50	0.78
1:B:420:ASP:OD1	1:B:532:ARG:HD3	1.84	0.77
1:A:180:LEU:HD22	1:A:299:ARG:HB3	1.66	0.76
1:B:218:THR:OG1	1:B:221:GLN:HG3	1.89	0.71
1:B:361:ARG:HD2	4:B:2049:HOH:O	1.89	0.71
1:B:108:GLU:HB2	1:B:109:PRO:CD	2.21	0.70
1:A:163:GLU:OE1	4:A:2017:HOH:O	2.12	0.68
1:A:480:ASP:O	1:A:483:ILE:HG12	1.95	0.66
1:B:68:LEU:O	1:B:70:ASP:OD1	2.13	0.65
1:B:546:GLN:O	4:B:2074:HOH:O	2.14	0.65
1:A:183:ALA:O	1:A:184:HIS:HB3	1.95	0.64
1:B:183:ALA:O	1:B:184:HIS:ND1	2.30	0.64
1:A:9:LEU:HD11	1:B:58:ASP:HA	1.80	0.63
1:A:441:MET:HE3	1:A:462:LEU:HD13	1.79	0.63
1:B:502:ILE:HG23	1:B:506:LEU:HD12	1.80	0.63
1:B:508:ILE:CD1	1:B:562:CYS:HB2	2.29	0.63
1:B:108:GLU:HB2	1:B:109:PRO:HD3	1.81	0.62
1:B:124:ARG:HB2	1:B:570:LEU:O	1.99	0.61
1:B:124:ARG:NH1	1:B:572:ALA:HB2	2.14	0.61
1:B:301:THR:O	1:B:301:THR:CG2	2.45	0.60
1:A:68:LEU:O	1:A:70:ASP:N	2.35	0.60
1:A:242:HIS:HB2	4:A:2048:HOH:O	2.02	0.59
1:A:318:ILE:HD11	1:A:491:LEU:HD21	1.83	0.59
1:B:124:ARG:HH11	1:B:572:ALA:CB	2.11	0.59
1:A:301:THR:HG22	1:A:302:ASN:H	1.68	0.58
1:B:226:PHE:CE2	1:B:345:VAL:HG12	2.38	0.58
1:A:413:ASN:O	1:A:417:TYR:HD2	1.88	0.57
1:B:166:LEU:HD22	1:B:383:MET:HE1	1.87	0.56
1:B:11:ARG:NH1	1:B:15:GLU:OE2	2.38	0.56
1:A:181:TRP:NE1	1:A:187:GLN:NE2	2.55	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:TRP:CD1	1:A:503:MET:HE2	2.42	0.54
1:B:426:LEU:O	1:B:430:VAL:HG23	2.07	0.54
1:A:158[A]:HIS:HB3	1:A:161:GLN:OE1	2.06	0.54
1:A:301:THR:HG22	1:A:302:ASN:N	2.23	0.54
1:A:173:HIS:NE2	1:A:301:THR:HG23	2.22	0.54
1:B:412:ASP:OD1	1:B:522:ARG:HD2	2.08	0.53
1:A:165:GLY:HA2	1:A:167:TRP:CZ3	2.43	0.53
1:A:470:LEU:HD12	1:A:479:ILE:HD11	1.89	0.53
1:B:508:ILE:HD13	1:B:562:CYS:HB2	1.90	0.53
1:A:297:ASN:OD1	1:A:306:LYS:HE3	2.08	0.52
1:B:495:ARG:NE	1:B:550:GLU:OE2	2.29	0.52
1:A:260:ARG:NH2	4:A:2044:HOH:O	2.42	0.52
1:B:252:ASP:OD1	1:B:254:ARG:HB2	2.09	0.51
1:A:336:LEU:HD22	1:A:433:LEU:HD11	1.92	0.51
1:B:166:LEU:HG	1:B:169:GLY:HA2	1.91	0.51
1:B:242:HIS:HB2	4:B:2032:HOH:O	2.10	0.51
1:A:64:MET:HG2	1:A:65:MET:N	2.27	0.49
1:A:214:ALA:HB2	1:A:222:VAL:HG21	1.94	0.49
1:B:106:ASP:HB2	1:B:109:PRO:HG2	1.94	0.49
1:B:11:ARG:O	1:B:15:GLU:HG3	2.13	0.49
1:B:533:VAL:O	1:B:537:LEU:HG	2.13	0.49
1:A:133:ILE:HG12	1:A:174:PRO:O	2.12	0.49
1:B:388:PHE:CE1	1:B:514:THR:HG23	2.48	0.48
1:A:173:HIS:NE2	1:A:301:THR:CG2	2.77	0.48
1:A:444:HIS:HB2	1:A:509:ASN:OD1	2.13	0.48
1:B:307:ASN:HB3	1:B:312:LEU:HD21	1.96	0.48
1:A:158[B]:HIS:HB2	1:A:161:GLN:OE1	2.14	0.47
1:A:181:TRP:CD1	1:A:187:GLN:NE2	2.82	0.47
1:A:124:ARG:HD3	1:A:570:LEU:O	2.13	0.47
1:A:428:ARG:HG2	1:A:540:ILE:HG12	1.95	0.47
1:B:578:ALA:N	4:B:2078:HOH:O	2.48	0.47
1:B:329:HIS:O	1:B:333:LEU:HG	2.14	0.46
1:B:571:ALA:HB3	1:B:578:ALA:HB2	1.97	0.46
1:A:181:TRP:HE1	1:A:187:GLN:NE2	2.13	0.46
1:B:427:LEU:HD23	1:B:506:LEU:HD22	1.98	0.46
1:B:26:LEU:C	1:B:26:LEU:HD23	2.40	0.46
1:B:84:PHE:HA	1:B:583:LEU:HD13	1.97	0.46
1:A:388:PHE:O	1:A:390:ARG:NH1	2.49	0.46
1:A:470:LEU:CD1	1:A:479:ILE:HD11	2.45	0.46
1:A:98:ALA:C	1:A:100:GLY:N	2.74	0.46
1:A:470:LEU:HD12	1:A:479:ILE:CD1	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:PHE:CZ	1:A:423:GLN:HG2	2.51	0.45
1:B:318:ILE:HD11	1:B:491:LEU:CD2	2.46	0.45
1:A:249:PHE:O	1:A:255:VAL:HG21	2.16	0.45
1:B:211:HIS:CE1	4:B:2049:HOH:O	2.70	0.45
1:A:228:ASP:O	1:A:231:PRO:HD2	2.17	0.45
1:B:344:VAL:HG22	1:B:367:ILE:HG12	1.99	0.45
1:B:305:ARG:NH2	2:B:1588:AMP:O3P	2.50	0.44
1:B:301:THR:O	1:B:302:ASN:HB3	2.17	0.44
1:B:184:HIS:C	1:B:186:GLY:H	2.25	0.44
1:A:258:LEU:HD11	1:A:360:PHE:CZ	2.53	0.44
1:B:388:PHE:CZ	1:B:514:THR:HG23	2.53	0.43
1:B:522:ARG:HG2	1:B:524:GLN:HE22	1.83	0.43
1:B:69:PRO:C	1:B:70:ASP:OD1	2.61	0.43
1:B:226:PHE:CE2	1:B:345:VAL:CG1	3.01	0.43
1:A:301:THR:CG2	1:A:302:ASN:H	2.30	0.43
1:A:181:TRP:CD1	1:A:187:GLN:HE21	2.36	0.43
1:B:274:ALA:HB1	1:B:283:TRP:HB3	2.00	0.43
1:A:338:ALA:HA	1:A:462:LEU:O	2.18	0.42
1:B:164:GLN:NE2	1:B:195:GLN:HA	2.34	0.42
1:A:470:LEU:HB3	1:A:475:GLY:C	2.45	0.42
1:B:139:LEU:HA	1:B:139:LEU:HD12	1.80	0.42
1:A:286:ASP:O	1:A:287:ASP:C	2.62	0.42
1:B:420:ASP:CG	1:B:532:ARG:HD3	2.43	0.42
1:A:64:MET:HE3	1:A:78:VAL:HG11	2.00	0.42
1:A:247:GLN:OE1	1:A:247:GLN:HA	2.19	0.42
1:B:337:VAL:HG21	1:B:459:GLN:HG2	2.01	0.42
1:A:442:GLU:HG2	1:A:442:GLU:O	2.20	0.42
1:B:46:LYS:HD3	1:B:101:ASP:OD1	2.20	0.42
1:A:84:PHE:CZ	1:A:586:PRO:HD3	2.54	0.42
1:B:29:GLU:HG2	1:B:564:THR:HG22	2.02	0.42
1:A:541:GLN:HE22	1:A:552:ASP:CG	2.28	0.41
1:B:106:ASP:O	1:B:107:PHE:C	2.63	0.41
1:B:536:GLN:O	1:B:540:ILE:HD12	2.20	0.41
1:A:226:PHE:C	1:A:272:ARG:NH2	2.78	0.41
1:A:381:SER:C	1:A:382:ILE:HG13	2.44	0.41
1:A:301:THR:HB	1:A:305:ARG:HH21	1.85	0.41
1:B:308:ALA:HA	1:B:362:GLU:HG3	2.03	0.41
1:A:248:LEU:O	1:A:251:GLN:HB2	2.20	0.41
1:B:132:GLN:OE1	1:B:569:ARG:NH2	2.53	0.41
1:A:136:SER:O	1:A:140:VAL:HG23	2.20	0.41
1:A:228:ASP:OD2	1:A:230:GLN:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LYS:HB3	1:A:60:LYS:HE2	1.90	0.41
1:A:68:LEU:HD23	1:A:68:LEU:HA	1.84	0.41
1:A:299:ARG:NH2	1:A:569:ARG:CZ	2.84	0.41
1:B:26:LEU:HD22	1:B:66:ILE:HD13	2.02	0.41
1:A:66:ILE:HD12	1:A:74:LEU:HD22	2.03	0.41
1:A:83:THR:HG21	1:A:585:SER:O	2.21	0.41
1:B:36:TYR:HB3	1:B:67:GLY:O	2.21	0.40
1:A:506:LEU:HD23	1:A:506:LEU:HA	1.88	0.40
1:A:583:LEU:HA	1:A:584:PRO:HD3	1.85	0.40
1:B:301:THR:O	1:B:302:ASN:CB	2.69	0.40
1:A:541:GLN:C	1:A:543:GLU:H	2.29	0.40
1:B:212:ILE:HG21	1:B:219:PRO:HA	2.02	0.40
1:A:543:GLU:O	1:A:543:GLU:HG2	2.21	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	571/620 (92%)	538 (94%)	29 (5%)	4 (1%)	18	34
1	B	562/620 (91%)	530 (94%)	26 (5%)	6 (1%)	11	22
All	All	1133/1240 (91%)	1068 (94%)	55 (5%)	10 (1%)	14	27

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	PRO
1	A	184	HIS
1	B	70	ASP
1	B	185	LEU
1	B	464	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	183	ALA
1	A	464	ASP
1	A	481	ASP
1	B	69	PRO
1	B	280	ILE

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	487/522 (93%)	475 (98%)	12 (2%)	42	69
1	B	481/522 (92%)	473 (98%)	8 (2%)	53	78
All	All	968/1044 (93%)	948 (98%)	20 (2%)	47	74

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	150	GLN
1	A	180	LEU
1	A	181	TRP
1	A	182	PRO
1	A	219	PRO
1	A	281	ARG
1	A	400	THR
1	A	403	ARG
1	A	479	ILE
1	A	528	LEU
1	A	582	ARG
1	B	60	LYS
1	B	215	ASN
1	B	281	ARG
1	B	354	GLU
1	B	386	THR
1	B	531	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	582	ARG
1	B	585	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	150	GLN
1	A	202	GLN
1	A	269	GLN
1	A	500	ASN
1	A	536	GLN
1	B	164	GLN
1	B	195	GLN
1	B	202	GLN
1	B	329	HIS
1	B	363	GLN
1	B	395	GLN
1	B	453	GLN
1	B	458	GLN
1	B	500	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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	SO4	A	1589	-	4,4,4	0.30	0	6,6,6	0.68	0
3	SO4	B	1589	-	4,4,4	0.21	0	6,6,6	0.39	0
2	AMP	A	1588	-	25,25,25	1.39	3 (12%)	37,38,38	2.29	11 (29%)
2	AMP	B	1588	-	25,25,25	1.48	4 (16%)	37,38,38	2.07	10 (27%)

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	A	1588	-	-	5/10/26/26	0/3/3/3
2	AMP	B	1588	-	-	4/10/26/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1588	AMP	C5-C4	5.00	1.48	1.39
2	A	1588	AMP	C5-C4	4.10	1.46	1.39
2	A	1588	AMP	C5-N7	-3.00	1.33	1.39
2	B	1588	AMP	C8-N7	2.49	1.36	1.31
2	B	1588	AMP	C5-N7	-2.43	1.34	1.39
2	B	1588	AMP	C5-C6	2.40	1.47	1.41
2	A	1588	AMP	C8-N9	-2.11	1.33	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1588	AMP	C5-C4-N3	-6.24	118.12	126.72
2	B	1588	AMP	C5-C4-N3	-5.78	118.75	126.72
2	A	1588	AMP	N3-C4-N9	5.53	136.58	127.17
2	A	1588	AMP	N3-C2-N1	-4.57	121.66	128.58
2	B	1588	AMP	N3-C2-N1	-4.46	121.84	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1588	AMP	N3-C4-N9	4.32	134.52	127.17
2	A	1588	AMP	C2-N3-C4	4.04	121.70	111.83
2	B	1588	AMP	C2-N3-C4	4.03	121.67	111.83
2	B	1588	AMP	C4-C5-N7	-3.61	106.46	110.58
2	A	1588	AMP	C4-N9-C8	3.49	109.40	105.74
2	A	1588	AMP	C4-C5-N7	-3.38	106.72	110.58
2	A	1588	AMP	C5-N7-C8	3.27	108.59	103.45
2	B	1588	AMP	C2-N1-C6	3.06	123.76	118.73
2	A	1588	AMP	N9-C8-N7	-2.80	109.96	113.94
2	B	1588	AMP	O4'-C1'-N9	2.79	113.45	108.09
2	A	1588	AMP	C2-N1-C6	2.75	123.25	118.73
2	A	1588	AMP	O5'-P-O1P	-2.63	99.32	106.44
2	B	1588	AMP	C6-C5-N7	2.36	136.65	132.09
2	B	1588	AMP	C5-N7-C8	2.29	107.05	103.45
2	B	1588	AMP	O3P-P-O2P	2.25	116.25	107.80
2	A	1588	AMP	N6-C6-N1	2.10	123.06	118.38

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1588	AMP	C5'-O5'-P-O2P
2	A	1588	AMP	C5'-O5'-P-O3P
2	B	1588	AMP	C5'-O5'-P-O1P
2	A	1588	AMP	O4'-C4'-C5'-O5'
2	A	1588	AMP	C3'-C4'-C5'-O5'
2	B	1588	AMP	C5'-O5'-P-O3P
2	A	1588	AMP	C5'-O5'-P-O1P
2	B	1588	AMP	C5'-O5'-P-O2P
2	B	1588	AMP	O4'-C1'-N9-C8

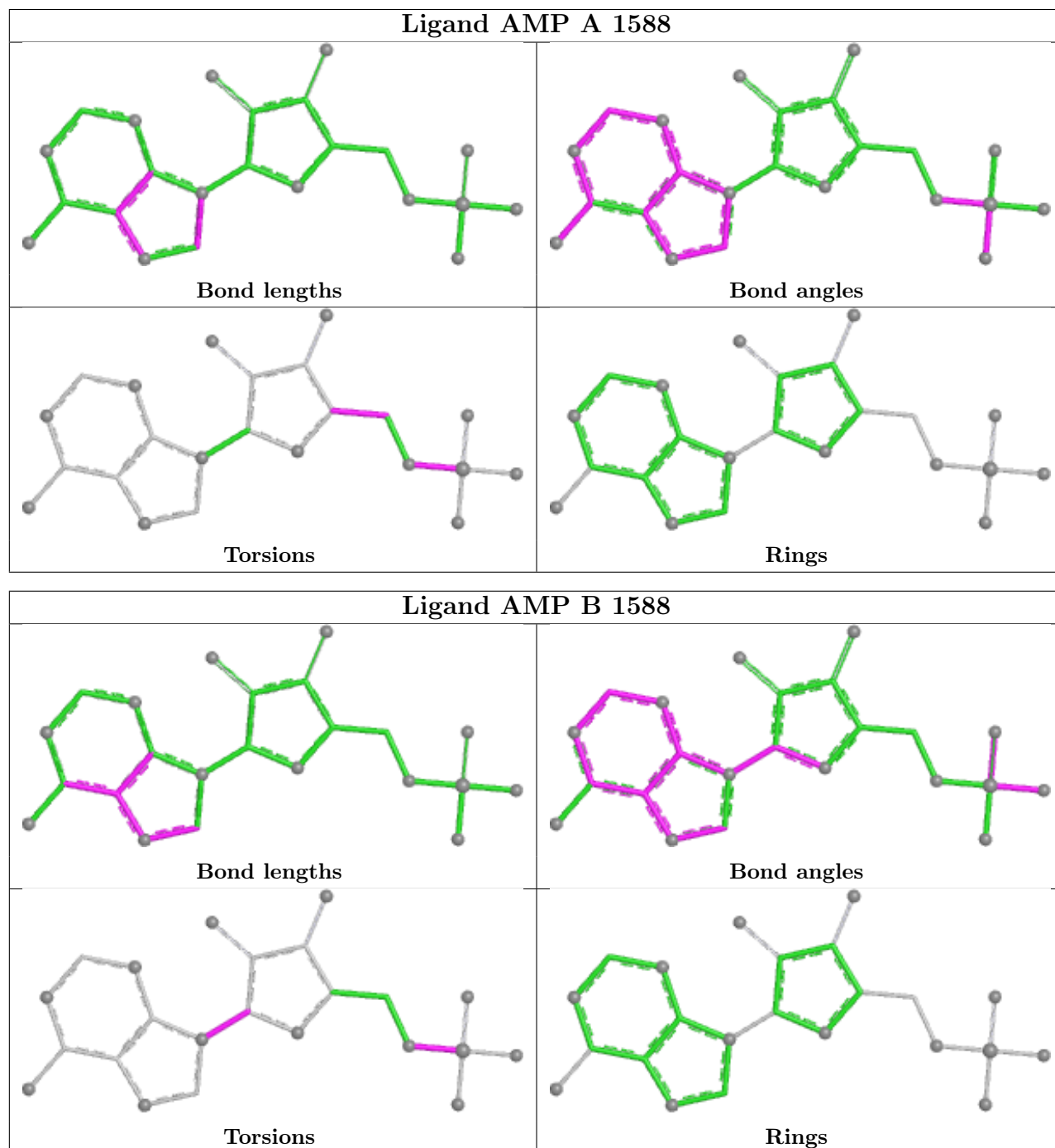
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1588	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

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	575/620 (92%)	0.43	20 (3%)	47 42	26, 47, 66, 75	2 (0%)
1	B	570/620 (91%)	0.37	21 (3%)	45 40	19, 46, 66, 80	2 (0%)
All	All	1145/1240 (92%)	0.40	41 (3%)	46 41	19, 47, 66, 80	4 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	144	VAL	7.3
1	A	120[A]	HIS	7.0
1	B	304	VAL	6.1
1	A	69	PRO	3.7
1	A	482	ASP	3.1
1	B	353	GLY	3.0
1	A	303	CYS	3.0
1	B	417	TYR	3.0
1	B	69	PRO	2.8
1	B	97	GLN	2.7
1	B	187	GLN	2.6
1	A	334	GLY	2.5
1	A	7	ASP	2.4
1	A	302	ASN	2.4
1	B	323	ARG	2.3
1	B	579	SER	2.3
1	B	406	TYR	2.3
1	A	158[A]	HIS	2.3
1	B	185	LEU	2.3
1	B	320	ARG	2.2
1	A	414	ALA	2.2
1	B	558	HIS	2.2
1	A	180	LEU	2.2
1	A	331	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	587	TRP	2.2
1	B	587	TRP	2.2
1	A	318	ILE	2.2
1	A	409	ALA	2.1
1	B	572	ALA	2.1
1	A	330	ALA	2.1
1	A	100	GLY	2.1
1	A	379	GLU	2.1
1	B	358	HIS	2.1
1	A	578	ALA	2.1
1	A	328	GLN	2.0
1	B	183	ALA	2.0
1	B	350	ALA	2.0
1	B	123	GLY	2.0
1	B	148	GLY	2.0
1	A	579	SER	2.0
1	B	233	SER	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.

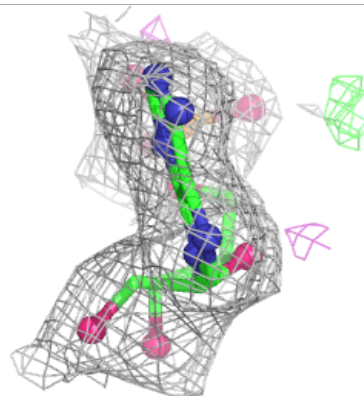
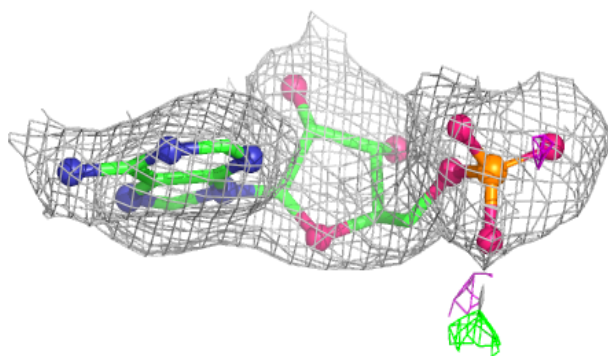
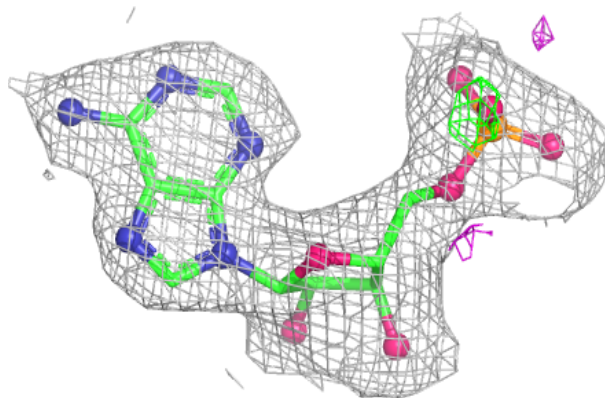
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AMP	A	1588	23/23	0.95	0.09	41,44,51,55	0
2	AMP	B	1588	23/23	0.95	0.08	48,52,57,58	0
3	SO4	B	1589	5/5	0.96	0.11	42,43,47,48	0
3	SO4	A	1589	5/5	0.97	0.08	45,46,51,51	0

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.

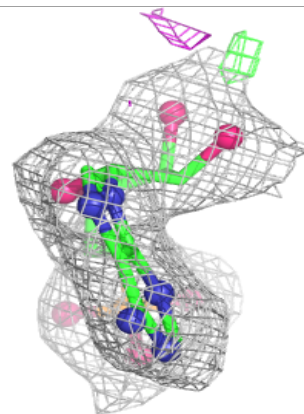
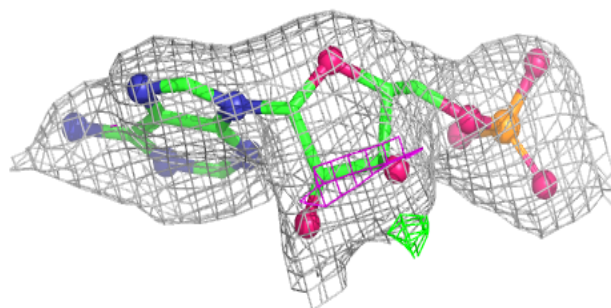
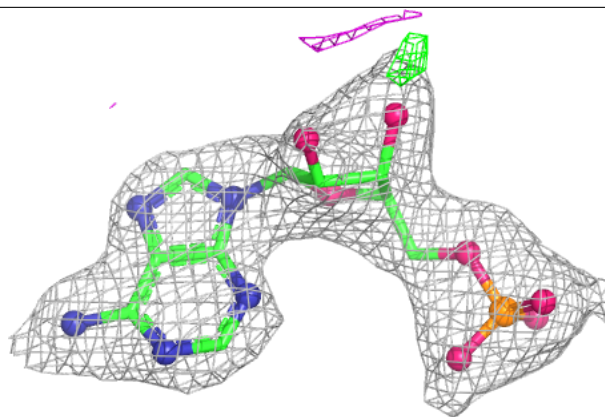
Electron density around AMP A 1588:

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



Electron density around AMP B 1588:

$2mF_o-DF_c$ (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.