Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 12:58 PM EDT

PDB ID	:	5SVB
Title	:	Mechanism of ATP-Dependent Acetone Carboxylation, Acetone Carboxylase AMP bound structure
Authors	:	Eilers, B.J.; Mus, F.; Alleman, A.B.; Kabasakal, B.V.; Murray, J.W.; Nocek, B.P.; Dubois, J.L.; Peters, J.W.
Deposited on	:	2016-08-05
Resolution	:	2.65 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 (i) 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 (i)) were used in the production of this report:

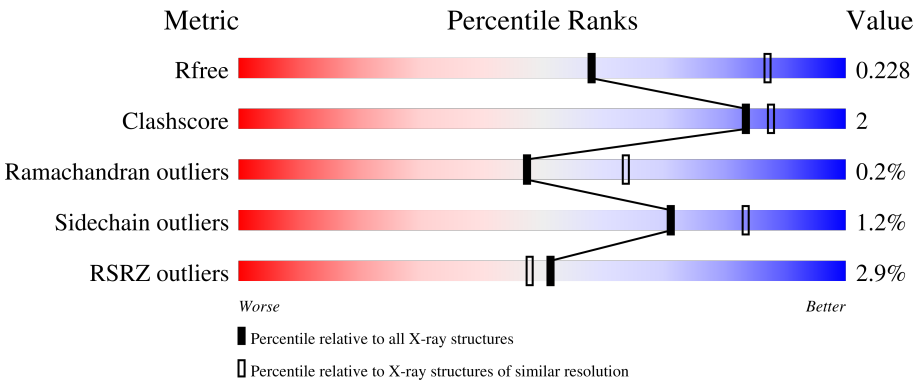
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 <=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	776	3% 87% 8% • •
1	D	776	4% 90% 5% • •
2	B	727	% 91% 6% •
2	E	727	3% 93% • •

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Mol	Chain	Length	Quality of chain
3	C	168	2% 93% 7%
3	F	168	4% 90% 8%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 50423 atoms, of which 24643 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 Acetone carboxylase alpha subunit.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S	Se			
1	A	746	11512	3712	5635	1032	1100	8	25	0	0	0
1	D	747	11516	3718	5633	1033	1099	8	25	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP Q8RM03
D	1	MSE	-	initiating methionine	UNP Q8RM03

- Molecule 2 is a protein called Acetone carboxylase beta subunit.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S	Se			
2	B	707	10806	3434	5353	950	1045	6	18	0	0	0
2	E	707	10767	3426	5328	945	1044	6	18	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MSE	-	initiating methionine	UNP Q8RM04
B	-8	HIS	-	expression tag	UNP Q8RM04
B	-7	HIS	-	expression tag	UNP Q8RM04
B	-6	HIS	-	expression tag	UNP Q8RM04
B	-5	HIS	-	expression tag	UNP Q8RM04
B	-4	HIS	-	expression tag	UNP Q8RM04
B	-3	HIS	-	expression tag	UNP Q8RM04
B	-2	SER	-	expression tag	UNP Q8RM04
B	-1	SER	-	expression tag	UNP Q8RM04
B	0	GLY	-	expression tag	UNP Q8RM04

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MSE	-	expression tag	UNP Q8RM04
E	-9	MSE	-	initiating methionine	UNP Q8RM04
E	-8	HIS	-	expression tag	UNP Q8RM04
E	-7	HIS	-	expression tag	UNP Q8RM04
E	-6	HIS	-	expression tag	UNP Q8RM04
E	-5	HIS	-	expression tag	UNP Q8RM04
E	-4	HIS	-	expression tag	UNP Q8RM04
E	-3	HIS	-	expression tag	UNP Q8RM04
E	-2	SER	-	expression tag	UNP Q8RM04
E	-1	SER	-	expression tag	UNP Q8RM04
E	0	GLY	-	expression tag	UNP Q8RM04
E	1	MSE	-	expression tag	UNP Q8RM04

- Molecule 3 is a protein called Acetone carboxylase gamma subunit.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S	Se			
3	C	167	2726	895	1342	230	250	5	4	0	0	0
			Total	C	H	N	O	S	Se			
3	F	165	2696	886	1329	228	244	5	4	0	0	0

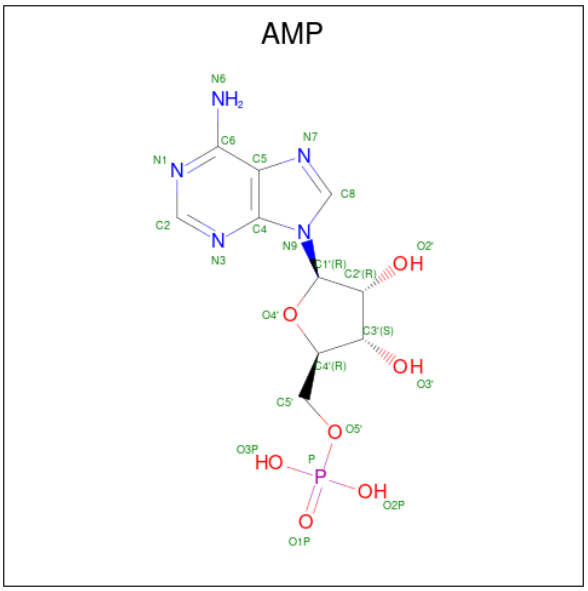
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MSE	-	initiating methionine	UNP Q8RM02
F	1	MSE	-	initiating methionine	UNP Q8RM02

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

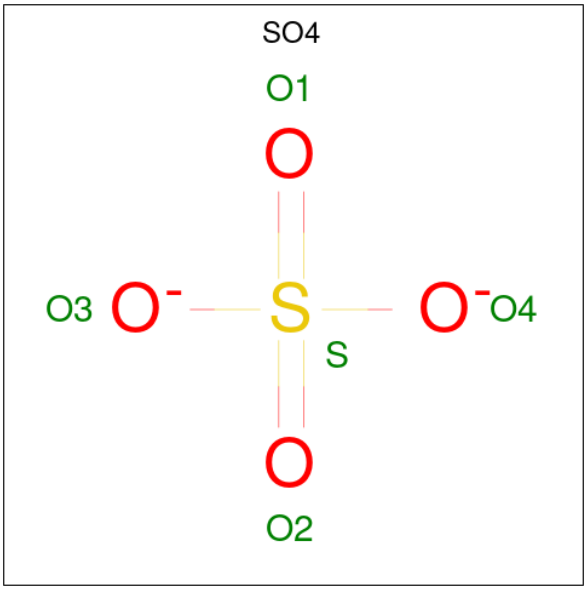
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
4	A	1	1	1	0	0
			Total	Mn		
4	D	1	1	1	0	0

- Molecule 5 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
5	B	1	34	10	11	5	7	1	0	0
			Total	C	H	N	O	P		
5	E	1	35	10	12	5	7	1	0	0

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



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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
7	C	1	1	1	0	0
7	F	1	1	1	0	0

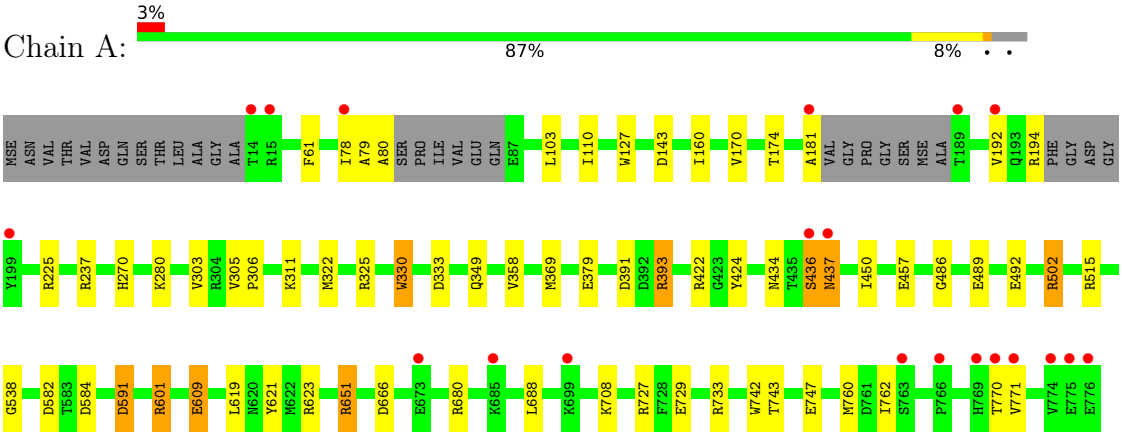
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	84	84	84	0	0
8	B	74	74	74	0	0
8	C	19	19	19	0	0
8	D	86	86	86	0	0
8	E	44	44	44	0	0
8	F	10	10	10	0	0

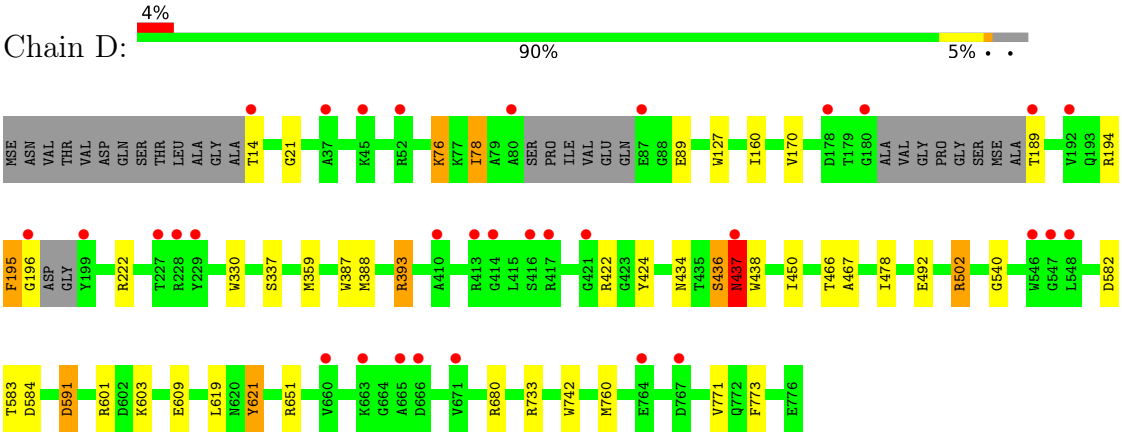
3 Residue-property plots (i)

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.

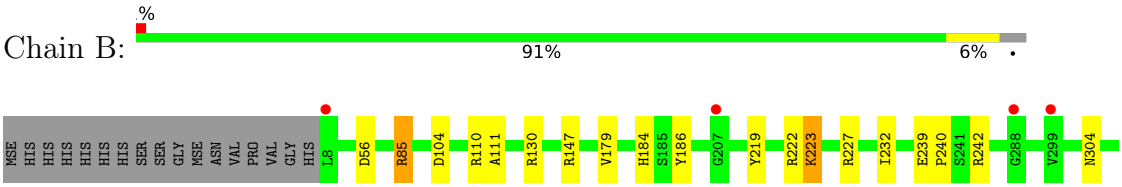
• Molecule 1: Acetone carboxylase alpha subunit

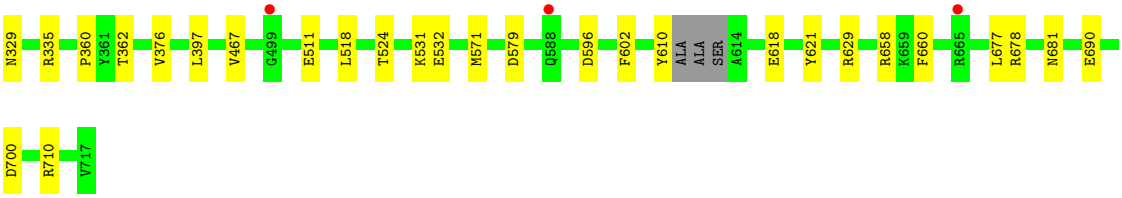


• Molecule 1: Acetone carboxylase alpha subunit



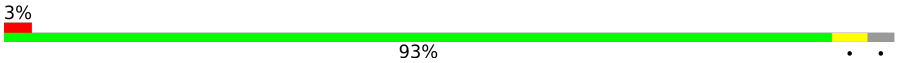
• Molecule 2: Acetone carboxylase beta subunit

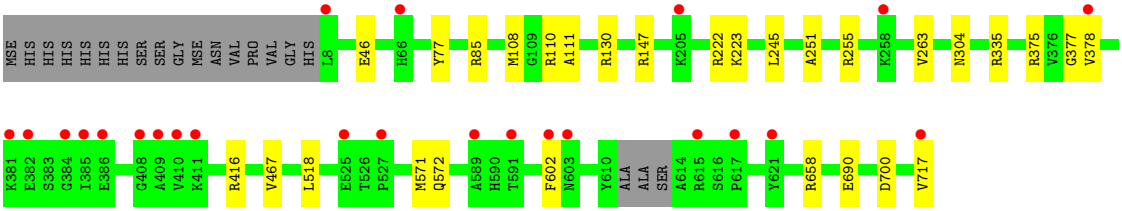




• Molecule 2: Acetone carboxylase beta subunit

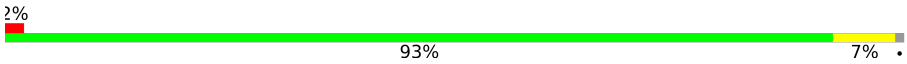
Chain E:

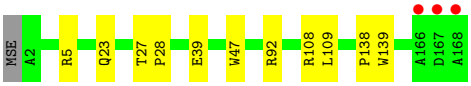




• Molecule 3: Acetone carboxylase gamma subunit

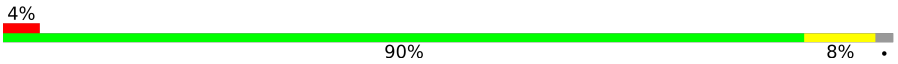
Chain C:

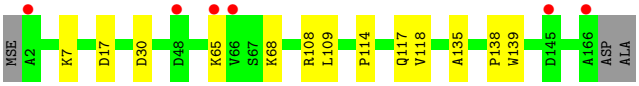




• Molecule 3: Acetone carboxylase gamma subunit

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.93Å 100.21Å 441.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.62 – 2.65 39.62 – 2.65	Depositor EDS
% Data completeness (in resolution range)	95.7 (39.62-2.65) 95.7 (39.62-2.65)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.93 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.198 , 0.227 0.200 , 0.228	Depositor DCC
R_{free} test set	5667 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	43.2	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 37.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	50423	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, MN, ZN, SO4

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	0.27	0/5999	0.44	0/8083
1	D	0.26	0/6006	0.43	0/8092
2	B	0.27	0/5549	0.44	0/7492
2	E	0.25	0/5535	0.43	0/7476
3	C	0.26	0/1427	0.41	0/1942
3	F	0.25	0/1410	0.41	0/1919
All	All	0.26	0/25926	0.43	0/35004

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	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	436	SER	Peptide
1	D	436	SER	Peptide

5.2 Too-close contacts (i)

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	5877	5635	5640	45	0
1	D	5883	5633	5643	30	0
2	B	5453	5353	5364	29	0
2	E	5439	5328	5336	16	0
3	C	1384	1342	1342	7	0
3	F	1367	1329	1329	8	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	B	23	11	12	0	0
5	E	23	12	12	0	0
6	B	5	0	0	0	0
6	E	5	0	0	0	0
7	C	1	0	0	0	0
7	F	1	0	0	0	0
8	A	84	0	0	2	0
8	B	74	0	0	2	0
8	C	19	0	0	0	0
8	D	86	0	0	2	0
8	E	44	0	0	0	0
8	F	10	0	0	0	0
All	All	25780	24643	24678	120	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 2.

All (120) 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:D:733:ARG:NH2	1:D:742:TRP:O	2.07	0.88
2:E:658:ARG:NH1	2:E:690:GLU:OE2	2.09	0.85
2:E:222:ARG:NH1	2:E:518:LEU:O	2.10	0.83
1:A:225:ARG:O	1:D:393:ARG:NH2	2.13	0.82
2:B:531:LYS:NZ	2:B:596:ASP:OD1	2.12	0.82
1:A:733:ARG:NH2	1:A:742:TRP:O	2.15	0.79
2:B:222:ARG:NH2	2:B:518:LEU:O	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:130:ARG:O	2:E:335:ARG:NH2	2.20	0.75
1:A:688:LEU:O	3:C:92:ARG:NH1	2.20	0.75
2:B:677:LEU:O	2:B:710:ARG:NH2	2.20	0.74
2:B:104:ASP:OD2	8:B:901:HOH:O	2.06	0.73
2:B:56:ASP:OD1	8:B:902:HOH:O	2.08	0.72
3:F:65:LYS:O	3:F:68:LYS:NZ	2.23	0.71
1:A:61:PHE:CZ	1:A:369:MSE:HG2	2.26	0.70
1:A:708:LYS:NZ	1:A:743:THR:O	2.20	0.70
1:D:583:THR:O	8:D:901:HOH:O	2.10	0.69
1:A:609:GLU:N	1:A:609:GLU:OE1	2.26	0.68
1:A:729:GLU:OE2	1:A:733:ARG:NH1	2.27	0.67
3:F:7:LYS:NZ	3:F:17:ASP:OD1	2.28	0.66
1:A:619:LEU:O	8:A:901:HOH:O	2.15	0.65
1:A:515:ARG:NH2	8:A:903:HOH:O	2.30	0.64
2:E:378:VAL:O	2:E:416:ARG:NH1	2.32	0.64
1:A:457:GLU:OE2	1:A:502:ARG:NH1	2.30	0.63
1:A:303:VAL:O	1:A:311:LYS:NZ	2.34	0.61
1:A:492:GLU:OE2	2:B:147:ARG:NH2	2.33	0.61
1:A:584:ASP:OD2	1:A:651:ARG:NH2	2.34	0.60
2:B:222:ARG:O	2:B:223:LYS:HB2	2.01	0.60
1:D:603:LYS:NZ	3:F:109:LEU:O	2.33	0.60
2:E:251:ALA:O	2:E:255:ARG:NH2	2.36	0.59
1:A:61:PHE:CE2	1:A:103:LEU:HD21	2.39	0.58
2:B:130:ARG:O	2:B:335:ARG:NH2	2.37	0.57
1:D:492:GLU:OE2	2:E:147:ARG:NH2	2.38	0.57
1:A:181:ALA:HA	1:D:195:PHE:O	2.05	0.56
1:A:369:MSE:SE	2:B:362:THR:HG21	2.55	0.56
1:A:79:ALA:O	1:A:80:ALA:CB	2.53	0.55
1:D:387:TRP:CE2	1:D:388:MSE:HE2	2.42	0.54
1:A:78:ILE:HG22	1:A:78:ILE:O	2.08	0.54
1:A:486:GLY:O	1:A:502:ARG:NH2	2.41	0.54
1:D:591:ASP:OD1	1:D:601:ARG:NH1	2.41	0.54
1:A:489:GLU:OE2	2:B:227:ARG:NH2	2.34	0.53
1:D:502:ARG:HG2	2:E:108:MSE:HE1	1.91	0.53
3:C:23:GLN:O	3:C:27:THR:HG22	2.09	0.53
2:B:579:ASP:OD1	2:B:610:TYR:OH	2.27	0.52
2:E:46:GLU:OE2	2:E:77:TYR:OH	2.24	0.52
1:A:325:ARG:NH2	1:A:379:GLU:OE2	2.43	0.52
1:A:436:SER:OG	1:A:623:ARG:HG3	2.09	0.52
2:B:360:PRO:HG3	3:C:28:PRO:HB3	1.91	0.52
1:D:584:ASP:OD2	1:D:651:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:27:THR:OG1	3:C:28:PRO:HD2	2.11	0.50
2:B:524:THR:OG1	2:B:618:GLU:O	2.28	0.50
1:A:280:LYS:O	1:A:422:ARG:NH2	2.42	0.50
2:B:571:MSE:HE2	2:B:602:PHE:CG	2.47	0.50
1:A:143:ASP:OD2	1:D:222:ARG:NE	2.46	0.49
1:A:436:SER:HB2	1:A:538:GLY:HA3	1.93	0.49
1:A:591:ASP:OD1	1:A:601:ARG:NH1	2.46	0.48
1:A:666:ASP:N	1:A:666:ASP:OD1	2.46	0.48
1:D:434:ASN:OD1	1:D:436:SER:HB3	2.13	0.48
1:A:770:THR:HG22	1:A:771:VAL:N	2.29	0.48
1:D:619:LEU:O	8:D:902:HOH:O	2.19	0.48
3:C:5:ARG:NH2	3:C:39:GLU:OE1	2.36	0.47
3:F:108:ARG:O	3:F:109:LEU:HB2	2.15	0.47
2:B:239:GLU:OE1	2:B:242:ARG:NH1	2.46	0.47
3:F:138:PRO:O	3:F:139:TRP:HB2	2.14	0.47
1:A:391:ASP:HA	1:A:762:ILE:CD1	2.45	0.46
1:A:393:ARG:HB2	1:A:760:MSE:HE2	1.96	0.46
2:B:304:ASN:O	2:B:467:VAL:HG22	2.15	0.46
1:A:333:ASP:OD2	1:A:727:ARG:NH2	2.48	0.46
3:C:138:PRO:O	3:C:139:TRP:HB2	2.16	0.46
3:C:108:ARG:O	3:C:109:LEU:HB2	2.16	0.46
1:D:76:LYS:O	1:D:78:ILE:N	2.45	0.46
1:D:189:THR:HG22	1:D:609:GLU:CD	2.37	0.45
1:A:760:MSE:HG2	1:D:450:ILE:HD11	1.97	0.45
2:B:219:TYR:O	2:B:227:ARG:HG3	2.17	0.45
2:E:717:VAL:HG23	2:E:717:VAL:O	2.17	0.45
1:A:160:ILE:HD11	1:A:170:VAL:HG22	1.99	0.44
1:D:466:THR:HG22	1:D:467:ALA:N	2.32	0.44
2:E:700:ASP:OD1	2:E:700:ASP:N	2.50	0.44
1:A:582:ASP:OD2	1:A:601:ARG:NH2	2.50	0.44
2:B:678:ARG:N	2:B:681:ASN:OD1	2.37	0.44
1:D:160:ILE:HD11	1:D:170:VAL:HG22	2.00	0.44
1:A:322:MSE:HE3	1:A:330:TRP:CE3	2.52	0.44
1:D:582:ASP:OD2	1:D:601:ARG:NH2	2.51	0.44
2:B:658:ARG:NH1	2:B:690:GLU:OE2	2.46	0.43
1:A:110:ILE:CG2	1:A:358:VAL:HG21	2.49	0.43
1:A:110:ILE:HG23	1:A:358:VAL:HG21	2.00	0.42
1:A:306:PRO:HB2	1:D:189:THR:OG1	2.19	0.42
1:D:337:SER:HB3	1:D:388:MSE:HE1	2.01	0.42
2:E:110:ARG:O	2:E:111:ALA:HB3	2.19	0.42
2:E:245:LEU:CD2	2:E:263:VAL:HG11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:304:ASN:O	2:E:467:VAL:HG22	2.19	0.42
1:A:192:VAL:CG1	1:A:305:VAL:CG2	2.98	0.42
2:E:375:ARG:O	2:E:377:GLY:N	2.53	0.42
1:A:422:ARG:HG2	1:A:424:TYR:CE2	2.55	0.42
2:B:571:MSE:HE3	2:B:621:TYR:CD1	2.54	0.42
2:B:110:ARG:O	2:B:111:ALA:HB3	2.19	0.42
2:B:700:ASP:N	2:B:700:ASP:OD1	2.52	0.42
3:F:114:PRO:HA	3:F:117:GLN:O	2.19	0.42
2:B:571:MSE:HE2	2:B:602:PHE:CD2	2.54	0.42
1:D:78:ILE:HG22	1:D:78:ILE:O	2.20	0.42
1:D:422:ARG:HG2	1:D:424:TYR:CE2	2.54	0.42
2:E:571:MSE:HE2	2:E:602:PHE:CG	2.55	0.42
2:B:511:GLU:OE2	2:B:629:ARG:NE	2.51	0.41
1:D:437:ASN:HB2	1:D:621:TYR:O	2.21	0.41
1:A:174:THR:OG1	1:A:237:ARG:NH1	2.49	0.41
2:B:179:VAL:HG21	2:B:232:ILE:HA	2.01	0.41
2:B:184:HIS:HA	2:B:186:TYR:CE2	2.55	0.41
1:D:337:SER:CB	1:D:388:MSE:HE1	2.50	0.41
2:E:222:ARG:O	2:E:223:LYS:HB2	2.21	0.41
3:F:30:ASP:OD1	3:F:30:ASP:N	2.49	0.41
1:A:192:VAL:HG11	1:A:305:VAL:CG2	2.50	0.41
1:A:434:ASN:OD1	1:A:436:SER:HB3	2.20	0.41
2:B:397:LEU:O	2:B:660:PHE:HA	2.21	0.41
1:D:359:MSE:CG	1:D:478:ILE:HD11	2.51	0.41
1:D:194:ARG:C	1:D:196:GLY:H	2.25	0.40
1:A:270:HIS:CE1	2:B:362:THR:CG2	3.05	0.40
2:B:85:ARG:HD2	2:B:240:PRO:HB2	2.03	0.40
1:A:450:ILE:HD11	1:D:760:MSE:HG2	2.04	0.40
1:D:14:THR:HB	1:D:21:GLY:HA2	2.03	0.40
1:D:771:VAL:HG23	1:D:773:PHE:CE2	2.56	0.40
3:F:118:VAL:O	3:F:135:ALA:HA	2.22	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	738/776 (95%)	709 (96%)	28 (4%)	1 (0%)	51	69
1	D	739/776 (95%)	708 (96%)	27 (4%)	4 (0%)	29	43
2	B	703/727 (97%)	685 (97%)	16 (2%)	2 (0%)	41	56
2	E	703/727 (97%)	682 (97%)	21 (3%)	0	100	100
3	C	165/168 (98%)	158 (96%)	7 (4%)	0	100	100
3	F	163/168 (97%)	154 (94%)	9 (6%)	0	100	100
All	All	3211/3342 (96%)	3096 (96%)	108 (3%)	7 (0%)	47	64

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	437	ASN
1	D	437	ASN
2	B	223	LYS
1	D	195	PHE
1	D	78	ILE
2	B	376	VAL
1	D	540	GLY

5.3.2 Protein sidechains (i)

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	600/595 (101%)	586 (98%)	14 (2%)	50	68
1	D	600/595 (101%)	589 (98%)	11 (2%)	59	75
2	B	572/569 (100%)	569 (100%)	3 (0%)	88	94
2	E	569/569 (100%)	567 (100%)	2 (0%)	91	95
3	C	155/151 (103%)	154 (99%)	1 (1%)	86	93
3	F	153/151 (101%)	153 (100%)	0	100	100
All	All	2649/2630 (101%)	2618 (99%)	31 (1%)	71	83

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	TRP
1	A	194	ARG
1	A	330	TRP
1	A	349	GLN
1	A	393	ARG
1	A	437	ASN
1	A	502	ARG
1	A	591	ASP
1	A	601	ARG
1	A	609	GLU
1	A	621	TYR
1	A	651	ARG
1	A	680	ARG
1	A	747	GLU
2	B	85	ARG
2	B	329	ASN
2	B	532	GLU
3	C	47	TRP
1	D	76	LYS
1	D	89	GLU
1	D	127	TRP
1	D	330	TRP
1	D	393	ARG
1	D	437	ASN
1	D	438	TRP
1	D	502	ARG
1	D	591	ASP
1	D	621	TYR
1	D	680	ARG
2	E	85	ARG
2	E	572	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	SO4	B	802	-	4,4,4	0.14	0	6,6,6	0.04	0
6	SO4	E	802	-	4,4,4	0.14	0	6,6,6	0.05	0
5	AMP	E	801	-	22,25,25	1.16	2 (9%)	25,38,38	3.36	4 (16%)
5	AMP	B	801	-	22,25,25	1.16	2 (9%)	25,38,38	3.29	4 (16%)

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
5	AMP	E	801	-	-	0/6/26/26	0/3/3/3
5	AMP	B	801	-	-	0/6/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	801	AMP	C5-C4	-2.96	1.33	1.40
5	E	801	AMP	C5-C4	-2.86	1.33	1.40
5	E	801	AMP	C6-N6	2.73	1.44	1.34
5	B	801	AMP	C6-N6	2.65	1.43	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	801	AMP	C1'-N9-C4	10.57	145.22	126.64
5	B	801	AMP	C1'-N9-C4	9.81	143.87	126.64
5	B	801	AMP	C5-C6-N6	9.34	134.55	120.35
5	E	801	AMP	C5-C6-N6	9.28	134.46	120.35
5	E	801	AMP	N6-C6-N1	-6.31	105.47	118.57
5	B	801	AMP	N6-C6-N1	-6.28	105.54	118.57
5	B	801	AMP	N3-C2-N1	-5.95	119.37	128.68
5	E	801	AMP	N3-C2-N1	-5.71	119.75	128.68

There are no chirality outliers.

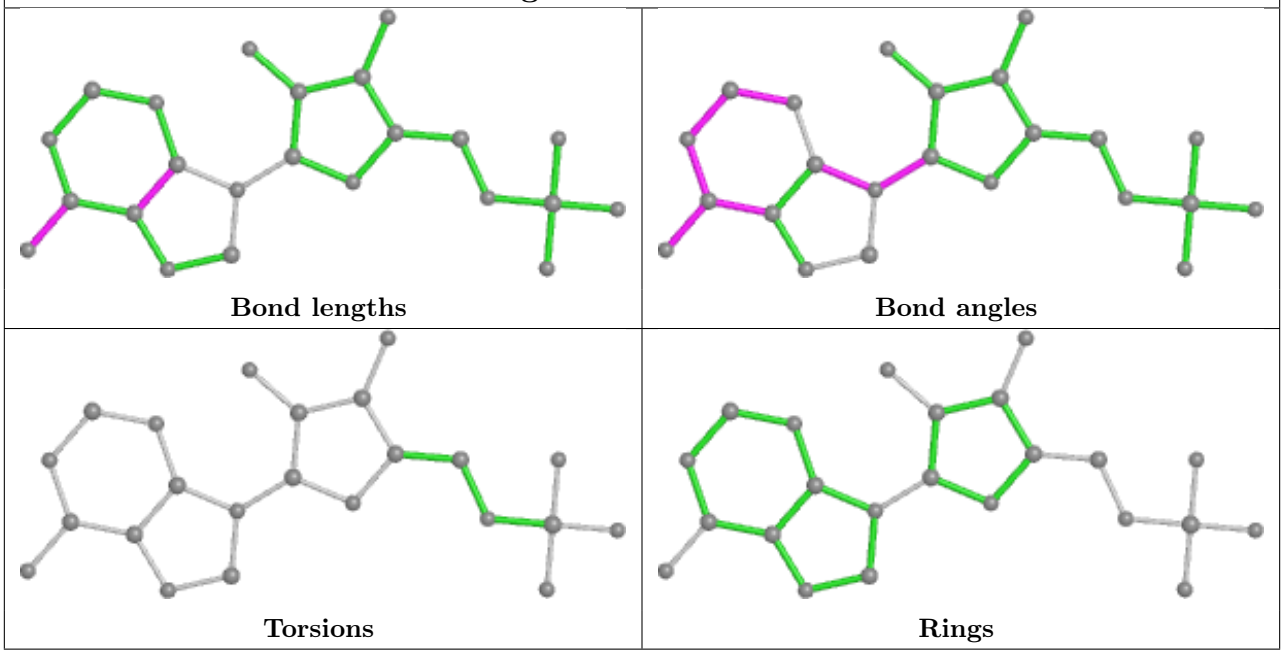
There are no torsion outliers.

There are no ring outliers.

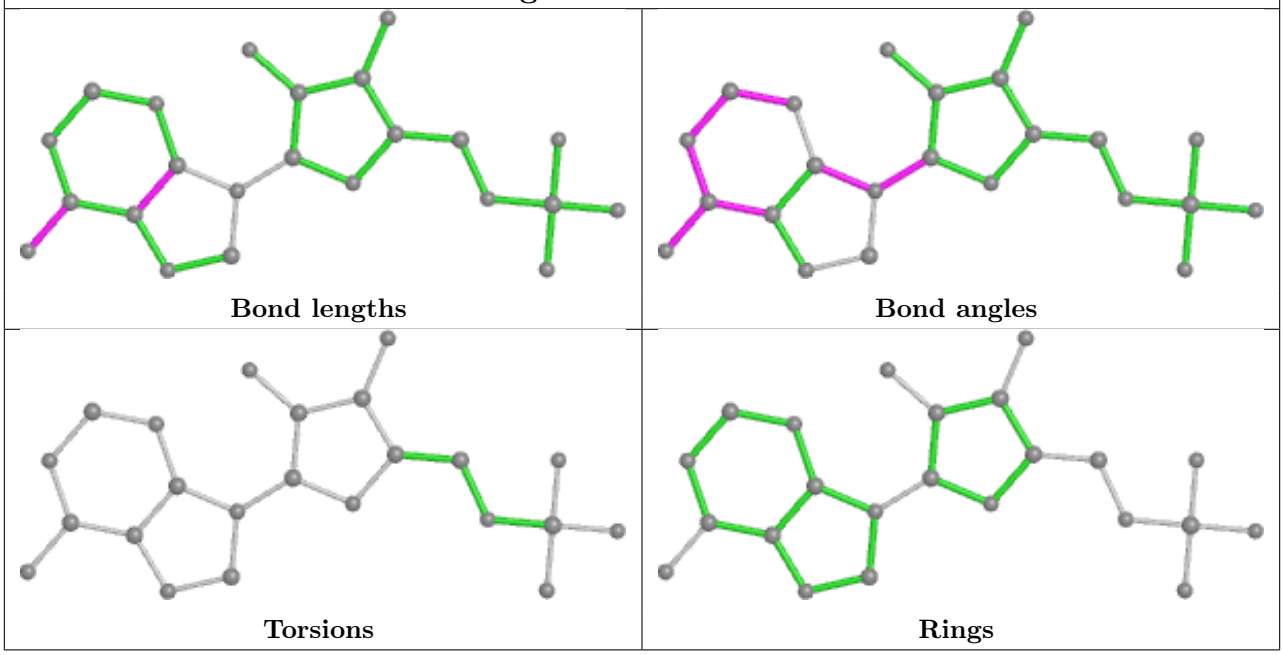
No monomer is involved in short contacts.

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 then 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 AMP E 801



Ligand AMP B 801



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	721/776 (92%)	0.13	20 (2%)	53	49	30, 41, 67, 108	0
1	D	722/776 (93%)	0.17	32 (4%)	34	31	31, 41, 68, 101	0
2	B	689/727 (94%)	0.07	7 (1%)	82	81	30, 41, 62, 101	0
2	E	689/727 (94%)	0.26	24 (3%)	44	40	31, 50, 69, 101	0
3	C	163/168 (97%)	-0.07	3 (1%)	68	66	30, 41, 53, 91	0
3	F	161/168 (95%)	0.19	6 (3%)	41	38	31, 45, 64, 80	0
All	All	3145/3342 (94%)	0.15	92 (2%)	51	48	30, 43, 67, 108	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	199	TYR	8.8
2	E	717	VAL	5.6
1	A	770	THR	5.6
1	D	189	THR	5.2
2	E	8	LEU	5.2
1	A	189	THR	5.1
1	D	180	GLY	4.7
1	D	178	ASP	4.6
1	D	14	THR	4.4
1	A	181	ALA	4.1
1	D	196	GLY	4.0
1	A	14	THR	3.9
1	D	665	ALA	3.7
2	E	408	GLY	3.7
1	D	547	GLY	3.6
1	A	436	SER	3.5
2	B	8	LEU	3.5
1	A	78	ILE	3.5
1	D	80	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	87	GLU	3.5
2	B	207	GLY	3.4
2	E	589	ALA	3.4
1	D	227	THR	3.4
2	E	410	VAL	3.4
3	F	2	ALA	3.3
1	D	37	ALA	3.3
1	A	771	VAL	3.3
1	A	774	VAL	3.3
1	D	414	GLY	3.3
2	E	525	GLU	3.2
3	F	166	ALA	3.2
2	E	66	HIS	3.1
2	E	381	LYS	3.0
3	C	166	ALA	3.0
3	C	168	ALA	3.0
3	F	65	LYS	3.0
1	A	437	ASN	3.0
2	E	409	ALA	2.9
2	E	258	LYS	2.9
3	F	66	VAL	2.9
2	E	527	PRO	2.9
2	E	382	GLU	2.8
1	A	766	PRO	2.7
1	D	417	ARG	2.7
3	C	167	ASP	2.7
1	D	666	ASP	2.6
1	A	763	SER	2.6
2	E	378	VAL	2.6
1	A	685	LYS	2.6
1	D	660	VAL	2.5
2	E	615	ARG	2.5
2	B	665	ARG	2.5
1	A	199	TYR	2.4
3	F	48	ASP	2.4
1	D	228	ARG	2.4
2	E	603	ASN	2.4
2	E	621	TYR	2.4
2	E	617	PRO	2.4
2	E	591	THR	2.3
1	D	52	ARG	2.3
2	E	385	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	546	TRP	2.3
2	E	411	LYS	2.3
1	A	776	GLU	2.3
2	B	299	VAL	2.3
2	E	386	GLU	2.3
2	B	588	GLN	2.3
1	A	15	ARG	2.3
1	D	410	ALA	2.3
3	F	145	ASP	2.3
1	D	548	LEU	2.3
2	E	602	PHE	2.3
1	A	192	VAL	2.3
2	B	499	GLY	2.2
1	D	45	LYS	2.2
1	A	769	HIS	2.2
1	D	437	ASN	2.1
1	D	192	VAL	2.1
1	D	767	ASP	2.1
1	D	764	GLU	2.1
1	D	229	TYR	2.1
1	D	671	VAL	2.1
1	A	775	GLU	2.1
1	D	416	SER	2.1
2	E	205	LYS	2.1
2	E	384	GLY	2.1
1	D	663	LYS	2.1
1	A	673	GLU	2.1
1	D	421	GLY	2.1
1	A	699	LYS	2.1
1	D	413	ARG	2.0
2	B	288	GLY	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 monosaccharides in this entry.

6.4 Ligands (i)

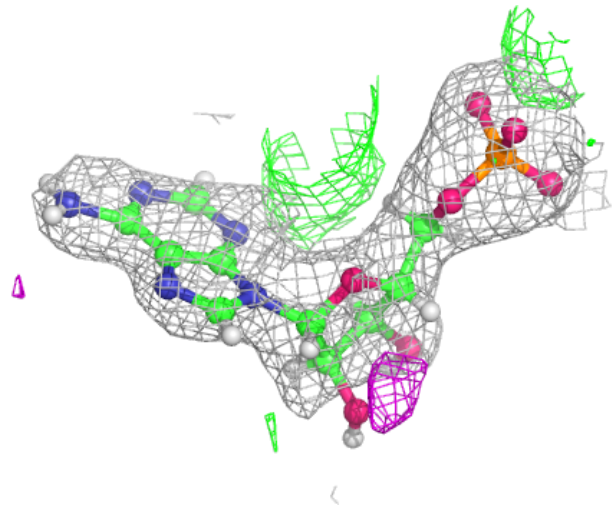
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

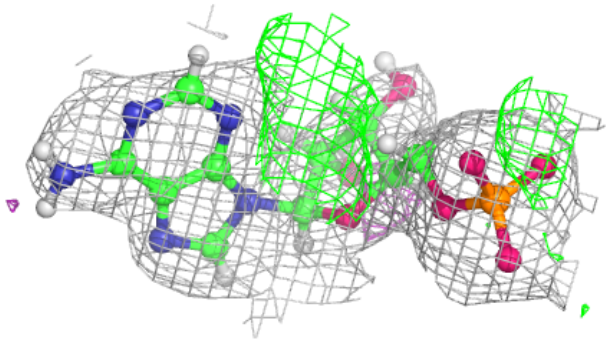
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	ZN	C	201	1/1	0.88	0.14	111,111,111,111	0
5	AMP	E	801	23/23	0.92	0.21	47,68,83,89	0
7	ZN	F	201	1/1	0.92	0.16	100,100,100,100	1
4	MN	D	801	1/1	0.93	0.11	55,55,55,55	0
6	SO4	E	802	5/5	0.94	0.26	70,72,72,72	0
4	MN	A	801	1/1	0.94	0.15	55,55,55,55	0
6	SO4	B	802	5/5	0.94	0.39	63,64,65,66	0
5	AMP	B	801	23/23	0.96	0.19	29,35,45,47	0

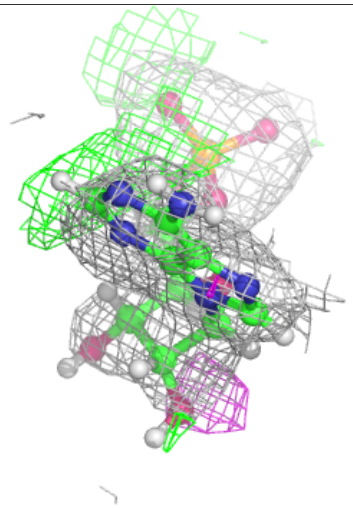
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AMP E 801:

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

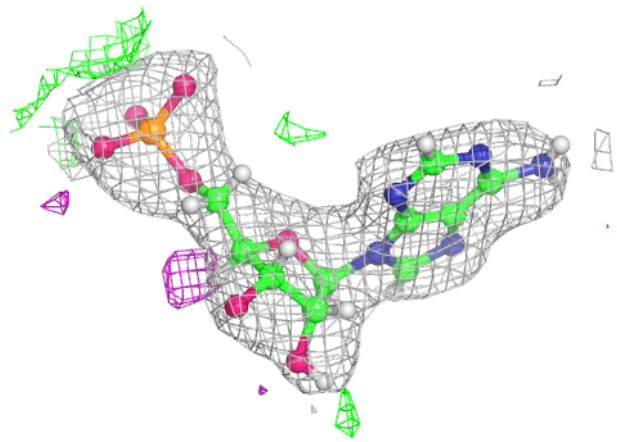


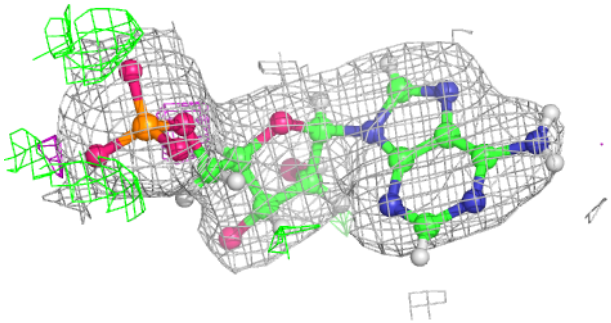


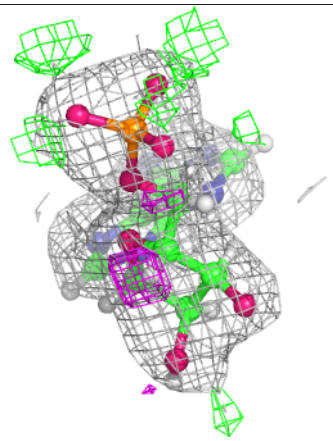


Electron density around AMP B 801:

$2mF_o$-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.