



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:17 AM UTC

PDB ID : 2VD6 / pdb_00002vd6
Title : Human adenylosuccinate lyase in complex with its substrate N6-(1,2-Dicarboxyethyl)-AMP, and its products AMP and fumarate.
Authors : Stenmark, P.; Moche, M.; Arrowsmith, C.; Berglund, H.; Busam, R.; Collins, R.; Dahlgren, L.G.; Edwards, A.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Hallberg, B.M.; Holmberg-schiavone, L.; Johansson, I.; Kallas, A.; Karlberg, T.; Kotenyova, T.; Lehtio, L.; Nilsson, M.; Nyman, T.; Ogg, D.; Persson, C.; Sagemark, J.; Sundstrom, M.; Thorsell, A.G.; Tresaugues, L.; van den Berg, S.; Weigelt, J.; Welin, M.; Nordlund, P.; Structural Genomics Consortium (SGC)
Deposited on : 2007-09-30
Resolution : 2.00 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)

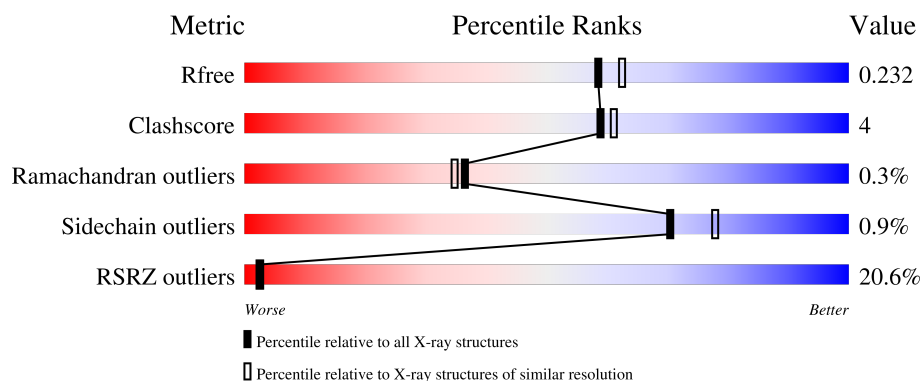
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	503	
1	B	503	

Continued on next page...

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

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	C	503	30% 81% 10% 9%
1	D	503	24% 83% 8% 8%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15817 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 ADENYLOSUCCINATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	4	0
			3706	2333	657	690	26			
1	B	461	Total	C	N	O	S	0	1	0
			3685	2322	654	683	26			
1	C	457	Total	C	N	O	S	0	4	0
			3681	2318	656	682	25			
1	D	462	Total	C	N	O	S	0	3	0
			3704	2334	657	687	26			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP P30566
A	-20	HIS	-	expression tag	UNP P30566
A	-19	HIS	-	expression tag	UNP P30566
A	-18	HIS	-	expression tag	UNP P30566
A	-17	HIS	-	expression tag	UNP P30566
A	-16	HIS	-	expression tag	UNP P30566
A	-15	HIS	-	expression tag	UNP P30566
A	-14	SER	-	expression tag	UNP P30566
A	-13	SER	-	expression tag	UNP P30566
A	-12	GLY	-	expression tag	UNP P30566
A	-11	VAL	-	expression tag	UNP P30566
A	-10	ASP	-	expression tag	UNP P30566
A	-9	LEU	-	expression tag	UNP P30566
A	-8	GLY	-	expression tag	UNP P30566
A	-7	THR	-	expression tag	UNP P30566
A	-6	GLU	-	expression tag	UNP P30566
A	-5	ASN	-	expression tag	UNP P30566
A	-4	LEU	-	expression tag	UNP P30566
A	-3	TYR	-	expression tag	UNP P30566
A	-2	PHE	-	expression tag	UNP P30566
A	-1	GLN	-	expression tag	UNP P30566

Continued on next page...

Continued from previous page...

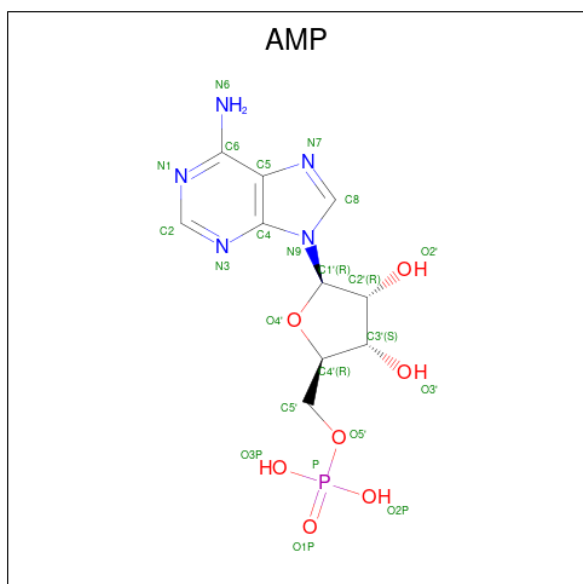
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P30566
B	-21	MET	-	expression tag	UNP P30566
B	-20	HIS	-	expression tag	UNP P30566
B	-19	HIS	-	expression tag	UNP P30566
B	-18	HIS	-	expression tag	UNP P30566
B	-17	HIS	-	expression tag	UNP P30566
B	-16	HIS	-	expression tag	UNP P30566
B	-15	HIS	-	expression tag	UNP P30566
B	-14	SER	-	expression tag	UNP P30566
B	-13	SER	-	expression tag	UNP P30566
B	-12	GLY	-	expression tag	UNP P30566
B	-11	VAL	-	expression tag	UNP P30566
B	-10	ASP	-	expression tag	UNP P30566
B	-9	LEU	-	expression tag	UNP P30566
B	-8	GLY	-	expression tag	UNP P30566
B	-7	THR	-	expression tag	UNP P30566
B	-6	GLU	-	expression tag	UNP P30566
B	-5	ASN	-	expression tag	UNP P30566
B	-4	LEU	-	expression tag	UNP P30566
B	-3	TYR	-	expression tag	UNP P30566
B	-2	PHE	-	expression tag	UNP P30566
B	-1	GLN	-	expression tag	UNP P30566
B	0	SER	-	expression tag	UNP P30566
C	-21	MET	-	expression tag	UNP P30566
C	-20	HIS	-	expression tag	UNP P30566
C	-19	HIS	-	expression tag	UNP P30566
C	-18	HIS	-	expression tag	UNP P30566
C	-17	HIS	-	expression tag	UNP P30566
C	-16	HIS	-	expression tag	UNP P30566
C	-15	HIS	-	expression tag	UNP P30566
C	-14	SER	-	expression tag	UNP P30566
C	-13	SER	-	expression tag	UNP P30566
C	-12	GLY	-	expression tag	UNP P30566
C	-11	VAL	-	expression tag	UNP P30566
C	-10	ASP	-	expression tag	UNP P30566
C	-9	LEU	-	expression tag	UNP P30566
C	-8	GLY	-	expression tag	UNP P30566
C	-7	THR	-	expression tag	UNP P30566
C	-6	GLU	-	expression tag	UNP P30566
C	-5	ASN	-	expression tag	UNP P30566
C	-4	LEU	-	expression tag	UNP P30566
C	-3	TYR	-	expression tag	UNP P30566

Continued on next page...

Continued from previous page...

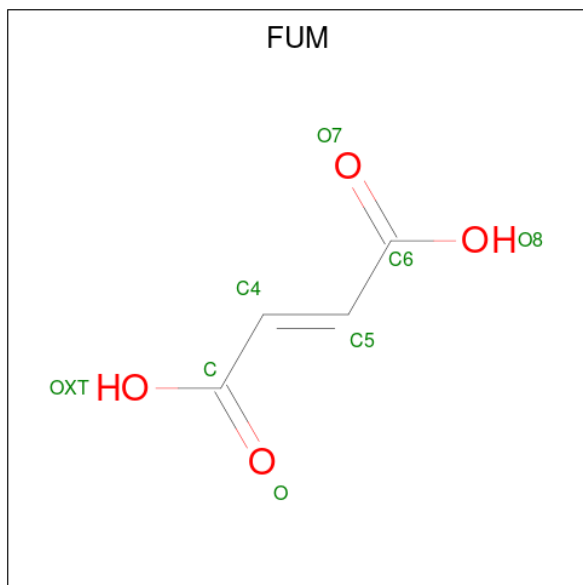
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	PHE	-	expression tag	UNP P30566
C	-1	GLN	-	expression tag	UNP P30566
C	0	SER	-	expression tag	UNP P30566
D	-21	MET	-	expression tag	UNP P30566
D	-20	HIS	-	expression tag	UNP P30566
D	-19	HIS	-	expression tag	UNP P30566
D	-18	HIS	-	expression tag	UNP P30566
D	-17	HIS	-	expression tag	UNP P30566
D	-16	HIS	-	expression tag	UNP P30566
D	-15	HIS	-	expression tag	UNP P30566
D	-14	SER	-	expression tag	UNP P30566
D	-13	SER	-	expression tag	UNP P30566
D	-12	GLY	-	expression tag	UNP P30566
D	-11	VAL	-	expression tag	UNP P30566
D	-10	ASP	-	expression tag	UNP P30566
D	-9	LEU	-	expression tag	UNP P30566
D	-8	GLY	-	expression tag	UNP P30566
D	-7	THR	-	expression tag	UNP P30566
D	-6	GLU	-	expression tag	UNP P30566
D	-5	ASN	-	expression tag	UNP P30566
D	-4	LEU	-	expression tag	UNP P30566
D	-3	TYR	-	expression tag	UNP P30566
D	-2	PHE	-	expression tag	UNP P30566
D	-1	GLN	-	expression tag	UNP P30566
D	0	SER	-	expression tag	UNP P30566

- 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	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is FUMARIC ACID (CCD ID: FUM) (formula: $C_4H_4O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	4	4		
3	C	1	Total	C	O	0	0
			8	4	4		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

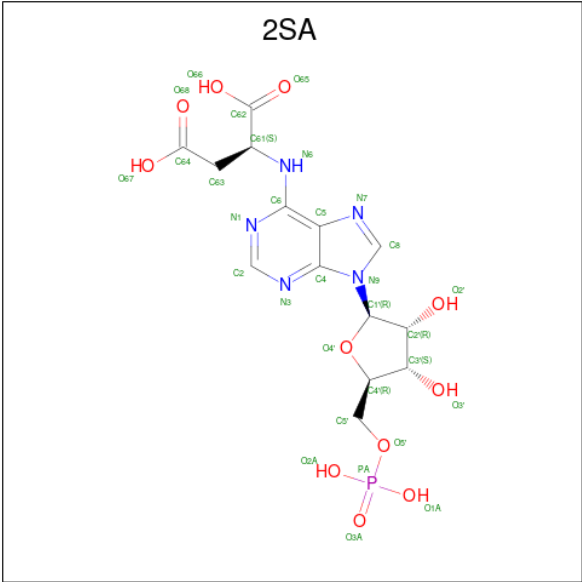


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	0
			2	2		
5	B	2	Total	Cl	0	0
			2	2		
5	C	1	Total	Cl	0	0
			1	1		
5	D	2	Total	Cl	0	0
			2	2		

- Molecule 6 is 2-[9-(3,4-DIHYDROXY-5-PHOSPHONOXYMETHYL-TETRAHYDRO-FURAN-2-YL)-9H-PURIN-6-YLAMINO]-SUCCINIC ACID (CCD ID: 2SA) (formula: C₁₄H₁₈N₅O₁₁P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			31	14	5	11	1		
6	D	1	Total	C	N	O	P	0	0
			31	14	5	11	1		

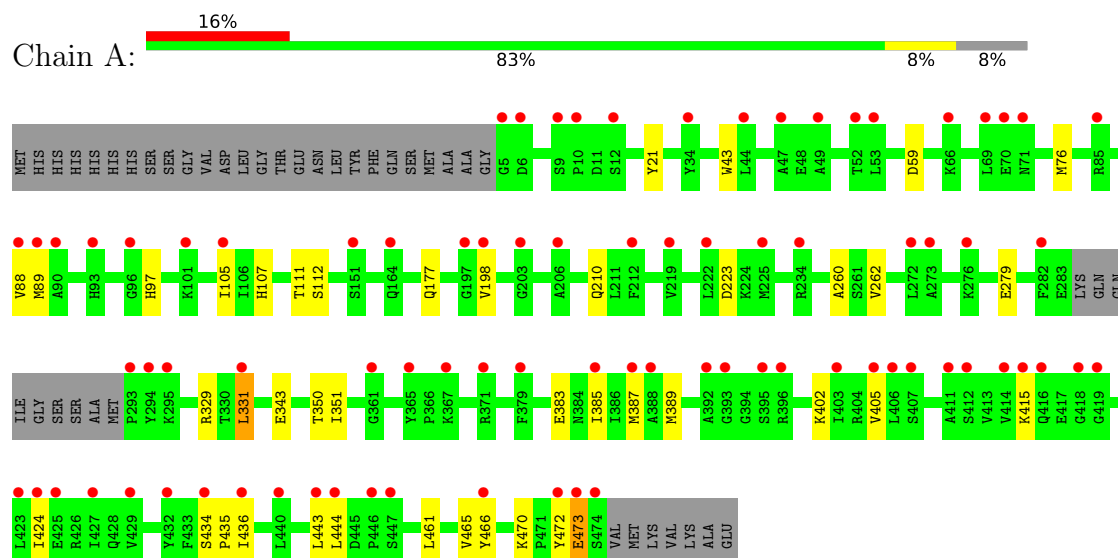
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	247	Total	O	0	0
			247	247		
7	B	158	Total	O	0	0
			158	158		
7	C	235	Total	O	0	0
			235	235		
7	D	240	Total	O	0	0
			240	240		

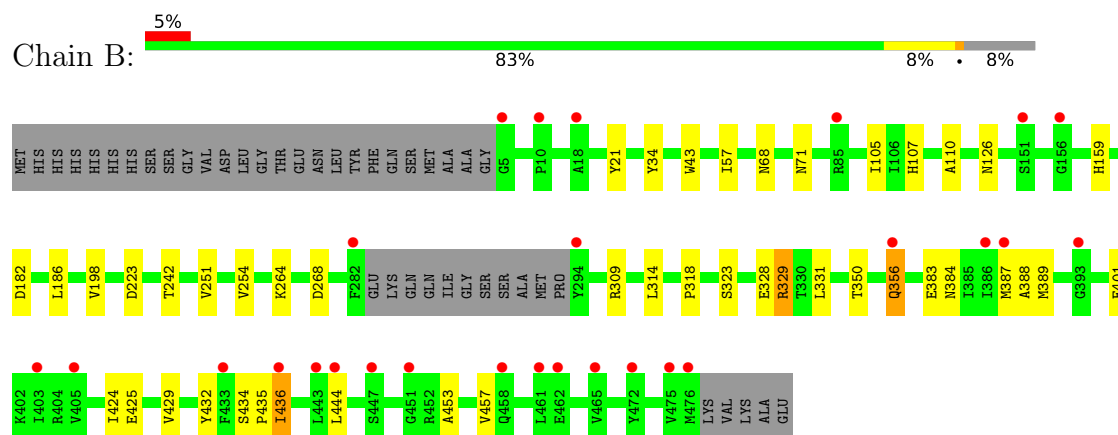
3 Residue-property plots [i](#)

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.

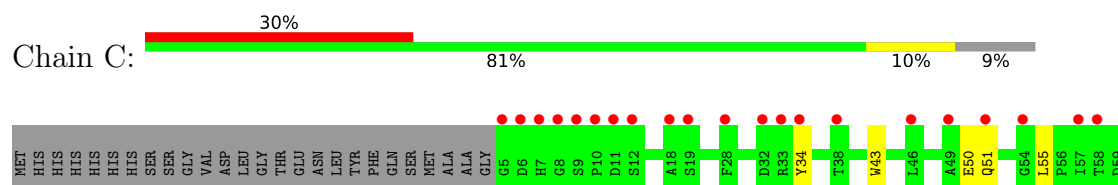
• Molecule 1: ADENYLOSUCCINATE LYASE

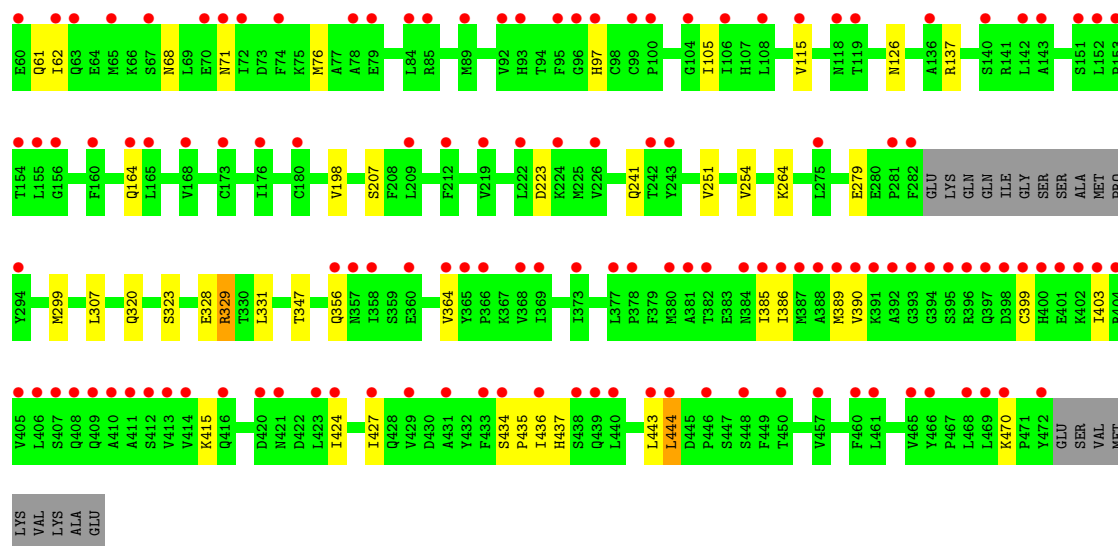


• Molecule 1: ADENYLOSUCCINATE LYASE

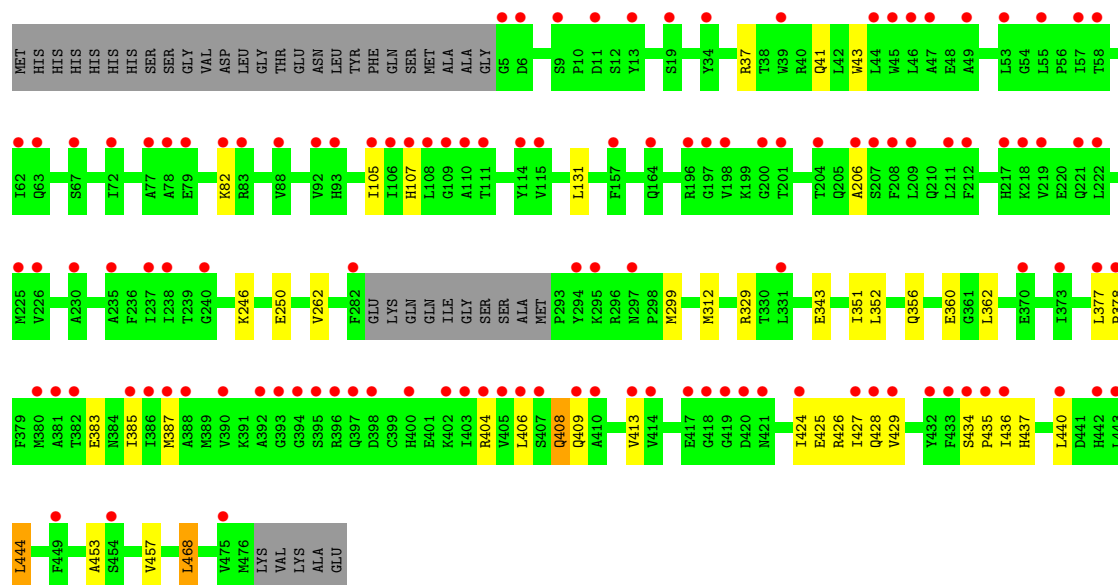
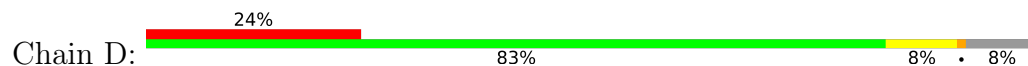


• Molecule 1: ADENYLOSUCCINATE LYASE





• Molecule 1: ADENYLOSUCCINATE LYASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.30Å 128.10Å 190.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 50.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.00) 99.7 (50.00-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.95 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.3.0040	Depositor
R, R_{free}	0.192 , 0.229 0.197 , 0.232	Depositor DCC
R_{free} test set	7207 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.0	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	0.91	EDS
Total number of atoms	15817	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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: FUM, 2SA, AMP, CL, GOL

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	0.58	2/3778 (0.1%)	0.78	0/5101
1	B	0.51	0/3756	0.77	0/5071
1	C	0.57	2/3752 (0.1%)	0.78	1/5066 (0.0%)
1	D	0.54	0/3779	0.77	0/5102
All	All	0.55	4/15065 (0.0%)	0.77	1/20340 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	61	GLN	CD-OE1	8.16	1.39	1.23
1	C	61	GLN	CD-NE2	6.19	1.46	1.33
1	A	59	ASP	CG-OD2	5.81	1.36	1.25
1	A	59	ASP	CG-OD1	5.04	1.34	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	61	GLN	OE1-CD-NE2	7.40	130.00	122.60

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	3706	0	3711	37	0
1	B	3685	0	3698	35	0
1	C	3681	0	3689	35	0
1	D	3704	0	3718	29	0
2	A	23	0	12	3	0
2	C	23	0	12	3	0
3	A	8	0	1	2	0
3	C	8	0	1	2	0
4	A	6	0	8	0	0
4	B	12	0	16	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
6	B	31	0	14	1	0
6	D	31	0	14	1	0
7	A	247	0	0	3	0
7	B	158	0	0	0	0
7	C	235	0	0	0	0
7	D	240	0	0	1	0
All	All	15817	0	14910	131	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 (131) 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:328:GLU:O	1:B:329:ARG:HB2	1.64	0.98
1:B:424:ILE:CD1	1:B:444:LEU:HD11	2.04	0.88
1:D:424:ILE:HD12	1:D:444:LEU:HD21	1.58	0.86
1:A:424:ILE:HD12	1:A:444:LEU:HD11	1.60	0.84
1:A:331:LEU:HD13	1:B:159:HIS:CE1	2.16	0.81
1:B:424:ILE:HD12	1:B:444:LEU:HD11	1.61	0.80
1:A:424:ILE:CD1	1:A:444:LEU:HD11	2.16	0.76
1:B:57:ILE:HG23	1:B:105:ILE:HD13	1.68	0.75
1:B:383:GLU:HG3	1:B:387:MET:HE2	1.69	0.75
1:C:164[B]:GLN:NE2	1:D:206:ALA:HB3	2.04	0.72
1:A:385:ILE:HG23	1:A:436:ILE:CD1	2.20	0.72
1:A:383:GLU:OE2	1:A:387:MET:HE3	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:ILE:HG23	1:C:436:ILE:CD1	2.26	0.65
1:A:343:GLU:OE2	1:D:343:GLU:OE2	2.15	0.64
1:D:43:TRP:HE1	1:D:107:HIS:CD2	2.17	0.62
1:B:424:ILE:HD11	1:B:444:LEU:HD11	1.80	0.61
1:C:76:MET:HE1	1:C:97:HIS:CD2	2.35	0.61
1:D:43:TRP:HE1	1:D:107:HIS:HD2	1.49	0.61
1:B:424:ILE:CD1	1:B:444:LEU:CD1	2.78	0.60
1:D:425:GLU:O	1:D:429:VAL:HG22	2.04	0.58
1:B:389:MET:HE2	1:B:432:TYR:CE2	2.38	0.58
1:A:105:ILE:C	1:A:105:ILE:HD12	2.29	0.58
1:D:385:ILE:HD13	1:D:427:ILE:HD13	1.85	0.58
1:C:34:TYR:OH	1:C:126:ASN:ND2	2.37	0.57
1:C:403:ILE:HD11	1:C:427:ILE:HD11	1.86	0.56
1:D:37:ARG:HH12	1:D:41:GLN:HE21	1.54	0.56
1:D:406:LEU:HD22	1:D:426:ARG:HB3	1.88	0.55
1:B:424:ILE:HD12	1:B:444:LEU:CD1	2.33	0.55
1:A:111:THR:HG22	7:A:2054:HOH:O	2.05	0.55
1:B:68:ASN:ND2	1:B:71:ASN:HD22	2.05	0.54
1:A:415:LYS:NZ	1:C:279:GLU:OE2	2.32	0.54
1:C:403:ILE:HD11	1:C:427:ILE:CD1	2.39	0.52
1:D:105:ILE:C	1:D:105:ILE:HD12	2.35	0.52
1:B:43:TRP:HE1	1:B:107:HIS:CD2	2.27	0.52
1:B:242:THR:HG23	1:B:329:ARG:HG3	1.91	0.51
1:A:385:ILE:HG23	1:A:436:ILE:HD11	1.92	0.51
2:C:1000:AMP:N6	3:C:1001:FUM:C4	2.73	0.51
1:A:76:MET:HE1	1:A:97:HIS:CG	2.45	0.51
1:C:76:MET:HE1	1:C:97:HIS:CG	2.44	0.51
1:C:328:GLU:O	1:C:329:ARG:HB3	2.10	0.51
1:A:88:VAL:HG21	1:A:112:SER:HB3	1.94	0.49
1:A:331:LEU:HD13	1:B:159:HIS:NE2	2.27	0.49
1:D:429:VAL:O	1:D:429:VAL:HG23	2.11	0.49
1:A:76:MET:HE1	1:A:97:HIS:CB	2.42	0.49
1:B:384:ASN:HA	1:B:387:MET:HE3	1.95	0.49
1:D:424:ILE:CD1	1:D:444:LEU:HD21	2.37	0.49
1:A:88:VAL:HG12	1:A:89[B]:MET:HE2	1.95	0.49
1:A:385:ILE:HG23	1:A:436:ILE:HD12	1.92	0.48
1:A:389:MET:HG2	1:A:436:ILE:HD13	1.95	0.48
1:C:105:ILE:C	1:C:105:ILE:HD12	2.39	0.48
1:A:402:LYS:O	1:A:405:VAL:HG22	2.14	0.48
1:C:389:MET:HG2	1:C:436:ILE:HD13	1.96	0.48
1:D:436:ILE:C	1:D:436:ILE:HD12	2.39	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:ILE:HG23	1:C:436:ILE:HD12	1.93	0.47
1:B:198:VAL:HG22	1:B:223:ASP:HA	1.96	0.47
1:C:424:ILE:HD12	1:C:444:LEU:CD1	2.43	0.47
1:C:68:ASN:ND2	1:C:71:ASN:HD22	2.13	0.47
1:A:466:TYR:HE1	7:A:2247:HOH:O	1.97	0.47
1:C:251:VAL:O	1:C:254:VAL:HG22	2.15	0.47
1:B:107:HIS:CD2	1:B:110:ALA:HB3	2.50	0.47
6:B:1002:2SA:N7	6:B:1002:2SA:H61	2.30	0.47
2:C:1000:AMP:N6	3:C:1001:FUM:C5	2.78	0.46
1:D:409:GLN:O	1:D:413:VAL:HG23	2.15	0.46
1:C:137:ARG:HD2	1:C:356[A]:GLN:NE2	2.30	0.46
1:C:434:SER:N	1:C:435:PRO:CD	2.78	0.46
1:D:468:LEU:HD13	7:D:2236:HOH:O	2.14	0.46
1:D:404:ARG:O	1:D:408:GLN:HG2	2.16	0.46
1:D:428:GLN:HG3	1:D:440:LEU:HD13	1.98	0.46
1:B:264:LYS:NZ	1:B:268:ASP:OD2	2.39	0.46
2:A:1000:AMP:N6	3:A:1001:FUM:C4	2.79	0.45
1:D:434:SER:N	1:D:435:PRO:CD	2.79	0.45
1:D:299:MET:O	1:D:299:MET:HE3	2.16	0.45
1:D:246:LYS:O	1:D:250:GLU:HG2	2.16	0.45
1:A:385:ILE:HD12	1:A:443:LEU:HD13	1.98	0.45
1:A:279:GLU:OE2	1:C:415:LYS:NZ	2.42	0.45
1:A:260:ALA:HA	1:B:323[B]:SER:OG	2.17	0.45
1:B:436:ILE:O	1:B:436:ILE:HG23	2.16	0.45
1:D:262:VAL:HG11	1:D:351:ILE:CG2	2.48	0.44
1:A:210:GLN:OE1	1:B:387:MET:HE1	2.18	0.44
1:C:385:ILE:HD13	1:C:443:LEU:HD13	2.00	0.44
1:B:34:TYR:OH	1:B:126:ASN:ND2	2.46	0.43
6:D:1002:2SA:H61	6:D:1002:2SA:N7	2.33	0.43
1:C:434:SER:HA	1:C:437:HIS:ND1	2.34	0.43
1:D:383:GLU:HG3	1:D:387:MET:HE3	2.01	0.43
1:C:424:ILE:HD12	1:C:444:LEU:HD13	2.01	0.43
1:D:434:SER:HA	1:D:437:HIS:ND1	2.34	0.43
1:B:434:SER:N	1:B:435:PRO:CD	2.82	0.43
1:B:331:LEU:HB3	1:C:299:MET:HE1	2.00	0.43
1:C:43:TRP:CE2	1:C:115:VAL:HG11	2.54	0.43
1:A:472:TYR:O	1:A:473:GLU:C	2.62	0.42
1:A:21:TYR:HB3	1:A:350:THR:HG21	2.00	0.42
1:C:198:VAL:HG22	1:C:223:ASP:HA	2.00	0.42
1:C:389:MET:HG3	1:C:399:CYS:SG	2.59	0.42
1:B:309:ARG:HD3	1:C:320:GLN:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:ILE:O	1:C:390:VAL:HG23	2.20	0.42
1:A:111:THR:HG22	1:A:112:SER:N	2.34	0.42
1:B:436:ILE:O	1:B:436:ILE:CG2	2.66	0.42
1:A:177:GLN:NE2	7:A:2096:HOH:O	2.53	0.42
2:A:1000:AMP:N6	3:A:1001:FUM:C5	2.83	0.42
1:B:425:GLU:O	1:B:429:VAL:HG22	2.19	0.42
1:C:329:ARG:C	1:C:329:ARG:HD3	2.45	0.42
1:D:377:LEU:N	1:D:378:PRO:CD	2.83	0.42
1:A:111:THR:HG22	1:A:112:SER:H	1.85	0.42
1:D:356[A]:GLN:NE2	1:D:360:GLU:OE2	2.52	0.42
1:A:461:LEU:HD23	1:A:465:VAL:HG21	2.01	0.42
1:D:131:LEU:HD22	1:D:352:LEU:HD12	2.02	0.42
1:A:424:ILE:CD1	1:A:444:LEU:CD1	2.95	0.41
1:B:182:ASP:O	1:B:186:LEU:HD13	2.19	0.41
1:A:43:TRP:HE1	1:A:107:HIS:CD2	2.37	0.41
1:A:331:LEU:HD21	2:A:1000:AMP:C4	2.54	0.41
1:B:314:LEU:O	1:B:318:PRO:HD2	2.21	0.41
1:D:453:ALA:O	1:D:457:VAL:HG23	2.20	0.41
1:A:43:TRP:HE1	1:A:107:HIS:HD2	1.68	0.41
1:C:50:GLU:HB3	1:C:55:LEU:HD12	2.02	0.41
1:A:262:VAL:HG11	1:A:351:ILE:CG2	2.50	0.41
1:B:453:ALA:O	1:B:457:VAL:HG23	2.20	0.41
1:C:307:LEU:HB3	1:C:347:THR:HG23	2.03	0.41
1:D:37:ARG:HH12	1:D:41:GLN:NE2	2.19	0.41
1:A:198:VAL:HG22	1:A:223:ASP:HA	2.02	0.41
1:B:251:VAL:O	1:B:254:VAL:HG22	2.20	0.41
1:A:88:VAL:HG12	1:A:89[B]:MET:CE	2.51	0.41
1:A:434[B]:SER:N	1:A:435:PRO:CD	2.83	0.41
1:C:331:LEU:HD21	2:C:1000:AMP:C6	2.56	0.40
1:C:51:GLN:OE1	1:C:62:ILE:HD12	2.20	0.40
1:B:21:TYR:HB3	1:B:350:THR:HG21	2.04	0.40
1:B:242:THR:HG23	1:B:329:ARG:CG	2.52	0.40
1:B:356:GLN:HE21	1:B:356:GLN:HA	1.87	0.40
1:B:388:ALA:C	1:B:436:ILE:HD11	2.47	0.40
1:C:323[B]:SER:OG	1:D:312:MET:SD	2.79	0.40
1:C:328:GLU:O	1:C:329:ARG:CB	2.69	0.40
1:C:241:GLN:HB3	1:C:329:ARG:HG2	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	461/503 (92%)	450 (98%)	9 (2%)	2 (0%)	30	27
1	B	458/503 (91%)	449 (98%)	8 (2%)	1 (0%)	43	42
1	C	457/503 (91%)	451 (99%)	5 (1%)	1 (0%)	43	42
1	D	461/503 (92%)	450 (98%)	10 (2%)	1 (0%)	43	42
All	All	1837/2012 (91%)	1800 (98%)	32 (2%)	5 (0%)	36	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	ARG
1	B	329	ARG
1	C	329	ARG
1	D	329	ARG
1	A	473	GLU

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	408/438 (93%)	406 (100%)	2 (0%)	81	87
1	B	405/438 (92%)	402 (99%)	3 (1%)	76	82
1	C	404/438 (92%)	399 (99%)	5 (1%)	63	70
1	D	408/438 (93%)	403 (99%)	5 (1%)	63	70
All	All	1625/1752 (93%)	1610 (99%)	15 (1%)	70	78

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	331	LEU
1	A	470	LYS
1	B	356	GLN
1	B	401	GLU
1	B	436	ILE
1	C	207	SER
1	C	264	LYS
1	C	364	VAL
1	C	444	LEU
1	C	470	LYS
1	D	82	LYS
1	D	362	LEU
1	D	408	GLN
1	D	444	LEU
1	D	468	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	97	HIS
1	A	107	HIS
1	A	177	GLN
1	A	408	GLN
1	B	68	ASN
1	B	97	HIS
1	B	107	HIS
1	B	210	GLN
1	B	356	GLN
1	B	409	GLN
1	C	63	GLN
1	C	68	ASN
1	C	91	HIS
1	C	97	HIS
1	C	126	ASN
1	C	184	GLN
1	C	397	GLN
1	C	408	GLN
1	D	7	HIS
1	D	41	GLN
1	D	107	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	126	ASN
1	D	375	GLN
1	D	408	GLN
1	D	409	GLN
1	D	458	GLN

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 18 ligands modelled in this entry, 7 are monoatomic - leaving 11 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	$\# Z > 2$
4	GOL	B	1004	-	5,5,5	0.42	0	5,5,5	0.58	0
3	FUM	C	1001	-	7,7,7	1.12	1 (14%)	8,8,8	0.95	0
4	GOL	C	1003	-	5,5,5	0.42	0	5,5,5	0.18	0
2	AMP	A	1000	-	25,25,25	1.32	4 (16%)	37,38,38	2.00	10 (27%)
6	2SA	D	1002	-	33,33,33	1.00	1 (3%)	47,49,49	1.72	11 (23%)
3	FUM	A	1001	-	7,7,7	1.18	0	8,8,8	0.93	0
2	AMP	C	1000	-	25,25,25	1.36	5 (20%)	37,38,38	1.93	10 (27%)
4	GOL	D	1003	-	5,5,5	0.32	0	5,5,5	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	1003	-	5,5,5	0.30	0	5,5,5	0.41	0
4	GOL	A	1003	-	5,5,5	0.28	0	5,5,5	0.26	0
6	2SA	B	1002	-	33,33,33	0.98	2 (6%)	47,49,49	1.82	13 (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
4	GOL	B	1004	-	-	4/4/4/4	-
3	FUM	C	1001	-	-	0/5/5/5	-
4	GOL	C	1003	-	-	2/4/4/4	-
2	AMP	A	1000	-	-	2/10/26/26	0/3/3/3
6	2SA	D	1002	-	-	4/22/38/38	0/3/3/3
3	FUM	A	1001	-	-	0/5/5/5	-
2	AMP	C	1000	-	-	2/10/26/26	0/3/3/3
4	GOL	D	1003	-	-	2/4/4/4	-
4	GOL	B	1003	-	-	2/4/4/4	-
4	GOL	A	1003	-	-	0/4/4/4	-
6	2SA	B	1002	-	-	7/22/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1000	AMP	C5-C4	4.18	1.46	1.39
2	A	1000	AMP	C5-C4	3.97	1.46	1.39
6	D	1002	2SA	C8-N7	2.53	1.36	1.31
6	B	1002	2SA	C8-N7	2.46	1.36	1.31
2	C	1000	AMP	C4-N9	-2.45	1.32	1.37
2	A	1000	AMP	C5-C6	2.37	1.47	1.41
2	C	1000	AMP	C5-C6	2.30	1.47	1.41
6	B	1002	2SA	C5-N7	-2.22	1.35	1.39
2	C	1000	AMP	C5-N7	-2.21	1.35	1.39
2	C	1000	AMP	C8-N7	2.19	1.35	1.31
2	A	1000	AMP	C8-N7	2.08	1.35	1.31
2	A	1000	AMP	C5-N7	-2.04	1.35	1.39
3	C	1001	FUM	OXT-C	-2.03	1.25	1.30

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	AMP	C5-C4-N3	-5.26	119.47	126.72
2	C	1000	AMP	C5-C4-N3	-5.20	119.56	126.72
6	D	1002	2SA	N1-C2-N3	-4.97	121.06	128.58
2	A	1000	AMP	N3-C4-N9	4.89	135.49	127.17
6	B	1002	2SA	C5-C4-N3	-4.77	120.14	126.72
6	B	1002	2SA	N1-C2-N3	-4.75	121.39	128.58
2	C	1000	AMP	N3-C4-N9	4.54	134.90	127.17
6	D	1002	2SA	C5-C4-N3	-4.04	121.15	126.72
2	A	1000	AMP	N3-C2-N1	-3.85	122.75	128.58
2	C	1000	AMP	N3-C2-N1	-3.82	122.80	128.58
2	A	1000	AMP	C4-N9-C8	3.81	109.74	105.74
2	C	1000	AMP	C2-N3-C4	3.72	120.93	111.83
6	D	1002	2SA	N9-C8-N7	-3.65	108.76	113.94
2	A	1000	AMP	C2-N3-C4	3.63	120.69	111.83
2	C	1000	AMP	C4-N9-C8	3.47	109.38	105.74
6	B	1002	2SA	N9-C8-N7	-3.39	109.13	113.94
6	D	1002	2SA	C63-C61-C62	-3.29	104.22	110.79
6	B	1002	2SA	C2-N3-C4	3.18	119.59	111.83
6	B	1002	2SA	C4-C5-N7	-2.99	107.16	110.58
6	D	1002	2SA	C2-N3-C4	2.88	118.87	111.83
6	B	1002	2SA	O4'-C1'-N9	2.82	113.51	108.09
6	D	1002	2SA	C5-N7-C8	2.70	107.69	103.45
6	B	1002	2SA	C63-C61-C62	-2.69	105.41	110.79
6	D	1002	2SA	C4-N9-C8	2.68	108.55	105.74
6	D	1002	2SA	C4-C5-N7	-2.68	107.52	110.58
6	B	1002	2SA	N3-C4-N9	2.66	131.69	127.17
6	B	1002	2SA	C5-N7-C8	2.58	107.51	103.45
6	B	1002	2SA	C4-C5-C6	2.58	118.92	116.78
2	A	1000	AMP	N9-C8-N7	-2.55	110.31	113.94
2	A	1000	AMP	C4-C5-N7	-2.48	107.75	110.58
2	C	1000	AMP	C4-C5-N7	-2.47	107.76	110.58
6	D	1002	2SA	N3-C4-N9	2.46	131.35	127.17
6	D	1002	2SA	C4-C5-C6	2.45	118.82	116.78
2	A	1000	AMP	C5-N7-C8	2.37	107.17	103.45
2	A	1000	AMP	N6-C6-N1	2.28	123.45	118.38
2	C	1000	AMP	N9-C8-N7	-2.28	110.70	113.94
2	A	1000	AMP	C5-C6-N6	-2.21	117.81	123.29
6	B	1002	2SA	C4-N9-C8	2.18	108.03	105.74
6	B	1002	2SA	C5-C4-N9	2.15	108.16	105.81
6	D	1002	2SA	C2-N1-C6	2.09	122.17	115.24
2	C	1000	AMP	C5-C6-N6	-2.09	118.11	123.29
2	C	1000	AMP	N6-C6-N1	2.07	122.99	118.38
6	B	1002	2SA	O67-C64-C63	2.04	120.35	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1000	AMP	C5-N7-C8	2.01	106.61	103.45

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1003	GOL	O1-C1-C2-C3
4	B	1004	GOL	C1-C2-C3-O3
4	C	1003	GOL	C1-C2-C3-O3
4	C	1003	GOL	O2-C2-C3-O3
4	D	1003	GOL	C1-C2-C3-O3
6	B	1002	2SA	N1-C6-N6-C61
6	D	1002	2SA	N1-C6-N6-C61
6	D	1002	2SA	C2'-C1'-N9-C4
4	B	1004	GOL	O1-C1-C2-C3
4	B	1003	GOL	O1-C1-C2-O2
4	B	1004	GOL	O2-C2-C3-O3
2	C	1000	AMP	C2'-C1'-N9-C8
6	D	1002	2SA	C2'-C1'-N9-C8
4	D	1003	GOL	O2-C2-C3-O3
6	B	1002	2SA	C2'-C1'-N9-C4
2	A	1000	AMP	C2'-C1'-N9-C8
6	B	1002	2SA	C2'-C1'-N9-C8
2	C	1000	AMP	C2'-C1'-N9-C4
6	B	1002	2SA	C5-C6-N6-C61
6	D	1002	2SA	C5-C6-N6-C61
2	A	1000	AMP	C2'-C1'-N9-C4
6	B	1002	2SA	C61-C63-C64-O67
6	B	1002	2SA	C61-C63-C64-O68
4	B	1004	GOL	O1-C1-C2-O2
6	B	1002	2SA	O4'-C1'-N9-C8

There are no ring outliers.

6 monomers are involved in 8 short contacts:

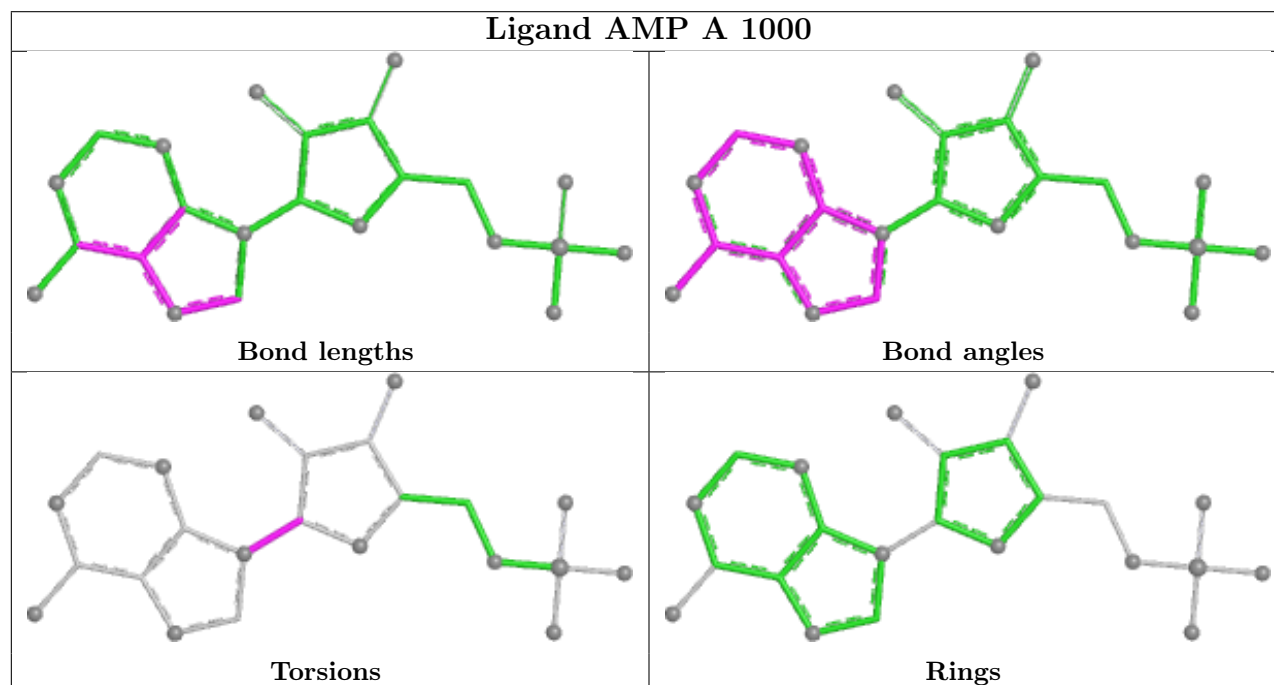
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1001	FUM	2	0
2	A	1000	AMP	3	0
6	D	1002	2SA	1	0
3	A	1001	FUM	2	0
2	C	1000	AMP	3	0

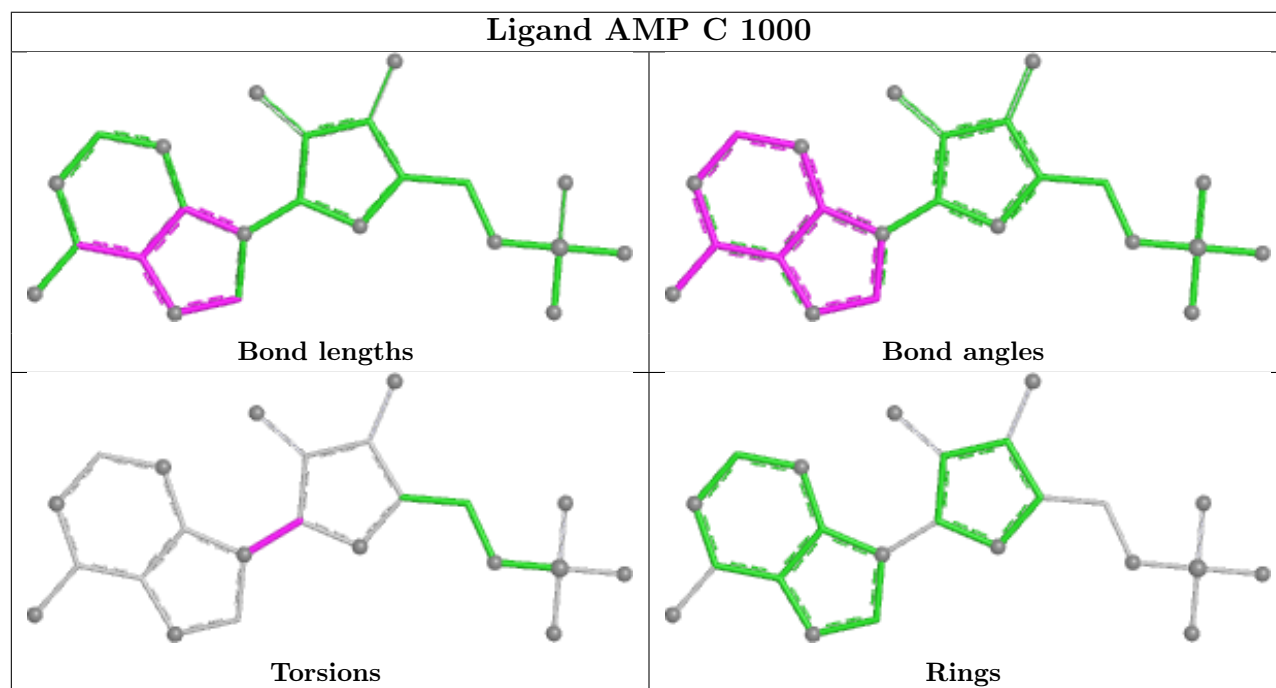
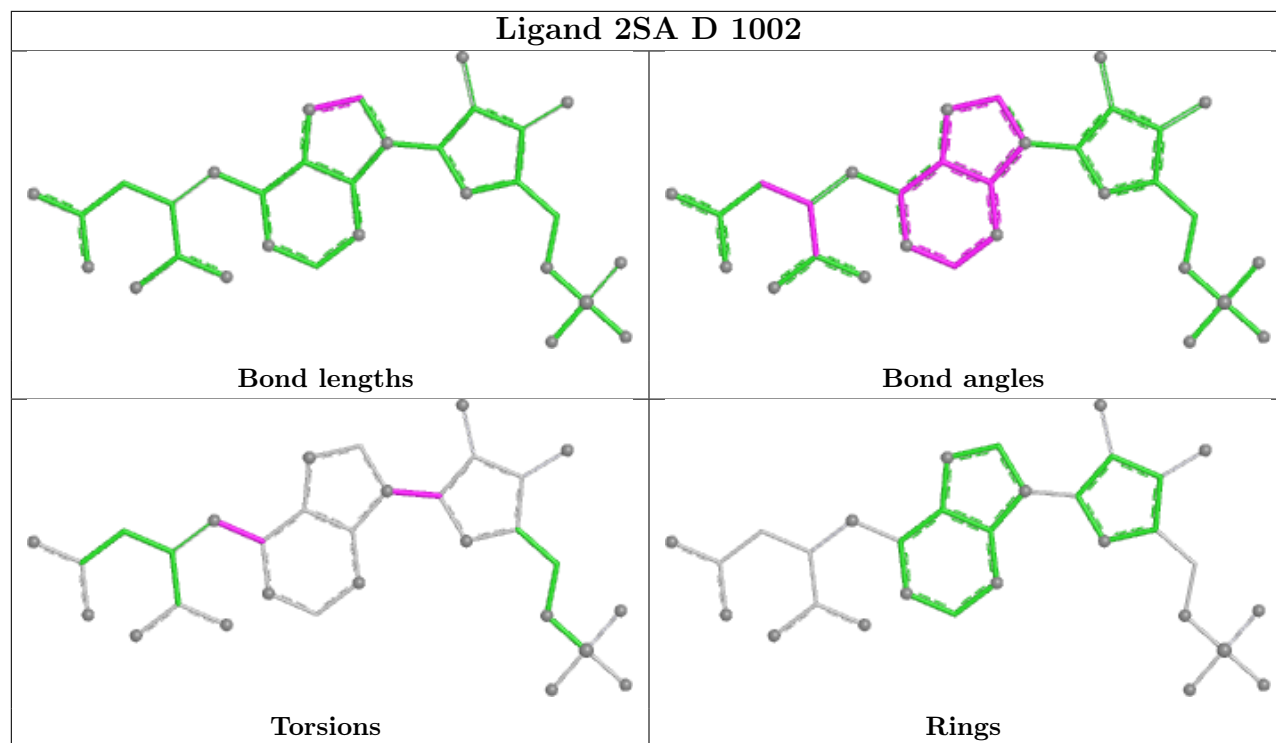
Continued on next page...

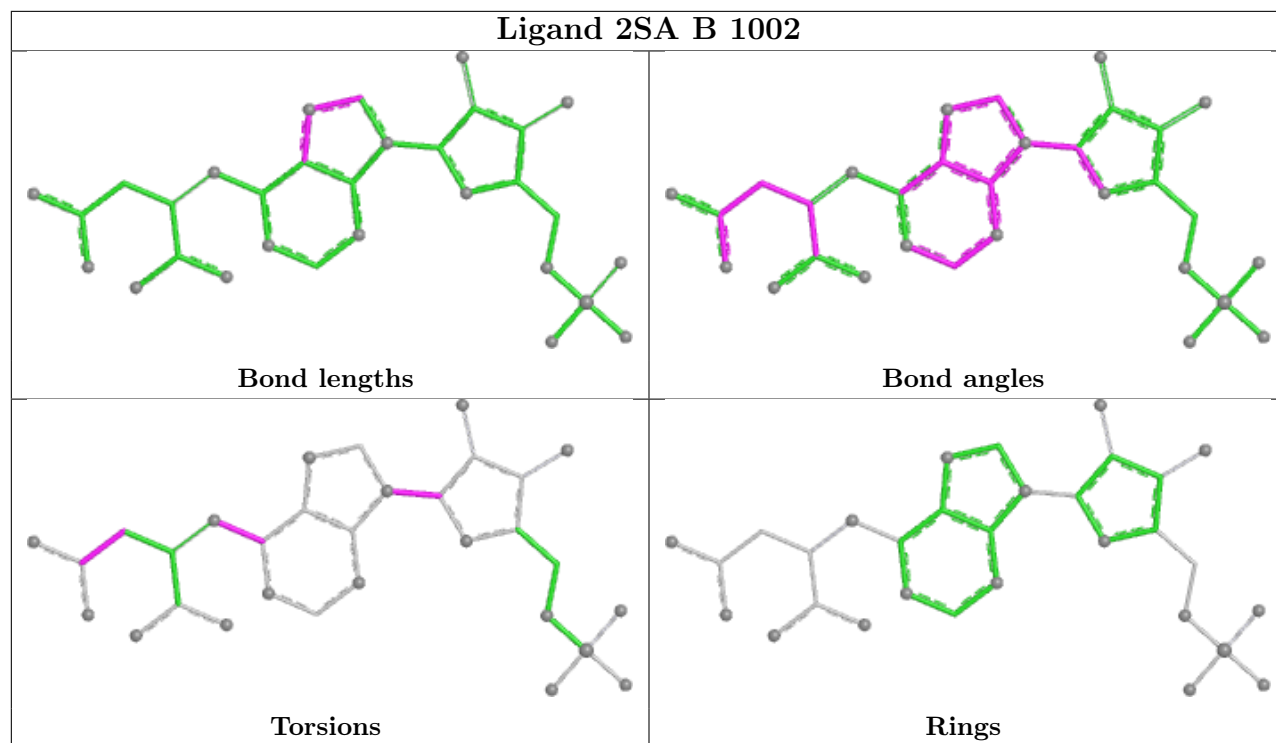
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1002	2SA	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	461/503 (91%)	1.27	82 (17%) 4 3	17, 34, 44, 55	4 (0%)
1	B	461/503 (91%)	0.92	27 (5%) 28 27	21, 34, 44, 50	1 (0%)
1	C	457/503 (90%)	1.71	151 (33%) 1 1	16, 33, 50, 61	4 (0%)
1	D	462/503 (91%)	1.46	119 (25%) 1 1	18, 33, 53, 63	3 (0%)
All	All	1841/2012 (91%)	1.34	379 (20%) 2 2	16, 33, 47, 63	12 (0%)

All (379) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	293	PRO	5.3
1	C	5	GLY	4.8
1	A	474	SER	4.8
1	C	436	ILE	4.7
1	D	397	GLN	4.6
1	C	423	LEU	4.6
1	C	294	TYR	4.6
1	C	93	HIS	4.6
1	C	394	GLY	4.5
1	D	475	VAL	4.4
1	A	5	GLY	4.3
1	C	431	ALA	4.3
1	C	390	VAL	4.3
1	C	427	ILE	4.3
1	D	403	ILE	4.2
1	C	395	SER	4.1
1	D	432	TYR	4.1
1	D	429	VAL	4.1
1	C	398	ASP	4.1
1	C	49	ALA	4.0
1	D	6	ASP	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	387	MET	4.0
1	A	294	TYR	4.0
1	C	385	ILE	4.0
1	D	5	GLY	4.0
1	D	395	SER	3.9
1	C	404	ARG	3.9
1	C	472	TYR	3.9
1	C	89	MET	3.8
1	C	386	ILE	3.8
1	C	212	PHE	3.8
1	B	282	PHE	3.7
1	D	393	GLY	3.6
1	C	400	HIS	3.6
1	C	397	GLN	3.6
1	D	427	ILE	3.6
1	C	97	HIS	3.6
1	C	8	GLY	3.6
1	C	392	ALA	3.5
1	B	294	TYR	3.5
1	D	396	ARG	3.5
1	D	436	ILE	3.5
1	B	5	GLY	3.5
1	C	403	ILE	3.5
1	D	419	GLY	3.5
1	C	446	PRO	3.4
1	C	411	ALA	3.4
1	C	438	SER	3.4
1	D	282	PHE	3.4
1	C	406	LEU	3.4
1	C	399	CYS	3.4
1	A	411	ALA	3.4
1	C	62	ILE	3.4
1	C	219	VAL	3.4
1	D	370	GLU	3.4
1	C	402	LYS	3.4
1	D	392	ALA	3.4
1	C	7	HIS	3.3
1	D	394	GLY	3.3
1	C	78	ALA	3.3
1	C	443	LEU	3.3
1	C	51	GLN	3.3
1	D	433	PHE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	6	ASP	3.3
1	D	405	VAL	3.3
1	D	388	ALA	3.3
1	C	444	LEU	3.3
1	C	387	MET	3.3
1	C	364	VAL	3.2
1	C	405	VAL	3.2
1	C	401	GLU	3.2
1	D	409	GLN	3.2
1	D	63	GLN	3.2
1	C	412	SER	3.2
1	D	440	LEU	3.2
1	D	385	ILE	3.1
1	C	433	PHE	3.1
1	D	108	LEU	3.1
1	A	466	TYR	3.1
1	A	473	GLU	3.1
1	D	390	VAL	3.1
1	A	436	ILE	3.1
1	D	11	ASP	3.1
1	A	88	VAL	3.1
1	A	295	LYS	3.1
1	A	444	LEU	3.1
1	D	238	ILE	3.1
1	D	402	LYS	3.0
1	A	403	ILE	3.0
1	C	106	ILE	3.0
1	C	96	GLY	3.0
1	C	60	GLU	3.0
1	C	408	GLN	3.0
1	A	419	GLY	3.0
1	D	197	GLY	3.0
1	A	52	THR	3.0
1	C	434	SER	3.0
1	D	449	PHE	3.0
1	C	381	ALA	2.9
1	A	423	LEU	2.9
1	C	469	LEU	2.9
1	A	418	GLY	2.9
1	C	72	ILE	2.9
1	D	294	TYR	2.9
1	A	71	ASN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	69	LEU	2.9
1	A	414	VAL	2.9
1	D	380	MET	2.9
1	C	57	ILE	2.9
1	C	70	GLU	2.9
1	A	282	PHE	2.9
1	A	387	MET	2.8
1	D	428	GLN	2.8
1	D	443	LEU	2.8
1	D	82	LYS	2.8
1	C	67	SER	2.8
1	D	157	PHE	2.8
1	A	93	HIS	2.8
1	C	85	ARG	2.8
1	C	388	ALA	2.8
1	C	99	CYS	2.8
1	D	57	ILE	2.8
1	D	424	ILE	2.8
1	C	384	ASN	2.8
1	D	49	ALA	2.8
1	C	429	VAL	2.8
1	D	226	VAL	2.8
1	B	403	ILE	2.8
1	A	412[A]	SER	2.8
1	D	67	SER	2.8
1	D	331	LEU	2.8
1	D	406	LEU	2.8
1	C	373	ILE	2.8
1	D	212	PHE	2.7
1	C	143	ALA	2.7
1	B	436	ILE	2.7
1	C	407	SER	2.7
1	C	448	SER	2.7
1	A	222	LEU	2.7
1	C	154	THR	2.7
1	C	165	LEU	2.7
1	C	382	THR	2.7
1	D	46	LEU	2.7
1	D	211	LEU	2.7
1	C	10	PRO	2.7
1	C	378	PRO	2.7
1	D	421	ASN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	385	ILE	2.7
1	C	224	LYS	2.7
1	D	240	GLY	2.7
1	A	53	LEU	2.7
1	C	209	LEU	2.7
1	D	93	HIS	2.7
1	C	180	CYS	2.7
1	C	58	THR	2.6
1	C	152	LEU	2.6
1	C	275	LEU	2.6
1	D	204	THR	2.6
1	C	366	PRO	2.6
1	D	378	PRO	2.6
1	C	11	ASP	2.6
1	A	219	VAL	2.6
1	C	393	GLY	2.6
1	A	273	ALA	2.6
1	C	357[A]	ASN	2.6
1	C	410	ALA	2.6
1	A	9	SER	2.6
1	A	365	TYR	2.6
1	C	243	TYR	2.6
1	D	34	TYR	2.6
1	C	156	GLY	2.6
1	D	111	THR	2.6
1	C	153	PRO	2.6
1	A	6	ASP	2.6
1	A	406	LEU	2.6
1	D	19[A]	SER	2.6
1	A	432	TYR	2.6
1	D	62	ILE	2.6
1	D	295	LYS	2.6
1	D	47	ALA	2.6
1	D	434	SER	2.6
1	D	208	PHE	2.5
1	C	63	GLN	2.5
1	A	427	ILE	2.5
1	C	92	VAL	2.5
1	D	88	VAL	2.5
1	A	96	GLY	2.5
1	D	209	LEU	2.5
1	D	222	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	417	GLU	2.5
1	D	413	VAL	2.5
1	C	466	TYR	2.5
1	C	9	SER	2.5
1	C	12	SER	2.5
1	D	407	SER	2.5
1	D	44	LEU	2.5
1	C	95	PHE	2.5
1	A	203	GLY	2.5
1	D	109	GLY	2.5
1	D	418	GLY	2.5
1	B	386	ILE	2.5
1	C	115	VAL	2.5
1	C	168	VAL	2.5
1	C	414	VAL	2.5
1	D	92	VAL	2.5
1	A	34	TYR	2.5
1	C	79	GLU	2.5
1	C	439	GLN	2.5
1	A	407	SER	2.5
1	C	242	THR	2.5
1	D	58	THR	2.5
1	D	382	THR	2.5
1	A	392	ALA	2.5
1	C	440	LEU	2.5
1	D	53	LEU	2.5
1	D	218	LYS	2.5
1	A	424	ILE	2.5
1	D	164	GLN	2.4
1	C	151	SER	2.4
1	C	391	LYS	2.4
1	A	379	PHE	2.4
1	C	457	VAL	2.4
1	D	72	ILE	2.4
1	D	79	GLU	2.4
1	D	219	VAL	2.4
1	A	395	SER	2.4
1	D	114	TYR	2.4
1	D	225	MET	2.4
1	C	84	LEU	2.4
1	D	400	HIS	2.4
1	B	451	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	54	GLY	2.4
1	C	71	ASN	2.4
1	B	462	GLU	2.4
1	C	282	PHE	2.4
1	C	460	PHE	2.4
1	B	475	VAL	2.4
1	D	386	ILE	2.4
1	A	447	SER	2.4
1	B	443	LEU	2.4
1	C	360	GLU	2.4
1	C	74	PHE	2.4
1	B	387	MET	2.4
1	C	33	ARG	2.4
1	A	472	TYR	2.3
1	D	381	ALA	2.3
1	B	444	LEU	2.3
1	C	118	ASN	2.3
1	C	420	ASP	2.3
1	A	276	LYS	2.3
1	C	389	MET	2.3
1	C	19	SER	2.3
1	D	198	VAL	2.3
1	D	454[A]	SER	2.3
1	D	217	HIS	2.3
1	C	164[A]	GLN	2.3
1	D	45	TRP	2.3
1	D	297	ASN	2.3
1	C	468	LEU	2.3
1	A	234	ARG	2.3
1	D	404	ARG	2.3
1	D	9	SER	2.3
1	A	105	ILE	2.3
1	C	413	VAL	2.3
1	D	115	VAL	2.3
1	D	414	VAL	2.3
1	D	221	GLN	2.3
1	A	388	ALA	2.3
1	D	110	ALA	2.3
1	C	377	LEU	2.3
1	A	70	GLU	2.3
1	C	28	PHE	2.3
1	B	356	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	369	ILE	2.3
1	C	424	ILE	2.3
1	A	198	VAL	2.3
1	A	429	VAL	2.3
1	A	85	ARG	2.3
1	A	47	ALA	2.3
1	A	66	LYS	2.3
1	A	361	GLY	2.3
1	A	415	LYS	2.3
1	D	230	ALA	2.3
1	A	331	LEU	2.3
1	C	461	LEU	2.3
1	A	425	GLU	2.2
1	D	107	HIS	2.2
1	B	151	SER	2.2
1	D	207	SER	2.2
1	A	212	PHE	2.2
1	C	358	ILE	2.2
1	B	405	VAL	2.2
1	A	49	ALA	2.2
1	A	89[A]	MET	2.2
1	A	440	LEU	2.2
1	C	365	TYR	2.2
1	C	409	GLN	2.2
1	B	447	SER	2.2
1	D	373	ILE	2.2
1	A	197	GLY	2.2
1	C	136	ALA	2.2
1	A	12	SER	2.2
1	A	151	SER	2.2
1	A	434[A]	SER	2.2
1	D	105	ILE	2.2
1	D	201	THR	2.2
1	D	420	ASP	2.2
1	B	465	VAL	2.2
1	C	104	GLY	2.2
1	C	416	GLN	2.2
1	D	77	ALA	2.2
1	A	272	LEU	2.2
1	C	108	LEU	2.2
1	C	155	LEU	2.2
1	C	222	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	140	SER	2.2
1	C	470	LYS	2.2
1	C	38	THR	2.2
1	C	450	THR	2.2
1	B	433	PHE	2.1
1	C	226	VAL	2.1
1	B	458	GLN	2.1
1	D	442	HIS	2.1
1	D	206	ALA	2.1
1	A	443	LEU	2.1
1	C	396	ARG	2.1
1	C	34	TYR	2.1
1	C	421	ASN	2.1
1	C	32	ASP	2.1
1	D	398	ASP	2.1
1	D	435	PRO	2.1
1	D	106	ILE	2.1
1	B	393	GLY	2.1
1	A	44	LEU	2.1
1	A	367	LYS	2.1
1	D	55	LEU	2.1
1	B	476	MET	2.1
1	C	380	MET	2.1
1	D	200	GLY	2.1
1	D	237	ILE	2.1
1	C	368	VAL	2.1
1	A	101	LYS	2.1
1	A	90	ALA	2.1
1	A	206	ALA	2.1
1	B	18	ALA	2.1
1	A	225	MET	2.1
1	A	10	PRO	2.1
1	A	396	ARG	2.1
1	D	196	ARG	2.1
1	A	393	GLY	2.1
1	B	156	GLY	2.1
1	C	176	ILE	2.1
1	A	405	VAL	2.1
1	C	160	PHE	2.1
1	C	465	VAL	2.1
1	D	39	TRP	2.1
1	C	18	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	410	ALA	2.1
1	D	377	LEU	2.0
1	A	164	GLN	2.0
1	A	416	GLN	2.0
1	C	356[A]	GLN	2.0
1	A	371	ARG	2.0
1	B	85	ARG	2.0
1	B	10	PRO	2.0
1	C	100	PRO	2.0
1	C	119	THR	2.0
1	B	472	TYR	2.0
1	D	13	TYR	2.0
1	C	65	MET	2.0
1	D	78	ALA	2.0
1	D	235	ALA	2.0
1	B	461	LEU	2.0
1	C	46	LEU	2.0
1	C	142	LEU	2.0
1	D	83	ARG	2.0
1	C	173	CYS	2.0
1	A	446	PRO	2.0
1	C	281	PRO	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
3	FUM	A	1001	8/8	0.77	0.13	41,41,42,43	0

Continued on next page...

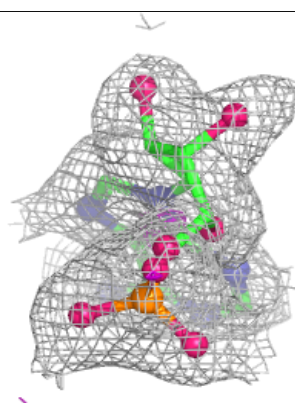
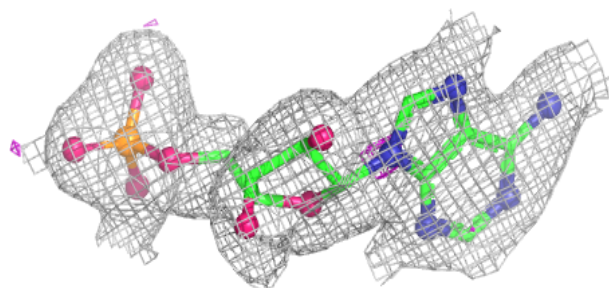
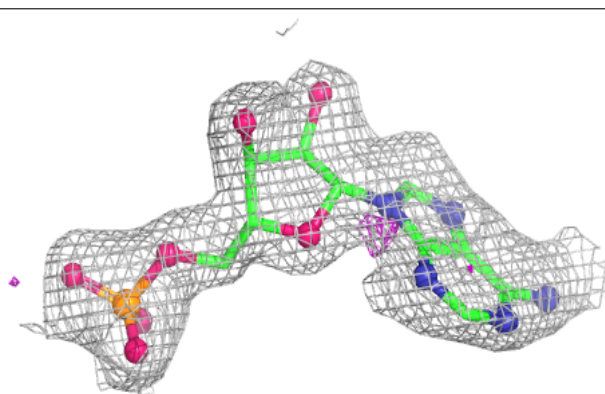
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	B	1004	6/6	0.77	0.16	49,50,51,51	0
4	GOL	C	1003	6/6	0.77	0.18	49,50,52,53	0
3	FUM	C	1001	8/8	0.81	0.15	41,42,43,44	0
4	GOL	B	1003	6/6	0.84	0.14	39,40,40,40	0
4	GOL	D	1003	6/6	0.86	0.12	33,35,35,36	0
4	GOL	A	1003	6/6	0.88	0.14	43,43,43,44	0
5	CL	A	2001	1/1	0.88	0.13	55,55,55,55	0
2	AMP	A	1000	23/23	0.90	0.10	26,36,37,37	0
2	AMP	C	1000	23/23	0.90	0.12	37,41,41,41	0
6	2SA	D	1002	31/31	0.92	0.09	18,20,22,24	0
5	CL	D	2001	1/1	0.93	0.06	29,29,29,29	0
6	2SA	B	1002	31/31	0.94	0.08	22,24,26,29	0
5	CL	A	2002	1/1	0.96	0.07	35,35,35,35	0
5	CL	D	2002	1/1	0.96	0.11	18,18,18,18	0
5	CL	B	2002	1/1	0.97	0.07	25,25,25,25	0
5	CL	C	2002	1/1	0.97	0.12	38,38,38,38	0
5	CL	B	2001	1/1	0.97	0.11	31,31,31,31	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.

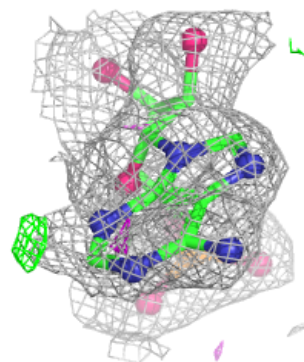
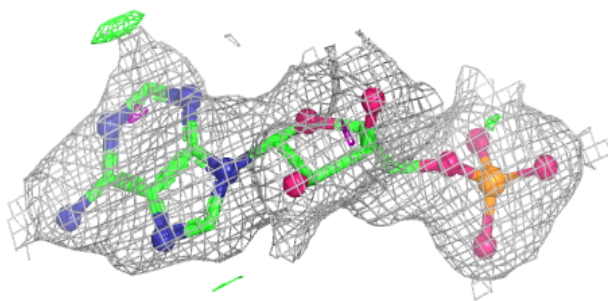
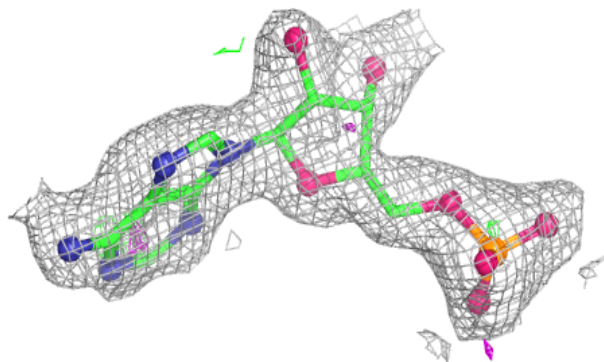
Electron density around AMP A 1000:

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

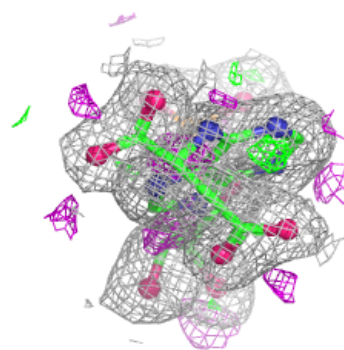
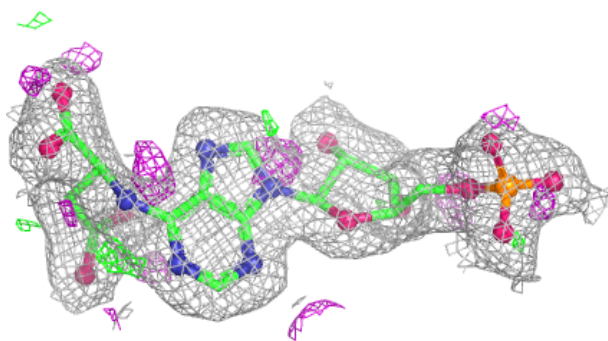
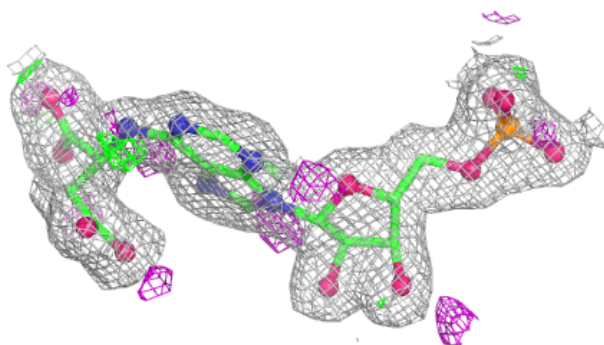


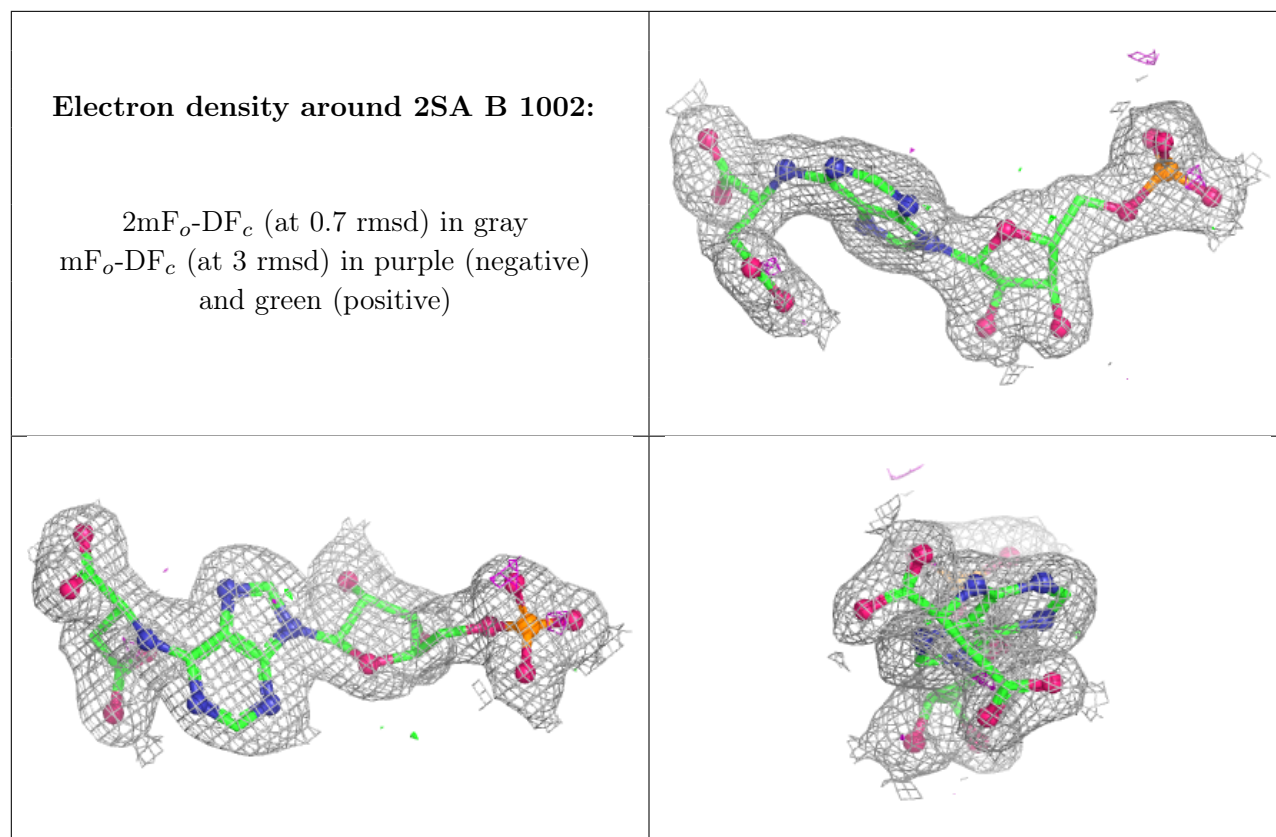
Electron density around AMP C 1000:

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

**Electron density around 2SA D 1002:**

$2mF_o-DF_c$ (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.