



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:48 PM UTC

PDB ID : 8HU6 / pdb_00008hu6
Title : AMP deaminase 2 in complex with AMP
Authors : Adachi, T.; Doi, S.
Deposited on : 2022-12-22
Resolution : 2.33 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

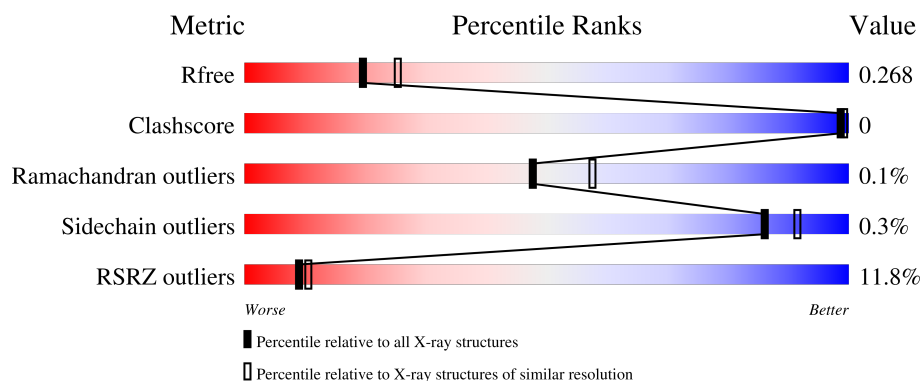
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	678	10% 89% • 9%
1	B	678	10% 92% • 7%
1	C	678	10% 89% • 9%
1	D	678	13% 89% • 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 41188 atoms, of which 20027 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 AMP deaminase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	614	Total	C	H	N	O	S	0	0	0
			9968	3209	4945	878	906	30			
1	B	629	Total	C	H	N	O	S	0	0	0
			10227	3286	5076	905	929	31			
1	C	619	Total	C	H	N	O	S	0	0	0
			10055	3234	4986	886	918	31			
1	D	621	Total	C	H	N	O	S	0	0	0
			10103	3247	5012	892	921	31			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	MET	-	initiating methionine	UNP Q01433
A	203	ASP	-	expression tag	UNP Q01433
A	204	TYR	-	expression tag	UNP Q01433
A	205	LYS	-	expression tag	UNP Q01433
A	206	ASP	-	expression tag	UNP Q01433
A	207	ASP	-	expression tag	UNP Q01433
A	208	ASP	-	expression tag	UNP Q01433
A	209	ASP	-	expression tag	UNP Q01433
A	210	LYS	-	expression tag	UNP Q01433
B	202	MET	-	initiating methionine	UNP Q01433
B	203	ASP	-	expression tag	UNP Q01433
B	204	TYR	-	expression tag	UNP Q01433
B	205	LYS	-	expression tag	UNP Q01433
B	206	ASP	-	expression tag	UNP Q01433
B	207	ASP	-	expression tag	UNP Q01433
B	208	ASP	-	expression tag	UNP Q01433
B	209	ASP	-	expression tag	UNP Q01433
B	210	LYS	-	expression tag	UNP Q01433
C	202	MET	-	initiating methionine	UNP Q01433
C	203	ASP	-	expression tag	UNP Q01433
C	204	TYR	-	expression tag	UNP Q01433

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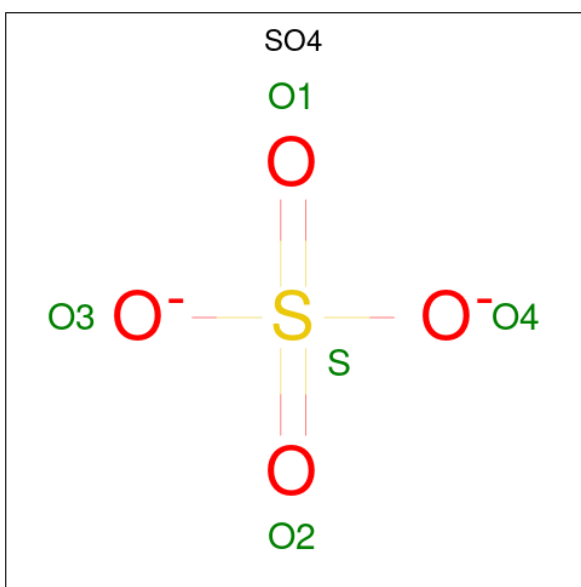
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Chain	Residue	Modelled	Actual	Comment	Reference
C	205	LYS	-	expression tag	UNP Q01433
C	206	ASP	-	expression tag	UNP Q01433
C	207	ASP	-	expression tag	UNP Q01433
C	208	ASP	-	expression tag	UNP Q01433
C	209	ASP	-	expression tag	UNP Q01433
C	210	LYS	-	expression tag	UNP Q01433
D	202	MET	-	initiating methionine	UNP Q01433
D	203	ASP	-	expression tag	UNP Q01433
D	204	TYR	-	expression tag	UNP Q01433
D	205	LYS	-	expression tag	UNP Q01433
D	206	ASP	-	expression tag	UNP Q01433
D	207	ASP	-	expression tag	UNP Q01433
D	208	ASP	-	expression tag	UNP Q01433
D	209	ASP	-	expression tag	UNP Q01433
D	210	LYS	-	expression tag	UNP Q01433

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

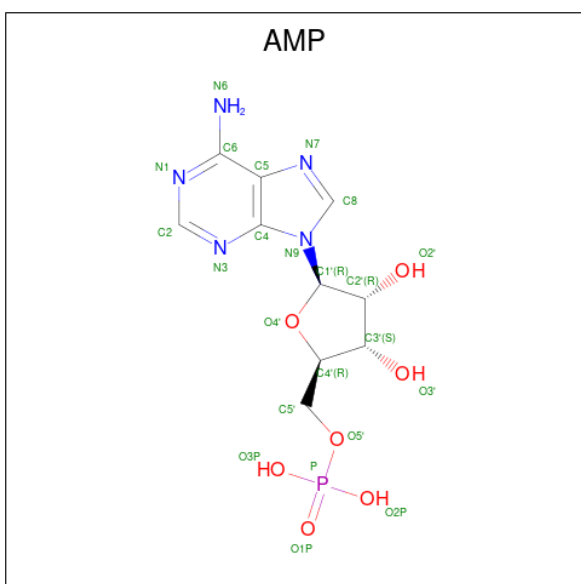
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

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



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		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	D	1	Total	C	H	N	O	P	0	0
			31	10	8	5	7	1		

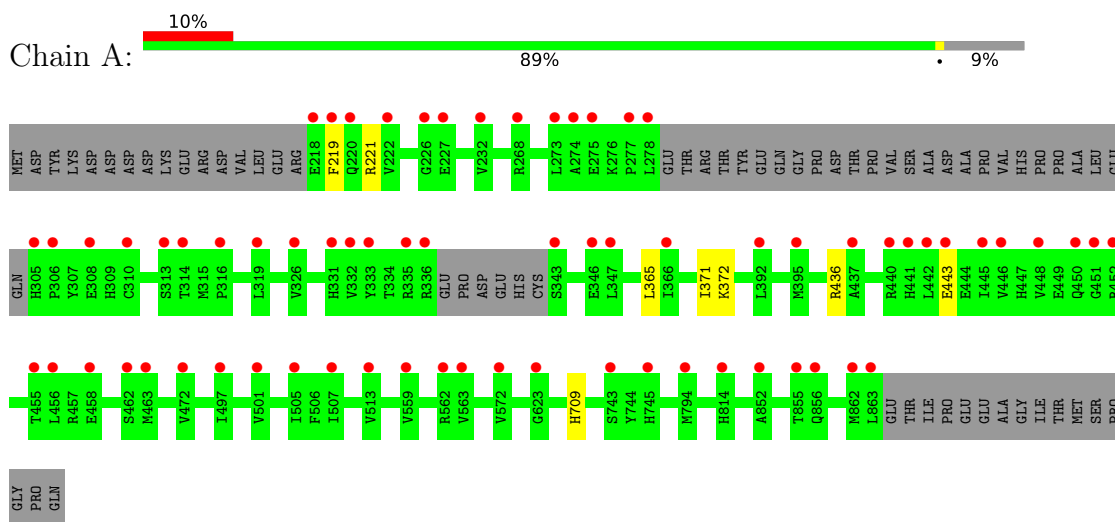
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	169	Total	O	0	0
			169	169		
5	B	179	Total	O	0	0
			179	179		
5	C	218	Total	O	0	0
			218	218		
5	D	214	Total	O	0	0
			214	214		

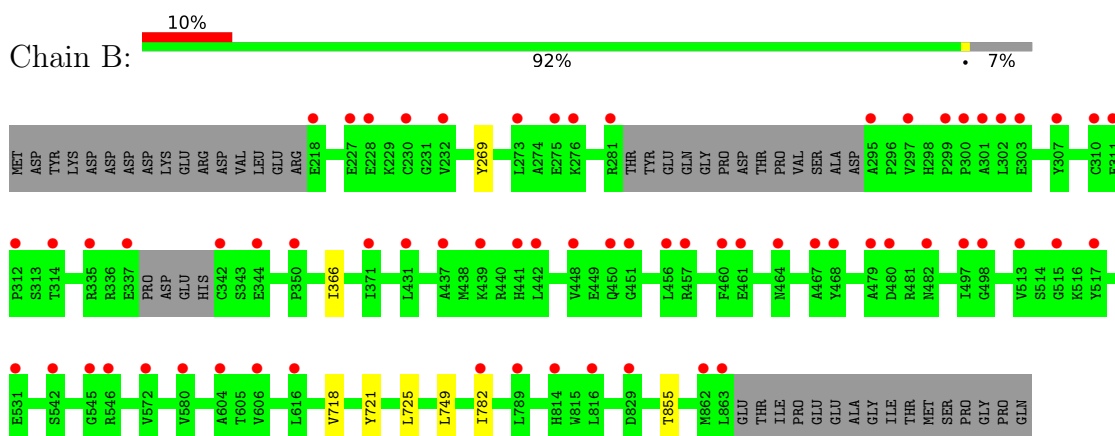
3 Residue-property plots [i](#)

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.

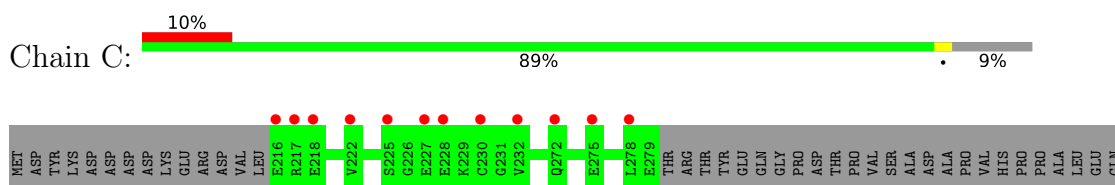
• Molecule 1: AMP deaminase 2

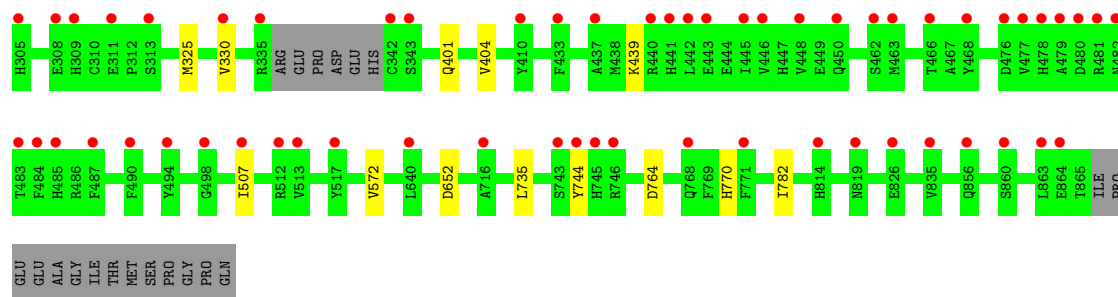


• Molecule 1: AMP deaminase 2

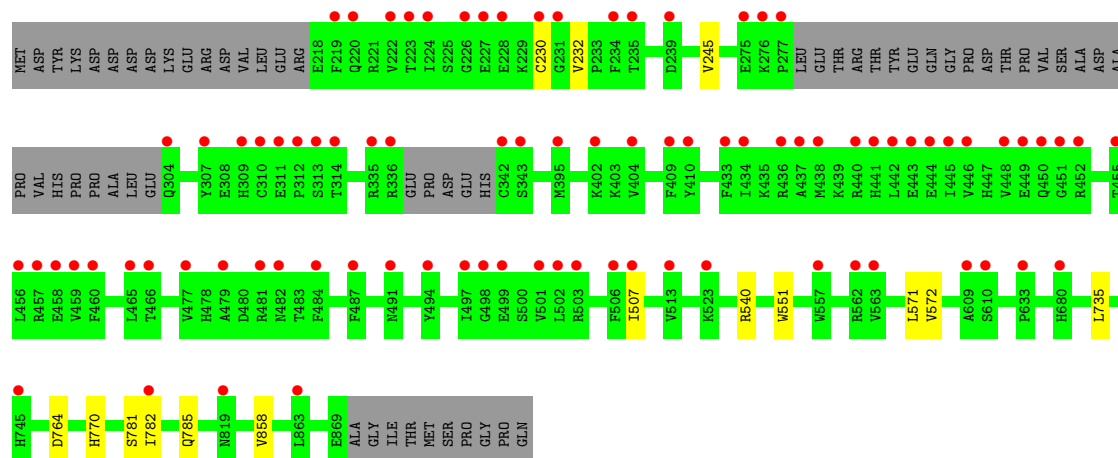
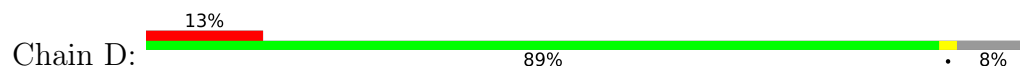


• Molecule 1: AMP deaminase 2





• Molecule 1: AMP deaminase 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	123.67Å 163.56Å 289.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.35 – 2.33 72.35 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.0 (72.35-2.33) 96.2 (72.35-2.33)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.237 , 0.268 0.238 , 0.268	Depositor DCC
R_{free} test set	6159 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.805	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	41188	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ZN, 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	0.22	0/5152	0.26	0/6976
1	B	0.21	0/5284	0.30	0/7156
1	C	0.22	0/5198	0.27	0/7037
1	D	0.27	0/5221	0.35	0/7068
All	All	0.23	0/20855	0.30	0/28237

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5023	4945	4942	3	0
1	B	5151	5076	5073	4	0
1	C	5069	4986	4983	6	0
1	D	5091	5012	5009	8	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	D	23	8	12	0	0
5	A	169	0	0	1	0
5	B	179	0	0	0	0
5	C	218	0	0	0	0
5	D	214	0	0	0	0
All	All	21161	20027	20019	20	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 0.

All (20) 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:735:LEU:HD23	1:D:770:HIS:CE1	2.30	0.67
1:D:230:CYS:SG	1:D:232:VAL:HG22	2.43	0.58
1:D:551:TRP:CH2	1:D:572:VAL:HG21	2.45	0.52
1:D:507:ILE:O	1:D:507:ILE:HG22	2.12	0.49
1:D:781:SER:O	1:D:785:GLN:HG2	2.14	0.48
1:A:365:LEU:HD11	1:A:371:ILE:HG21	1.98	0.46
1:A:219:PHE:CE2	1:A:221:ARG:HG2	2.51	0.46
1:C:401:GLN:O	1:C:404:VAL:HG12	2.15	0.45
1:C:325:MET:HG3	1:C:330:VAL:HG22	1.99	0.44
1:A:372:LYS:NZ	5:A:1014:HOH:O	2.51	0.43
1:C:782:ILE:HG12	1:D:782:ILE:HG12	2.01	0.43
1:C:572:VAL:O	1:C:572:VAL:HG13	2.19	0.42
1:B:721:TYR:CE2	1:B:725:LEU:HD11	2.54	0.42
1:B:749:LEU:HD23	1:B:749:LEU:C	2.43	0.42
1:C:744:TYR:CZ	1:C:782:ILE:HG22	2.56	0.41
1:C:735:LEU:HD23	1:C:770:HIS:CE1	2.56	0.41
1:B:366:ILE:HA	1:B:718:VAL:HG11	2.01	0.41
1:B:269:TYR:HB3	1:B:855:THR:HG21	2.03	0.41
1:D:540:ARG:HD3	1:D:571:LEU:HB2	2.03	0.40
1:D:245:VAL:HG21	1:D:858:VAL:HG21	2.02	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	608/678 (90%)	588 (97%)	19 (3%)	1 (0%)	43	50
1	B	623/678 (92%)	607 (97%)	16 (3%)	0	100	100
1	C	613/678 (90%)	597 (97%)	15 (2%)	1 (0%)	43	50
1	D	615/678 (91%)	598 (97%)	16 (3%)	1 (0%)	43	50
All	All	2459/2712 (91%)	2390 (97%)	66 (3%)	3 (0%)	48	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	764	ASP
1	D	764	ASP
1	A	709	HIS

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	553/612 (90%)	551 (100%)	2 (0%)	84	89
1	B	568/612 (93%)	567 (100%)	1 (0%)	87	93
1	C	559/612 (91%)	556 (100%)	3 (0%)	81	88
1	D	562/612 (92%)	562 (100%)	0	100	100
All	All	2242/2448 (92%)	2236 (100%)	6 (0%)	86	91

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	436	ARG
1	A	443	GLU
1	B	782	ILE
1	C	439	LYS
1	C	507	ILE
1	C	652	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	360	ASN
1	A	485	HIS
1	A	591	GLN
1	A	709	HIS
1	A	737	ASN
1	B	520	HIS
1	B	564	HIS
1	B	828	ASN
1	C	441	HIS
1	C	520	HIS
1	C	615	HIS
1	C	680	HIS
1	C	737	ASN
1	D	380	GLN
1	D	387	GLN
1	D	406	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	C	902	-	4,4,4	0.24	0	6,6,6	0.11	0
3	SO4	A	902	-	4,4,4	0.32	0	6,6,6	0.15	0
4	AMP	D	902	-	25,25,25	1.82	6 (24%)	37,38,38	3.10	10 (27%)
3	SO4	B	902	-	4,4,4	0.29	0	6,6,6	0.09	0
3	SO4	D	903	-	4,4,4	0.27	0	6,6,6	0.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AMP	D	902	-	-	2/10/26/26	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	902	AMP	C5-C4	4.77	1.47	1.39
4	D	902	AMP	C6-N6	4.56	1.45	1.34
4	D	902	AMP	C6-N1	-2.85	1.27	1.35
4	D	902	AMP	P-O3P	-2.69	1.44	1.54
4	D	902	AMP	P-O2P	-2.29	1.46	1.54
4	D	902	AMP	C2-N1	-2.07	1.30	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	902	AMP	C5-N7-C8	8.44	116.71	103.45
4	D	902	AMP	C4-C5-N7	-8.03	101.40	110.58
4	D	902	AMP	C4-N9-C8	7.89	114.02	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	902	AMP	N9-C8-N7	-7.04	103.95	113.94
4	D	902	AMP	C6-C5-N7	6.41	144.45	132.09
4	D	902	AMP	C2-N1-C6	4.36	125.90	118.73
4	D	902	AMP	O3P-P-O5'	2.62	113.50	106.67
4	D	902	AMP	C6-C5-C4	-2.22	114.15	117.18
4	D	902	AMP	O5'-P-O1P	2.19	112.36	106.44
4	D	902	AMP	C1'-N9-C8	-2.17	122.28	127.09

There are no chirality outliers.

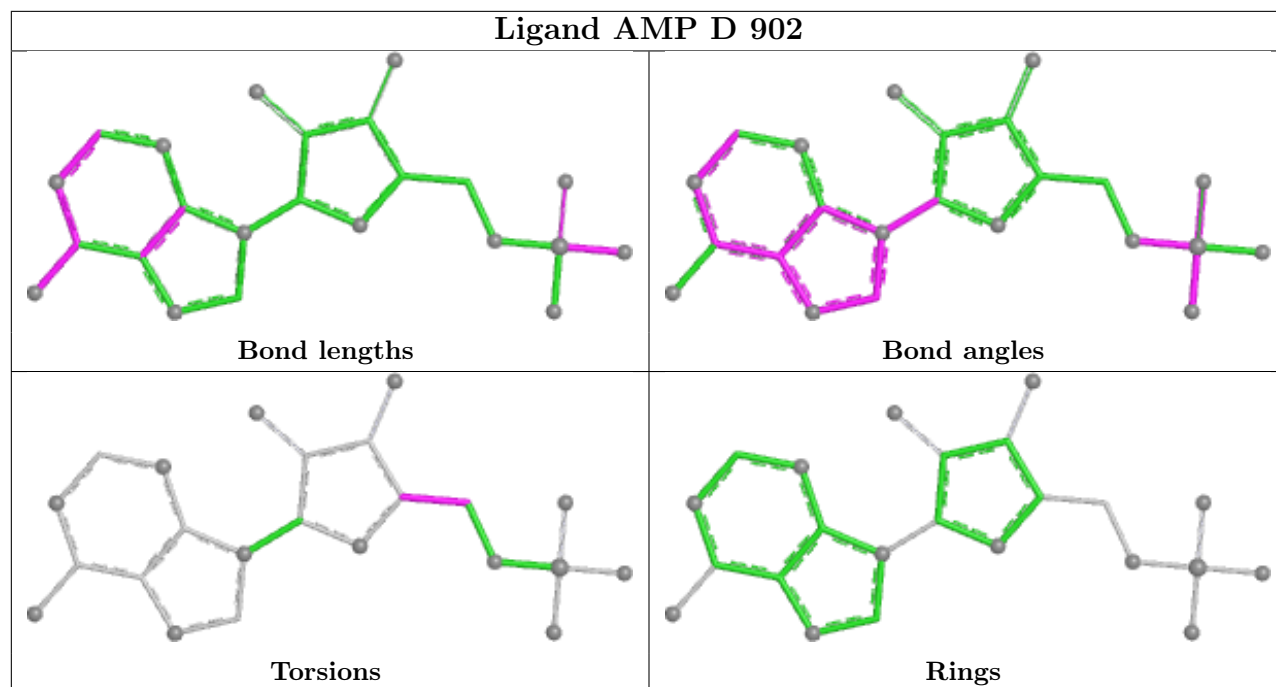
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	902	AMP	C3'-C4'-C5'-O5'
4	D	902	AMP	O4'-C4'-C5'-O5'

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 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	614/678 (90%)	1.00	69 (11%)	10 11	30, 45, 73, 101	0
1	B	629/678 (92%)	1.01	66 (10%)	11 13	30, 45, 73, 96	0
1	C	619/678 (91%)	0.90	70 (11%)	10 11	26, 43, 69, 93	0
1	D	621/678 (91%)	1.08	87 (14%)	6 7	30, 46, 78, 107	0
All	All	2483/2712 (91%)	1.00	292 (11%)	9 10	26, 45, 73, 107	0

All (292) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	863	LEU	5.0
1	A	220	GLN	4.5
1	D	446	VAL	4.4
1	C	441	HIS	4.3
1	B	451	GLY	4.2
1	C	216	GLU	4.1
1	D	481	ARG	4.1
1	A	275	GLU	3.9
1	B	342	CYS	3.9
1	C	442	LEU	3.9
1	D	456	LEU	3.9
1	D	459	VAL	3.8
1	A	445	ILE	3.8
1	D	451	GLY	3.7
1	D	227	GLU	3.6
1	D	443	GLU	3.6
1	D	445	ILE	3.6
1	A	505	ILE	3.6
1	B	448	VAL	3.5
1	D	310	CYS	3.5
1	C	484	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	231	GLY	3.4
1	A	440	ARG	3.4
1	D	304	GLN	3.4
1	B	297	VAL	3.3
1	D	239	ASP	3.3
1	A	442	LEU	3.3
1	A	451	GLY	3.3
1	A	226	GLY	3.3
1	B	230	CYS	3.3
1	B	863	LEU	3.2
1	D	498	GLY	3.2
1	D	745	HIS	3.2
1	A	562	ARG	3.1
1	A	443	GLU	3.1
1	D	482	ASN	3.1
1	A	448	VAL	3.1
1	D	442	LEU	3.1
1	B	281	ARG	3.1
1	D	224	ILE	3.1
1	D	434	ILE	3.1
1	C	487	PHE	3.1
1	D	487	PHE	3.1
1	D	452	ARG	3.1
1	A	441	HIS	3.1
1	D	276	LYS	3.1
1	D	441	HIS	3.0
1	C	437	ALA	3.0
1	A	446	VAL	3.0
1	C	494	TYR	3.0
1	A	343	SER	3.0
1	C	498	GLY	3.0
1	B	218	GLU	3.0
1	B	337	GLU	3.0
1	B	299	PRO	3.0
1	A	437	ALA	3.0
1	B	301	ALA	3.0
1	D	609	ALA	3.0
1	D	513	VAL	3.0
1	A	852	ALA	2.9
1	A	305	HIS	2.9
1	C	477	VAL	2.9
1	A	507	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	343	SER	2.9
1	C	342	CYS	2.9
1	A	743	SER	2.9
1	D	307	TYR	2.9
1	C	864	GLU	2.9
1	D	610	SER	2.8
1	C	517	TYR	2.8
1	A	319	LEU	2.8
1	B	606	VAL	2.8
1	D	444	GLU	2.8
1	C	445	ILE	2.8
1	A	277	PRO	2.8
1	A	306	PRO	2.8
1	D	440	ARG	2.8
1	D	234	PHE	2.8
1	D	562	ARG	2.8
1	B	437	ALA	2.8
1	B	464	ASN	2.7
1	D	230	CYS	2.7
1	B	275	GLU	2.7
1	D	311	GLU	2.7
1	D	466	THR	2.7
1	B	302	LEU	2.7
1	C	222	VAL	2.7
1	A	314	THR	2.7
1	C	308	GLU	2.7
1	B	442	LEU	2.7
1	A	274	ALA	2.7
1	C	478	HIS	2.7
1	C	745	HIS	2.7
1	C	466	THR	2.7
1	A	335	ARG	2.7
1	A	862	MET	2.7
1	B	468	TYR	2.6
1	B	482	ASN	2.6
1	B	531	GLU	2.6
1	C	218	GLU	2.6
1	A	513	VAL	2.6
1	D	448	VAL	2.6
1	D	277	PRO	2.6
1	C	640	LEU	2.6
1	A	218	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	227	GLU	2.6
1	D	449	GLU	2.6
1	D	436	ARG	2.6
1	C	482	ASN	2.6
1	A	326	VAL	2.6
1	A	497	ILE	2.6
1	C	863	LEU	2.6
1	A	346	GLU	2.6
1	D	228	GLU	2.5
1	B	335	ARG	2.5
1	C	746	ARG	2.5
1	B	479	ALA	2.5
1	D	680	HIS	2.5
1	D	275	GLU	2.5
1	D	342	CYS	2.5
1	A	623	GLY	2.5
1	B	300	PRO	2.5
1	D	226	GLY	2.5
1	A	331	HIS	2.5
1	A	745	HIS	2.5
1	C	309	HIS	2.5
1	A	501	VAL	2.5
1	B	782	ILE	2.5
1	B	303	GLU	2.5
1	A	268	ARG	2.5
1	A	336	ARG	2.5
1	C	335	ARG	2.5
1	B	450	GLN	2.5
1	B	461	GLU	2.5
1	C	481	ARG	2.5
1	C	507	ILE	2.5
1	D	497	ILE	2.5
1	B	295	ALA	2.5
1	D	437	ALA	2.5
1	C	275	GLU	2.4
1	C	512	ARG	2.4
1	D	455	THR	2.4
1	D	863	LEU	2.4
1	A	455	THR	2.4
1	A	222	VAL	2.4
1	A	472	VAL	2.4
1	D	501	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	782	ILE	2.4
1	A	273	LEU	2.4
1	D	494	TYR	2.4
1	A	856	GLN	2.4
1	C	217	ARG	2.4
1	D	220	GLN	2.4
1	A	308	GLU	2.4
1	A	219	PHE	2.4
1	B	460	PHE	2.4
1	D	507	ILE	2.4
1	B	616	LEU	2.4
1	B	431	LEU	2.4
1	C	225	SER	2.3
1	C	743	SER	2.3
1	D	438	MET	2.3
1	A	366	ILE	2.3
1	B	441	HIS	2.3
1	C	450	GLN	2.3
1	C	313	SER	2.3
1	B	457	ARG	2.3
1	C	440	ARG	2.3
1	A	332	VAL	2.3
1	C	228	GLU	2.3
1	C	311	GLU	2.3
1	D	404	VAL	2.3
1	D	235	THR	2.3
1	A	462	SER	2.3
1	C	814	HIS	2.3
1	D	458	GLU	2.3
1	C	232	VAL	2.3
1	C	448	VAL	2.3
1	D	460	PHE	2.3
1	D	563	VAL	2.3
1	B	456	LEU	2.3
1	C	480	ASP	2.3
1	D	312	PRO	2.3
1	D	410	TYR	2.3
1	C	462	SER	2.3
1	C	826	GLU	2.3
1	D	450	GLN	2.3
1	C	446	VAL	2.3
1	C	819	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	316	PRO	2.2
1	B	498	GLY	2.2
1	B	546	ARG	2.2
1	D	335	ARG	2.2
1	C	485	HIS	2.2
1	C	716	ALA	2.2
1	D	523	LYS	2.2
1	A	563	VAL	2.2
1	A	572	VAL	2.2
1	C	513	VAL	2.2
1	A	395	MET	2.2
1	A	463	MET	2.2
1	D	633	PRO	2.2
1	B	228	GLU	2.2
1	C	768	GLN	2.2
1	C	483	THR	2.2
1	C	744	TYR	2.2
1	D	313	SER	2.2
1	A	456	LEU	2.2
1	B	273	LEU	2.2
1	B	232	VAL	2.2
1	D	409	PHE	2.2
1	D	491	ASN	2.2
1	B	310	CYS	2.2
1	B	545	GLY	2.2
1	C	230	CYS	2.2
1	C	278	LEU	2.2
1	A	232	VAL	2.2
1	B	513	VAL	2.2
1	B	829	ASP	2.2
1	D	477	VAL	2.2
1	B	439	LYS	2.2
1	D	479	ALA	2.2
1	D	503	ARG	2.1
1	A	392	LEU	2.1
1	B	371	ILE	2.1
1	C	476	ASP	2.1
1	D	222	VAL	2.1
1	B	276	LYS	2.1
1	C	490	PHE	2.1
1	D	219	PHE	2.1
1	D	402	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	309	HIS	2.1
1	A	310	CYS	2.1
1	B	604	ALA	2.1
1	D	336	ARG	2.1
1	C	410	TYR	2.1
1	C	463	MET	2.1
1	A	458	GLU	2.1
1	C	433	PHE	2.1
1	D	433	PHE	2.1
1	D	506	PHE	2.1
1	B	542	SER	2.1
1	D	223	THR	2.1
1	A	278	LEU	2.1
1	B	227	GLU	2.1
1	B	344	GLU	2.1
1	B	816	LEU	2.1
1	D	499	GLU	2.1
1	B	307	TYR	2.1
1	C	468	TYR	2.1
1	A	450	GLN	2.1
1	C	835	VAL	2.1
1	A	855	THR	2.1
1	D	343	SER	2.1
1	C	479	ALA	2.1
1	A	347	LEU	2.1
1	A	814	HIS	2.1
1	B	350	PRO	2.1
1	B	515	GLY	2.1
1	D	484	PHE	2.1
1	A	452	ARG	2.1
1	D	457	ARG	2.1
1	B	314	THR	2.0
1	B	862	MET	2.0
1	D	395	MET	2.0
1	B	311	GLU	2.0
1	C	272	GLN	2.0
1	B	480	ASP	2.0
1	B	789	LEU	2.0
1	D	465	LEU	2.0
1	D	502	LEU	2.0
1	B	312	PRO	2.0
1	A	333	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	517	TYR	2.0
1	A	559	VAL	2.0
1	B	572	VAL	2.0
1	B	580	VAL	2.0
1	C	330	VAL	2.0
1	C	771	PHE	2.0
1	D	557	TRP	2.0
1	A	227	GLU	2.0
1	A	794	MET	2.0
1	A	313	SER	2.0
1	C	443	GLU	2.0
1	C	860	SER	2.0
1	D	314	THR	2.0
1	B	467	ALA	2.0
1	B	814	HIS	2.0
1	C	305	HIS	2.0
1	C	856	GLN	2.0
1	D	819	ASN	2.0
1	B	497	ILE	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.

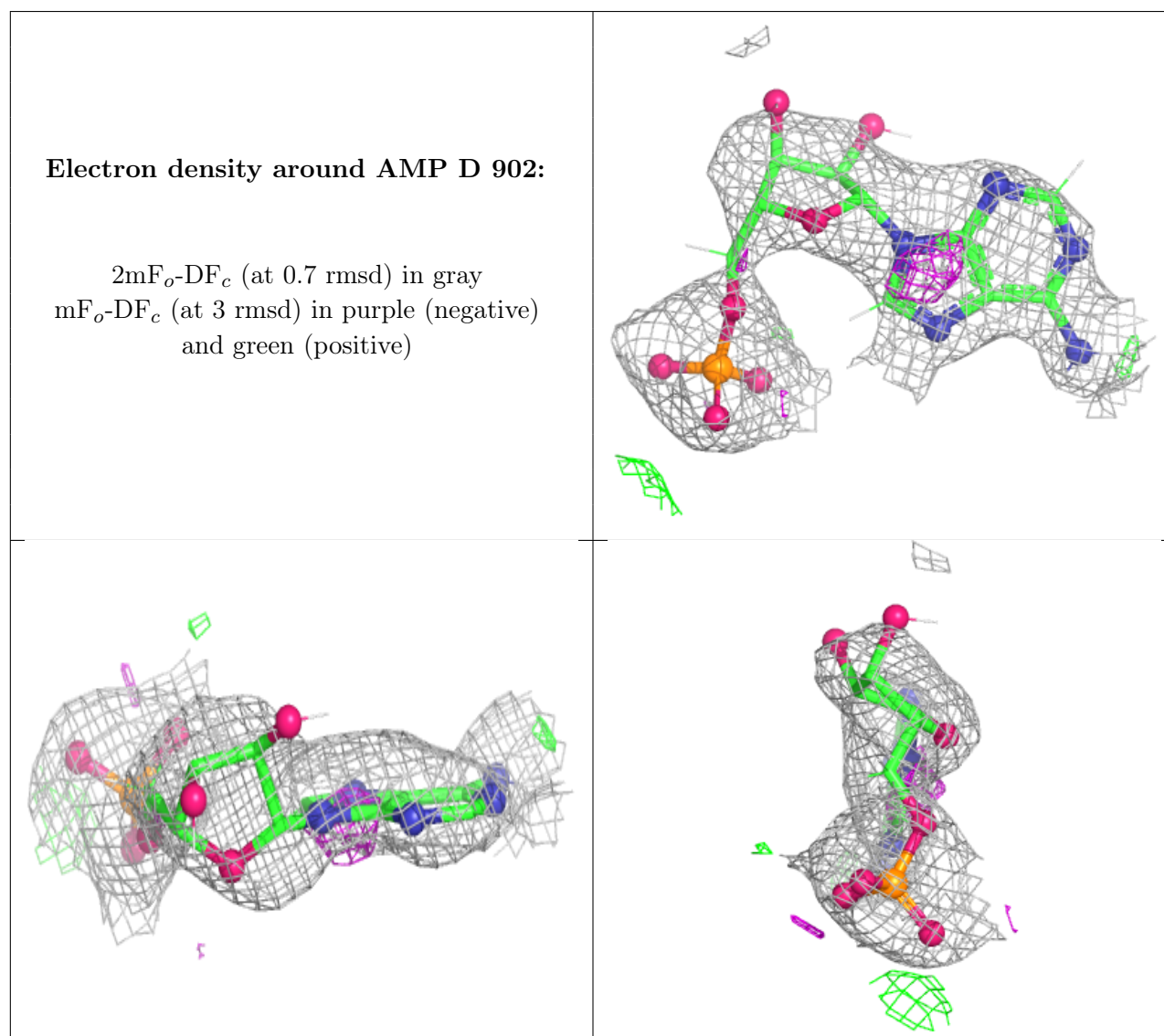
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	AMP	D	902	23/23	0.82	0.15	45,53,66,66	0
3	SO4	D	903	5/5	0.83	0.16	52,57,64,64	0
3	SO4	B	902	5/5	0.84	0.18	51,52,58,62	0
3	SO4	A	902	5/5	0.94	0.09	41,42,49,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	C	902	5/5	0.95	0.10	39,39,48,50	0
2	ZN	D	901	1/1	0.98	0.06	32,32,32,32	0
2	ZN	B	901	1/1	0.98	0.04	30,30,30,30	0
2	ZN	A	901	1/1	0.99	0.10	38,38,38,38	0
2	ZN	C	901	1/1	1.00	0.03	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.