

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	8HU6
Title	:	AMP deaminase 2 in complex with AMP
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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 (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 (1)) 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	:	2.31.3
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)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (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 <=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	А	678	90%	• 9%
1	В	678	<u>5%</u> 92%	• 7%
1	С	678	<mark>6%</mark> 89%	• 9%
1	D	678	89%	• 8%



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2 Entry composition (i)

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.

Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace
1	Δ	614	Total	С	Η	Ν	0	\mathbf{S}	0	0	0
1	A	014	9968	3209	4945	878	906	30	0		0
1	р	620	Total	С	Η	Ν	0	S	0	0	0
1	I D	029	10227	3286	5076	905	929	31	0		
1	1 0	610	Total	С	Η	Ν	0	S	0	0	0
	019	10055	3234	4986	886	918	31	0	0	0	
1	1 D	691	Total	С	Н	Ν	0	S	0	0	0
	021	10103	3247	5012	892	921	31	U	U	U	

• Molecule 1 is a protein called AMP deaminase 2.

There are 36 discrepancies between the modelled and reference sequences:

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



Chain	Residue	Modelled	Actual	Comment	Reference
С	205	LYS	-	expression tag	UNP Q01433
С	206	ASP	-	expression tag	UNP Q01433
С	207	ASP	-	expression tag	UNP Q01433
С	208	ASP	-	expression tag	UNP Q01433
С	209	ASP	-	expression tag	UNP Q01433
С	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 (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Zn 1 1	0	0
2	В	1	Total Zn 1 1	0	0
2	С	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

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





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	П	1	Total	С	Η	Ν	Ο	Р	0	0
4 D	1	31	10	8	5	7	1	0	0	

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	169	Total O 169 169	0	0
5	В	179	Total O 179 179	0	0
5	С	218	Total O 218 218	0	0
5	D	214	Total O 214 214	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: AMP deaminase 2







4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	123.67Å 163.56Å 289.38Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	72.35 - 2.33	Depositor
Resolution (A)	144.69 - 2.33	EDS
% Data completeness	99.0 (72.35-2.33)	Depositor
(in resolution range)	96.3(144.69-2.33)	EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.03 (at 2.34 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
B B.	0.237 , 0.268	Depositor
Π, Π_{free}	0.234 , 0.265	DCC
R_{free} test set	6159 reflections $(5.01%)$	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 , 46.1	EDS
L-test for $twinning^2$	$ < L >=0.44, < L^2>=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.

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.



¹Intensities estimated from amplitudes.

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, SO4, ZN $\,$

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).

Mal	Chain	Bond	lengths	Bond angles		
WIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.28	0/5152	0.46	0/6976	
1	В	0.28	0/5284	0.47	0/7156	
1	С	0.30	0/5198	0.48	0/7037	
1	D	0.30	0/5221	0.48	0/7068	
All	All	0.29	0/20855	0.47	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	А	5023	4945	4942	2	0
1	В	5151	5076	5073	3	0
1	С	5069	4986	4983	6	0
1	D	5091	5012	5009	8	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
3	А	5	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes						
3	В	5	0	0	0	0						
3	С	5	0	0	0	0						
3	D	5	0	0	0	0						
4	D	23	8	12	0	0						
5	А	169	0	0	0	0						
5	В	179	0	0	0	0						
5	С	218	0	0	0	0						
5	D	214	0	0	0	0						
All	All	21161	20027	20019	18	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 (18) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	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: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: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 (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	Perce	ntiles
1	А	608/678~(90%)	588 (97%)	19 (3%)	1 (0%)	47	55
1	В	623/678~(92%)	607~(97%)	16 (3%)	0	100	100
1	С	613/678~(90%)	597 (97%)	15 (2%)	1 (0%)	47	55
1	D	615/678~(91%)	598~(97%)	16 (3%)	1 (0%)	47	55
All	All	2459/2712 (91%)	2390 (97%)	66 (3%)	3 (0%)	51	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	764	ASP
1	D	764	ASP
1	А	709	HIS

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	Perce	entiles
1	А	553/612~(90%)	551 (100%)	2(0%)	91	95
1	В	568/612~(93%)	568 (100%)	0	100	100
1	С	559/612~(91%)	556 (100%)	3~(0%)	88	93
1	D	562/612~(92%)	561 (100%)	1 (0%)	93	96
All	All	2242/2448~(92%)	2236 (100%)	6 (0%)	92	96

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



Mol	Chain	Res	Type
1	А	436	ARG
1	А	443	GLU
1	С	439	LYS
1	С	607	HIS
1	С	652	ASP
1	D	591	GLN

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such side chains are listed below:

Mol	Chain	Res	Type
1	В	564	HIS
1	D	745	HIS

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 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 T	Turne	Chain	Dec	es Link	Bond lengths			Bond angles		
MOI	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	С	902	-	4,4,4	0.13	0	6,6,6	0.10	0
3	SO4	А	902	-	4,4,4	0.23	0	6,6,6	0.13	0



Mol Tyr	Turne	Chain	Bos	Tipk	Bond lengths			Bond angles		
	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	D	903	-	4,4,4	0.17	0	6,6,6	0.08	0
4	AMP	D	902	-	22,25,25	1.57	6 (27%)	25,38,38	2.09	4 (16%)
3	SO4	В	902	-	4,4,4	0.18	0	6,6,6	0.06	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	-	-	2/6/26/26	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	C6-N6	3.23	1.45	1.34
4	D	902	AMP	P-O3P	-2.61	1.44	1.54
4	D	902	AMP	C5-C4	2.52	1.47	1.40
4	D	902	AMP	C8-N7	-2.37	1.30	1.34
4	D	902	AMP	P-O2P	-2.22	1.46	1.54
4	D	902	AMP	C6-N1	-2.12	1.27	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	D	902	AMP	C4-C5-N7	-7.68	101.40	109.40
4	D	902	AMP	C2-N1-C6	4.18	125.90	118.75
4	D	902	AMP	O3P-P-O5'	2.54	113.50	106.73
4	D	902	AMP	O5'-P-O1P	2.10	112.36	106.47

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 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.



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, 95^{th} 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	А	614/678~(90%)	0.78	41 (6%)	17	25	27, 41, 66, 92	0
1	В	629/678~(92%)	0.75	32~(5%)	28	39	27, 41, 66, 88	0
1	С	619/678~(91%)	0.74	40 (6%)	18	26	24, 39, 62, 85	0
1	D	621/678~(91%)	0.82	47 (7%)	13	20	27, 42, 72, 96	0
All	All	2483/2712 (91%)	0.77	160 (6%)	19	27	24, 41, 67, 96	0

All (160) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	А	863	LEU	8.0
1	А	275	GLU	6.0
1	С	216	GLU	5.6
1	D	452	ARG	5.6
1	С	217	ARG	5.0
1	D	227	GLU	4.1
1	D	228	GLU	4.0
1	А	562	ARG	4.0
1	А	507	ILE	3.9
1	D	481	ARG	3.8
1	А	227	GLU	3.8
1	А	442	LEU	3.6
1	D	863	LEU	3.6
1	С	494	TYR	3.6
1	В	232	VAL	3.5
1	С	308	GLU	3.5
1	С	218	GLU	3.4
1	В	450	GLN	3.3
1	А	513	VAL	3.3
1	С	517	TYR	3.3
1	В	342	CYS	3.2



Mol	Chain	Res	Type	RSRZ
1	D	501	VAL	3.2
1	D	562	ARG	3.2
1	А	220	GLN	3.2
1	С	441	HIS	3.2
1	В	863	LEU	3.2
1	В	448	VAL	3.2
1	D	456	LEU	3.1
1	D	451	GLY	3.1
1	С	437	ALA	3.1
1	D	335	ARG	3.1
1	D	459	VAL	3.0
1	А	443	GLU	3.0
1	D	487	PHE	3.0
1	С	487	PHE	3.0
1	D	494	TYR	2.9
1	В	301	ALA	2.9
1	А	440	ARG	2.9
1	С	507	ILE	2.9
1	В	443	GLU	2.9
1	С	477	VAL	2.8
1	В	281	ARG	2.8
1	С	498	GLY	2.8
1	D	434	ILE	2.8
1	D	457	ARG	2.8
1	D	745	HIS	2.7
1	А	268	ARG	2.7
1	А	448	VAL	2.7
1	С	513	VAL	2.7
1	D	441	HIS	2.7
1	D	224	ILE	2.7
1	D	507	ILE	2.7
1	В	442	LEU	2.7
1	D	563	VAL	2.7
1	C	481	ARG	2.7
1	A	346	GLU	2.7
1	A	222	VAL	2.7
1	С	335	ARG	2.6
1	С	484	PHE	2.6
1	В	302	LEU	2.6
1	C	485	HIS	2.6
1	B	477	VAL	2.6
1	D	505	ILE	2.6



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Mol	Chain	Res	Type	RSRZ			
1	D	498	GLY	2.5			
1	А	437	ALA	2.5			
1	А	505	ILE	2.5			
1	В	297	VAL	2.5			
1	С	222	VAL	2.5			
1	D	782	ILE	2.5			
1	D	449	GLU	2.5			
1	D	443	GLU	2.5			
1	В	531	GLU	2.5			
1	А	852	ALA	2.5			
1	А	497	ILE	2.5			
1	С	744	TYR	2.5			
1	С	309	HIS	2.5			
1	В	571	LEU	2.4			
1	С	819	ASN	2.4			
1	А	451	GLY	2.4			
1	С	403	LYS	2.4			
1	D	735	LEU	2.4			
1	D	482	ASN	2.4			
1	В	487	PHE	2.4			
1	В	230	CYS	2.4			
1	В	403	LYS	2.4			
1	В	439	LYS	2.4			
1	А	445	ILE	2.4			
1	А	572	VAL	2.4			
1	В	218	GLU	2.4			
1	А	512	ARG	2.4			
1	А	464	ASN	2.4			
1	В	517	TYR	2.3			
1	D	448	VAL	2.3			
1	D	450	GLN	2.3			
1	С	482	ASN	2.3			
1	А	308	GLU	2.3			
1	D	276	LYS	2.3			
1	А	456	LEU	2.3			
1	В	222	VAL	2.3			
1	С	448	VAL	2.3			
1	В	582	ARG	2.3			
1	С	228	GLU	2.3			
1	A	862	MET	2.3			
1	С	232	VAL	2.3			
1	A	670	LEU	2.3			



8HU	J6
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Mol	Chain	Res	Type	RSRZ
1	D	310	CYS	2.3
1	D	811	VAL	2.3
1	С	864	GLU	2.2
1	С	858	VAL	2.2
1	D	786	VAL	2.2
1	D	445	ILE	2.2
1	А	673	LEU	2.2
1	А	326	VAL	2.2
1	В	546	ARG	2.2
1	D	546	ARG	2.2
1	А	559	VAL	2.2
1	В	303	GLU	2.2
1	В	441	HIS	2.2
1	В	456	LEU	2.2
1	С	640	LEU	2.2
1	А	786	VAL	2.2
1	В	299	PRO	2.2
1	В	513	VAL	2.2
1	С	512	ARG	2.2
1	С	342	CYS	2.2
1	А	273	LEU	2.2
1	С	227	GLU	2.2
1	D	313	SER	2.2
1	С	450	GLN	2.2
1	D	513	VAL	2.1
1	А	452	ARG	2.1
1	С	865	THR	2.1
1	D	506	PHE	2.1
1	D	270	LEU	2.1
1	А	226	GLY	2.1
1	А	745	HIS	2.1
1	А	277	PRO	2.1
1	А	314	THR	2.1
1	В	275	GLU	2.1
1	D	741	PHE	2.1
1	В	782	ILE	2.1
1	D	239	ASP	2.1
1	A	267	ARG	2.1
1	C	461	GLU	2.1
1	C	440	ARG	2.1
1	Ā	376	TYR	2.1
1	С	442	LEU	2.0



Mol	Chain	Res	Type	RSRZ
1	D	497	ILE	2.0
1	D	403	LYS	2.0
1	D	438	MET	2.0
1	С	466	THR	2.0
1	В	277	PRO	2.0
1	В	572	VAL	2.0
1	D	234	PHE	2.0
1	D	409	PHE	2.0
1	D	410	TYR	2.0
1	С	478	HIS	2.0
1	С	319	LEU	2.0
1	А	794	MET	2.0
1	А	856	GLN	2.0

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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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	SO4	D	903	5/5	0.85	0.15	52,57,64,64	0
4	AMP	D	902	23/23	0.89	0.28	$45,\!53,\!66,\!66$	0
3	SO4	В	902	5/5	0.92	0.20	$51,\!52,\!58,\!62$	0
3	SO4	А	902	5/5	0.96	0.16	41,42,49,50	0
2	ZN	В	901	1/1	0.97	0.17	30,30,30,30	0
2	ZN	D	901	1/1	0.97	0.20	32,32,32,32	0
3	SO4	С	902	5/5	0.98	0.16	39,39,48,50	0
2	ZN	А	901	1/1	0.99	0.21	38,38,38,38	0
2	ZN	С	901	1/1	0.99	0.16	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 (i)

There are no such residues in this entry.

