Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2017 – 02:10 PM EDT

PDB ID	:	1X6V
Title	:	The crystal structure of human 3'-phosphoadenosine-5'-phosphosulfate synthetase 1
Authors	:	Harjes, S.; Bayer, P.; Scheidig, A.J.
Deposited on	:	unknown
Resolution	:	1.75 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345
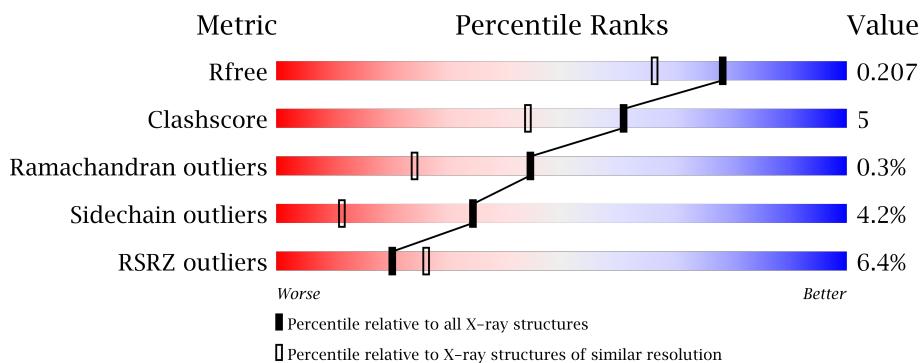
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
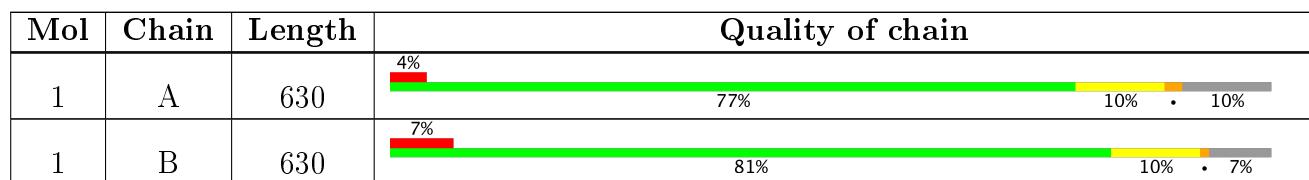
The reported resolution of this entry is 1.75 Å.

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}	100719	1762 (1.76-1.76)
Clashscore	112137	1889 (1.76-1.76)
Ramachandran outliers	110173	1868 (1.76-1.76)
Sidechain outliers	110143	1868 (1.76-1.76)
RSRZ outliers	101464	1770 (1.76-1.76)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	630	4% 77% 10% · 10%
1	B	630	7% 81% 10% · 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10326 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 Bifunctional 3'-phosphoadenosine 5'-phosphosulfate synthetase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	586	Total 4682	C 2965	N 823	O 861	S 33	0	3	0
1	A	564	Total 4524	C 2866	N 795	O 830	S 33	0	7	0

There are 14 discrepancies between the modelled and reference sequences:
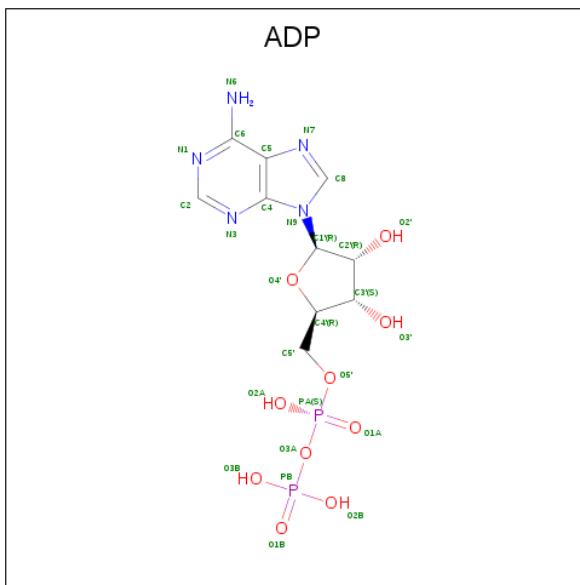
Chain	Residue	Modelled	Actual	Comment	Reference
B	416	SER	PHE	CONFLICT	UNP O43252
B	625	HIS	-	EXPRESSION TAG	UNP O43252
B	626	HIS	-	EXPRESSION TAG	UNP O43252
B	627	HIS	-	EXPRESSION TAG	UNP O43252
B	628	HIS	-	EXPRESSION TAG	UNP O43252
B	629	HIS	-	EXPRESSION TAG	UNP O43252
B	630	HIS	-	EXPRESSION TAG	UNP O43252
A	416	SER	PHE	CONFLICT	UNP O43252
A	625	HIS	-	EXPRESSION TAG	UNP O43252
A	626	HIS	-	EXPRESSION TAG	UNP O43252
A	627	HIS	-	EXPRESSION TAG	UNP O43252
A	628	HIS	-	EXPRESSION TAG	UNP O43252
A	629	HIS	-	EXPRESSION TAG	UNP O43252
A	630	HIS	-	EXPRESSION TAG	UNP O43252

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is A D E N O S I N E - 5 ' - D I P H O S P H A T E (three-letter code: ADP) (formula:

$C_{10}H_{15}N_5O_{10}P_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
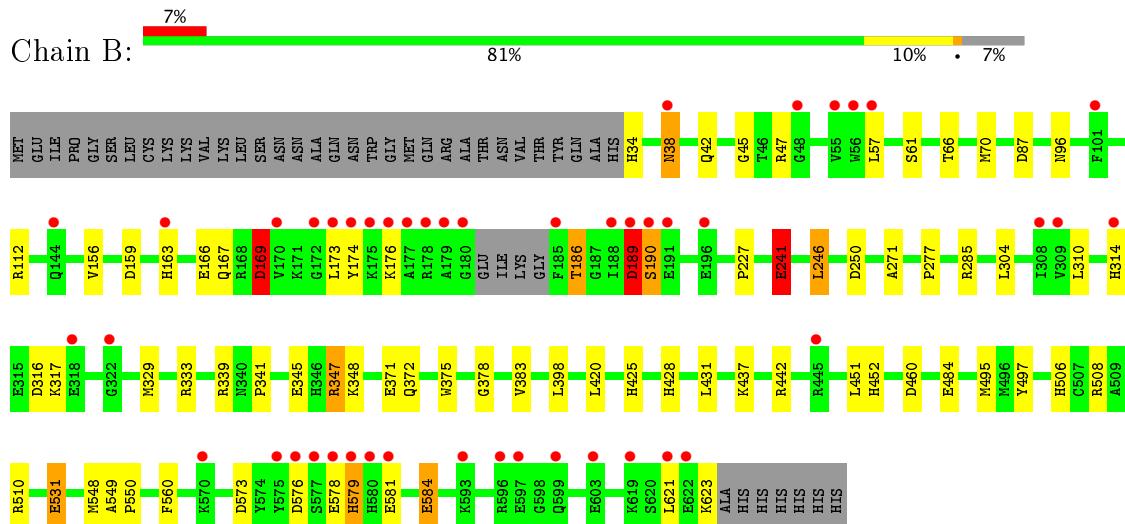
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	546	Total 546	O 546	0	0
4	A	545	Total 545	O 545	0	0
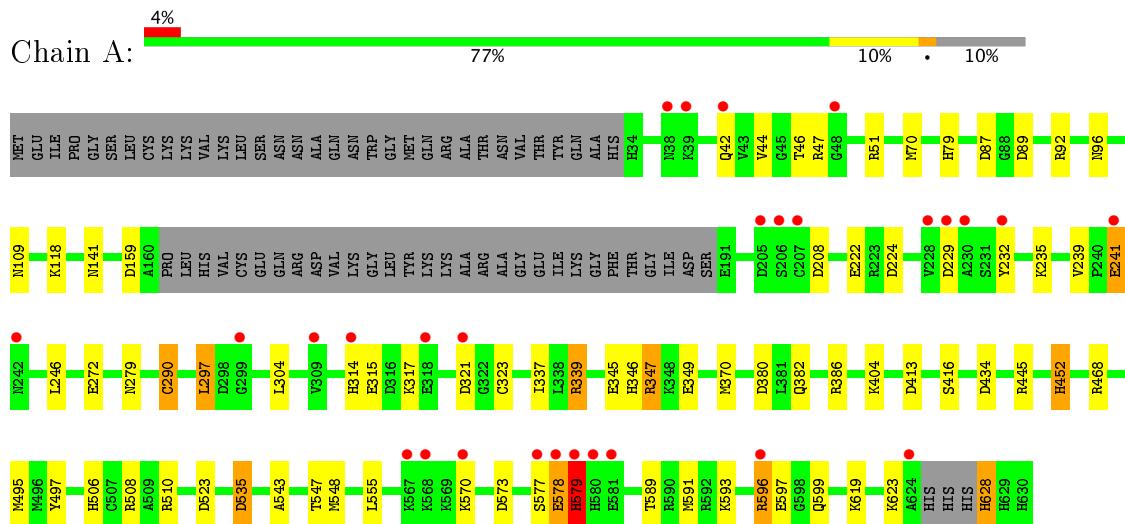
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: Bifunctional 3'-phosphoadenosine 5'-phosphosulfate synthetase 1

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4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.21Å 82.55Å 133.60Å 90.00° 105.10° 90.00°	Depositor
Resolution (Å)	129.10 – 1.75 28.45 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.7 (129.10-1.75) 99.7 (28.45-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.166 , 0.198 0.177 , 0.207	Depositor DCC
R_{free} test set	8203 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 52.1	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10326	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, CL

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	0.97	1/4663 (0.0%)	1.03	29/6316 (0.5%)
1	B	0.95	4/4810 (0.1%)	0.95	14/6513 (0.2%)
All	All	0.96	5/9473 (0.1%)	0.99	43/12829 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	460	ASP	CB-CG	-6.08	1.39	1.51
1	B	548	MET	CG-SD	5.33	1.95	1.81
1	A	272	GLU	CD-OE1	5.19	1.31	1.25
1	B	241	GLU	CD-OE2	5.10	1.31	1.25
1	B	347	ARG	CZ-NH1	5.00	1.39	1.33

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	523	ASP	CB-CG-OD2	9.21	126.59	118.30
1	B	339	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	A	323[A]	CYS	CA-CB-SG	8.49	129.29	114.00
1	A	323[B]	CYS	CA-CB-SG	8.49	129.29	114.00
1	A	347	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	A	573	ASP	CB-CG-OD2	8.34	125.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	404	LYS	CD-CE-NZ	7.18	128.22	111.70
1	B	339	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	B	576	ASP	CB-CG-OD2	6.77	124.39	118.30
1	A	224	ASP	CB-CG-OD2	6.64	124.28	118.30
1	B	285	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	208	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	290[A]	CYS	CA-CB-SG	6.37	125.46	114.00
1	A	290[B]	CYS	CA-CB-SG	6.37	125.46	114.00
1	B	347	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	297	LEU	CB-CG-CD1	6.30	121.72	111.00
1	A	87	ASP	CB-CG-OD1	6.25	123.92	118.30
1	B	189	ASP	CB-CG-OD2	6.25	123.92	118.30
1	B	285	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	A	380	ASP	CB-CG-OD2	6.23	123.90	118.30
1	A	92	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	573	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	159	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	316	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	339	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	B	548	MET	CG-SD-CE	-5.75	90.99	100.20
1	A	413	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	339	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	628	HIS	N-CA-C	5.64	126.22	111.00
1	B	169	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	548	MET	CG-SD-CE	-5.62	91.22	100.20
1	B	87	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	159	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	347	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	A	246	LEU	CA-CB-CG	5.42	127.78	115.30
1	A	321	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	591	MET	CG-SD-CE	-5.37	91.60	100.20
1	B	460	ASP	CB-CA-C	-5.35	99.69	110.40
1	A	434	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	70[A]	MET	CB-CG-SD	5.30	128.30	112.40
1	A	70[B]	MET	CB-CG-SD	5.30	128.30	112.40
1	A	468	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	535	ASP	CB-CG-OD1	5.06	122.86	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	628	HIS	CA

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	4524	0	4447	49	0
1	B	4682	0	4617	47	0
2	A	1	0	0	0	0
2	B	1	0	0	1	0
3	B	27	0	12	0	0
4	A	545	0	0	25	0
4	B	546	0	0	22	0
All	All	10326	0	9076	96	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 5.

All (96) 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:A:370:MET:CE	1:A:370:MET:SD	2.05	1.44
1:A:232:TYR:HB2	4:A:1147:HOH:O	1.64	0.96
1:B:314:HIS:HB3	4:B:1277:HOH:O	1.67	0.93
1:B:452:HIS:HD2	1:B:510:ARG:HE	1.11	0.91
1:A:452:HIS:HD2	1:A:510:ARG:HE	1.20	0.86
1:B:452:HIS:CD2	1:B:510:ARG:HE	1.94	0.85
1:A:345:GLU:OE2	4:A:1162:HOH:O	1.97	0.83
1:A:452:HIS:CD2	1:A:510:ARG:HE	1.96	0.82
1:B:250:ASP:HB2	4:B:1330:HOH:O	1.79	0.82
1:A:370:MET:HG3	4:A:1233:HOH:O	1.78	0.82
1:A:241:GLU:HB2	4:A:1181:HOH:O	1.81	0.80
1:B:38:ASN:HB2	4:B:1284:HOH:O	1.82	0.79
1:A:535:ASP:OD2	4:A:1170:HOH:O	2.01	0.79
1:B:347:ARG:N	4:B:1257:HOH:O	2.15	0.78
2:B:700:CL:CL	4:B:1275:HOH:O	2.39	0.77
1:A:628:HIS:HB2	4:A:1245:HOH:O	1.85	0.75
1:B:345:GLU:OE2	4:B:1270:HOH:O	2.05	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:HIS:HB3	4:A:1017:HOH:O	1.89	0.72
1:B:425:HIS:H	1:B:428:HIS:HD2	1.36	0.71
1:B:166:GLU:HG2	1:B:174:TYR:CD2	2.32	0.65
1:B:186:THR:HB	4:B:1269:HOH:O	1.97	0.65
1:A:141:ASN:HB2	4:A:1182:HOH:O	1.97	0.65
1:B:371:GLU:HB2	4:B:1273:HOH:O	1.96	0.64
1:B:452:HIS:HD2	1:B:510:ARG:NE	1.89	0.61
1:B:246:LEU:HD12	4:B:1165:HOH:O	2.00	0.61
1:B:428:HIS:HE1	4:B:1346:HOH:O	1.83	0.60
1:B:38:ASN:CB	4:B:1284:HOH:O	2.46	0.59
1:A:239[A]:VAL:CG1	1:A:382:GLN:CG	2.81	0.59
1:B:578:GLU:O	1:B:579:HIS:HB2	2.03	0.58
1:B:34:HIS:N	4:B:1258:HOH:O	2.35	0.58
1:B:189:ASP:HB2	4:B:1310:HOH:O	2.03	0.57
1:A:118:LYS:HD2	4:A:1195:HOH:O	2.03	0.57
1:A:619:LYS:HE2	4:A:1169:HOH:O	2.04	0.57
1:B:45:GLY:N	1:A:44:VAL:O	2.37	0.57
1:A:337:ILE:HD12	1:A:382:GLN:HE21	1.70	0.57
1:A:452:HIS:HE1	4:A:714:HOH:O	1.87	0.56
1:B:246:LEU:HD22	4:B:1295:HOH:O	2.04	0.56
1:B:66:THR:O	1:B:70[B]:MET:HG3	2.05	0.55
1:A:347:ARG:N	4:A:1017:HOH:O	2.39	0.55
1:A:506:HIS:O	1:A:510:ARG:HD3	2.07	0.55
1:B:47:ARG:HD3	1:B:227:PRO:HG2	1.89	0.54
1:A:597:GLU:HG3	1:A:599:GLN:HE21	1.72	0.54
1:A:623:LYS:O	4:A:1156:HOH:O	2.19	0.53
1:B:166:GLU:O	1:B:169:ASP:HB2	2.09	0.53
1:B:578:GLU:O	1:B:579:HIS:CB	2.56	0.53
1:A:452:HIS:HD2	1:A:510:ARG:NE	1.99	0.52
1:A:628:HIS:CD2	4:A:1245:HOH:O	2.63	0.52
1:B:531:GLU:HG2	4:B:1096:HOH:O	2.09	0.52
1:B:96:ASN:ND2	1:B:112:ARG:HD2	2.26	0.51
1:A:239[A]:VAL:CG1	1:A:382:GLN:HG3	2.40	0.50
1:B:420:LEU:HD11	1:B:451:LEU:HD11	1.92	0.50
1:A:386:ARG:HB2	4:A:1185:HOH:O	2.11	0.50
1:B:452:HIS:CD2	1:B:510:ARG:NE	2.73	0.49
1:B:452:HIS:HE1	4:B:815:HOH:O	1.94	0.49
1:A:241:GLU:CD	1:A:241:GLU:H	2.16	0.49
1:A:596:ARG:HG2	4:A:1146:HOH:O	2.12	0.49
1:B:484:GLU:HG3	4:B:1302:HOH:O	2.11	0.49
1:B:96:ASN:HD21	1:B:112:ARG:HD2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ARG:HG3	4:A:1168:HOH:O	2.12	0.48
1:B:57:LEU:HD23	1:B:156:VAL:HB	1.94	0.48
1:A:235:LYS:HZ3	1:A:279:ASN:HD21	1.61	0.48
1:A:452:HIS:CD2	1:A:510:ARG:NE	2.75	0.48
1:B:42:GLN:HA	4:B:1280:HOH:O	2.14	0.48
1:A:241:GLU:CG	4:A:1176:HOH:O	2.62	0.47
1:A:239[A]:VAL:HG12	1:A:382:GLN:HG3	1.97	0.47
1:B:271:ALA:HB2	1:B:383:VAL:HG21	1.95	0.47
1:A:349:GLU:CD	4:A:1173:HOH:O	2.53	0.46
1:A:386:ARG:HD2	4:A:1185:HOH:O	2.16	0.46
1:B:506:HIS:O	1:B:510:ARG:HD3	2.15	0.46
1:B:348:LYS:NZ	1:B:372:GLN:O	2.41	0.46
1:B:241:GLU:CD	1:B:241:GLU:N	2.69	0.46
1:A:89:ASP:C	4:A:1167:HOH:O	2.54	0.46
1:A:239[A]:VAL:HG12	1:A:382:GLN:CG	2.45	0.46
1:B:329:MET:HA	1:B:333:ARG:O	2.17	0.45
1:A:239[A]:VAL:HG12	1:A:382:GLN:OE1	2.16	0.45
1:A:241:GLU:HG3	4:A:1176:HOH:O	2.16	0.44
1:A:47:ARG:NH2	1:A:79:HIS:O	2.50	0.44
1:B:584:GLU:OE1	4:B:1299:HOH:O	2.21	0.44
1:A:416[A]:SER:HB2	4:A:916:HOH:O	2.17	0.43
1:B:190:SER:HB2	4:B:1269:HOH:O	2.19	0.43
1:A:96:ASN:ND2	1:A:109:ASN:OD1	2.48	0.43
1:A:495:MET:HG2	1:A:497:TYR:CZ	2.53	0.43
1:A:51:ARG:HD2	4:A:788:HOH:O	2.19	0.43
1:B:163:HIS:HE1	4:B:1274:HOH:O	2.02	0.43
1:A:314:HIS:CD2	4:A:1178:HOH:O	2.71	0.42
1:A:589:THR:O	1:A:593:LYS:HG3	2.19	0.42
1:B:341:PRO:HA	1:B:378:GLY:O	2.20	0.42
1:B:495:MET:HG2	1:B:497:TYR:CZ	2.55	0.41
1:A:241:GLU:CD	1:A:241:GLU:N	2.74	0.41
1:A:578:GLU:O	1:A:579:HIS:CB	2.68	0.41
1:B:317:LYS:HD2	1:B:375:TRP:CE2	2.56	0.41
1:B:163:HIS:CE1	4:B:1274:HOH:O	2.72	0.41
1:B:431:LEU:HG	1:B:560:PHE:CG	2.55	0.40
1:A:543:ALA:O	1:A:547:THR:HG23	2.21	0.40
1:B:549:ALA:HA	1:B:550:PRO:HD3	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	564/630 (90%)	551 (98%)	12 (2%)	1 (0%)	51	31
1	B	585/630 (93%)	576 (98%)	7 (1%)	2 (0%)	44	24
All	All	1149/1260 (91%)	1127 (98%)	19 (2%)	3 (0%)	44	24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	579	HIS
1	A	579	HIS
1	B	169	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	489/538 (91%)	468 (96%)	21 (4%)	33	11
1	B	504/538 (94%)	482 (96%)	22 (4%)	33	10
All	All	993/1076 (92%)	950 (96%)	43 (4%)	34	11

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	38	ASN
1	B	61	SER
1	B	167	GLN

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Mol	Chain	Res	Type
1	B	173	LEU
1	B	176	LYS
1	B	186	THR
1	B	189	ASP
1	B	190	SER
1	B	241	GLU
1	B	246	LEU
1	B	277	PRO
1	B	304	LEU
1	B	310	LEU
1	B	398	LEU
1	B	437	LYS
1	B	442	ARG
1	B	508	ARG
1	B	531	GLU
1	B	581	GLU
1	B	584	GLU
1	B	621	LEU
1	B	623	LYS
1	A	42	GLN
1	A	46	THR
1	A	222	GLU
1	A	229	ASP
1	A	241	GLU
1	A	290[A]	CYS
1	A	290[B]	CYS
1	A	297	LEU
1	A	304	LEU
1	A	315	GLU
1	A	317	LYS
1	A	445	ARG
1	A	452	HIS
1	A	508	ARG
1	A	555[A]	LEU
1	A	555[B]	LEU
1	A	570	LYS
1	A	577	SER
1	A	578	GLU
1	A	579	HIS
1	A	596	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	96	ASN
1	B	109	ASN
1	B	144	GLN
1	B	210	ASN
1	B	245	HIS
1	B	314	HIS
1	B	411	ASN
1	B	428	HIS
1	B	452	HIS
1	B	579	HIS
1	A	93	GLN
1	A	140	ASN
1	A	279	ASN
1	A	382	GLN
1	A	422	ASN
1	A	452	HIS
1	A	599	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	ADP	B	800	-	25,29,29	1.25	2 (8%)	24,45,45	2.10	2 (8%)

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
3	ADP	B	800	-	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	800	ADP	O4'-C4'	-2.41	1.39	1.45
3	B	800	ADP	C2-N3	3.71	1.38	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	800	ADP	N3-C2-N1	-9.25	120.80	128.86
3	B	800	ADP	O2B-PB-O1B	2.91	121.88	110.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	564/630 (89%)	-0.00	28 (4%)	30	36	12, 24, 47, 77	7 (1%)
1	B	586/630 (93%)	0.10	46 (7%)	14	18	12, 24, 52, 77	0
All	All	1150/1260 (91%)	0.05	74 (6%)	20	26	12, 24, 50, 77	7 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	179	ALA	7.8
1	B	189	ASP	7.3
1	B	175	LYS	7.0
1	A	577	SER	6.5
1	A	624	ALA	5.6
1	B	188	ILE	5.5
1	B	577	SER	4.7
1	B	578	GLU	4.5
1	B	190	SER	4.3
1	B	178	ARG	4.2
1	A	578	GLU	4.1
1	B	172	GLY	3.8
1	B	621	LEU	3.8
1	B	177	ALA	3.7
1	A	580	HIS	3.7
1	B	170	VAL	3.6
1	A	581	GLU	3.6
1	A	38	ASN	3.6
1	B	575	TYR	3.5
1	B	596	ARG	3.5
1	B	593	LYS	3.5
1	B	580	HIS	3.4
1	A	232	TYR	3.3
1	B	579	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	101	PHE	3.3
1	B	314	HIS	3.2
1	B	176	LYS	3.2
1	B	180	GLY	3.1
1	A	205	ASP	3.1
1	B	603	GLU	3.0
1	B	191	GLU	3.0
1	B	48	GLY	2.9
1	A	299	GLY	2.9
1	A	568	LYS	2.9
1	A	596	ARG	2.8
1	A	230	ALA	2.8
1	A	321	ASP	2.8
1	B	570	LYS	2.7
1	A	207	CYS	2.7
1	A	318	GLU	2.7
1	B	163	HIS	2.6
1	A	48	GLY	2.6
1	B	174	TYR	2.6
1	B	597	GLU	2.6
1	B	185	PHE	2.6
1	B	308	ILE	2.6
1	B	38	ASN	2.6
1	A	314	HIS	2.5
1	B	445	ARG	2.5
1	B	318	GLU	2.5
1	B	196	GLU	2.5
1	B	581	GLU	2.5
1	A	39	LYS	2.5
1	B	576	ASP	2.4
1	A	206	SER	2.3
1	A	579	HIS	2.3
1	A	241	GLU	2.3
1	B	144	GLN	2.3
1	B	622	GLU	2.3
1	B	309	VAL	2.3
1	B	173	LEU	2.3
1	B	55	VAL	2.2
1	B	56	TRP	2.2
1	B	619	LYS	2.2
1	B	599	GLN	2.2
1	A	242	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	322	GLY	2.1
1	A	229	ASP	2.1
1	A	42	GLN	2.1
1	B	57	LEU	2.1
1	A	570	LYS	2.0
1	A	228	VAL	2.0
1	A	309	VAL	2.0
1	A	567	LYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	CL	A	700	1/1	0.98	0.09	-0.57	31,31,31,31	0
3	ADP	B	800	27/27	0.98	0.06	-0.86	28,35,39,40	0
2	CL	B	700	1/1	0.99	0.04	-2.98	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.