Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2024 – 07:44 AM EST

PDB ID	:	1XRC
Title	:	CRYSTAL STRUCTURE OF S-ADENOSYLMETHIONINE SYNTHETASE
Authors	:	Takusagawa, F.; Kamitori, S.; Misaki, S.; Markham, G.D.
Deposited on	:	1995-10-26
Resolution	:	3.00 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:

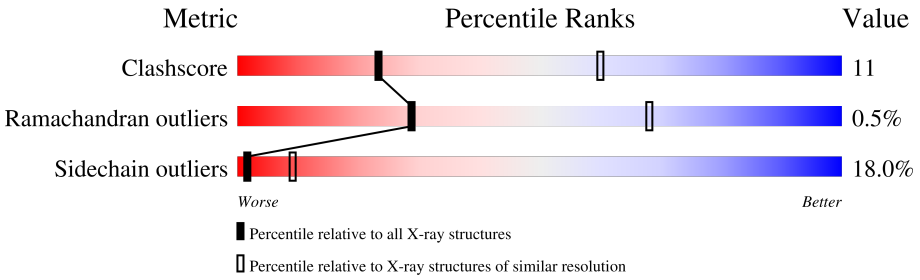
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	383	57% 31% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	384	-	X	-	-

2 Entry composition

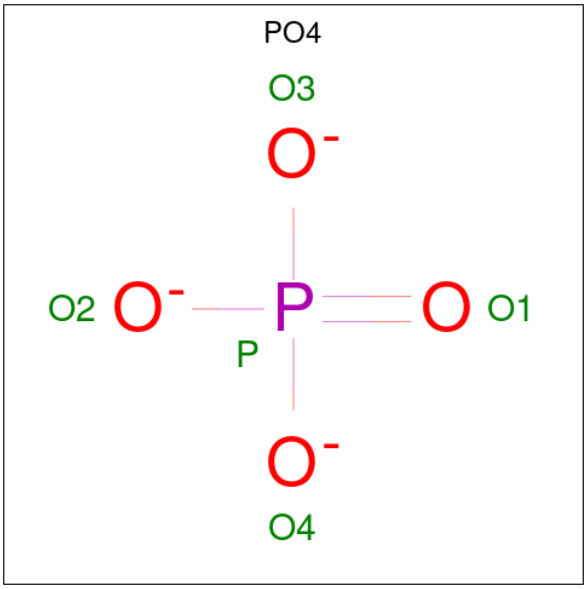
There are 4 unique types of molecules in this entry. The entry contains 3544 atoms, of which 632 are hydrogens and 0 are deuteriums.

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 S-ADENOSYLMETHIONINE SYNTHETASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	377	3530	1830	632	495	560	13	632	0	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0
			Total	O	P		
2	A	1	5	4	1	0	0

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Co		
3	A	2	2	2	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total K 2 2	0	0

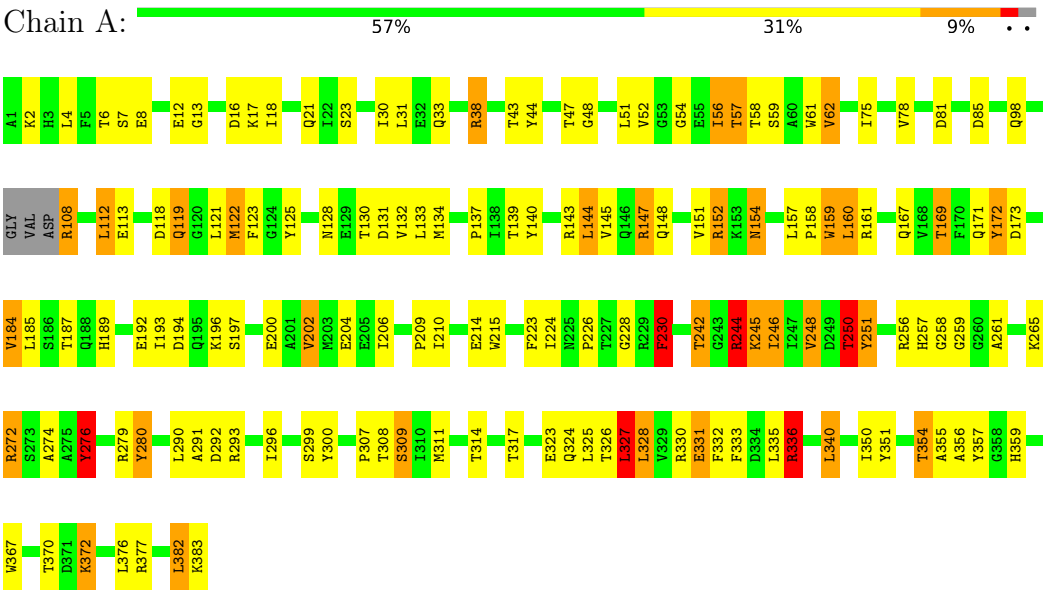
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

- Molecule 1: S-ADENOSYLMETHIONINE SYNTHETASE

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α, β, γ	128.90Å 128.90Å 139.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.00	Depositor
% Data completeness (in resolution range)	96.8 (10.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.197 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3544	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, CO, PO4

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	0.93	0/2956	1.72	52/4005 (1.3%)

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	0	19

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	250	THR	CA-CB-CG2	9.86	126.20	112.40
1	A	161	ARG	NE-CZ-NH2	-9.69	115.45	120.30
1	A	215	TRP	CD1-CG-CD2	9.26	113.70	106.30
1	A	250	THR	N-CA-CB	-9.04	93.12	110.30
1	A	362	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	A	61	TRP	CD1-CG-CD2	8.40	113.02	106.30
1	A	159	TRP	CD1-CG-CD2	8.12	112.80	106.30
1	A	159	TRP	CE2-CD2-CG	-7.99	100.91	107.30
1	A	159	TRP	CG-CD2-CE3	7.70	140.83	133.90
1	A	61	TRP	CE2-CD2-CG	-7.57	101.25	107.30
1	A	159	TRP	CB-CG-CD1	-7.55	117.18	127.00
1	A	16	ASP	CB-CG-OD1	7.53	125.08	118.30
1	A	276	TYR	CB-CG-CD2	-7.52	116.49	121.00
1	A	8	GLU	CA-CB-CG	7.44	129.78	113.40
1	A	382	LEU	CA-CB-CG	7.29	132.06	115.30
1	A	336	ARG	NE-CZ-NH2	-7.21	116.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	215	TRP	CE2-CD2-CG	-7.20	101.54	107.30
1	A	327	LEU	CA-CB-CG	7.01	131.44	115.30
1	A	161	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	152	ARG	NE-CZ-NH2	-6.97	116.82	120.30
1	A	279	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	A	367	TRP	CD1-CG-CD2	6.57	111.55	106.30
1	A	331	GLU	OE1-CD-OE2	-6.40	115.61	123.30
1	A	367	TRP	CE2-CD2-CG	-6.40	102.18	107.30
1	A	108	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	362	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	230	PHE	CB-CG-CD2	-6.32	116.38	120.80
1	A	244	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	A	38	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	215	TRP	CG-CD1-NE1	-6.25	103.85	110.10
1	A	314	THR	N-CA-C	-6.25	94.13	111.00
1	A	293	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	A	147	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	A	251	TYR	CB-CG-CD2	-5.89	117.47	121.00
1	A	261	ALA	CB-CA-C	-5.88	101.27	110.10
1	A	172	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	A	256	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	160	LEU	CA-CB-CG	5.72	128.46	115.30
1	A	331	GLU	N-CA-CB	5.61	120.70	110.60
1	A	118	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	363	GLU	N-CA-C	5.47	125.76	111.00
1	A	78	VAL	N-CA-CB	-5.31	99.81	111.50
1	A	61	TRP	CG-CD1-NE1	-5.28	104.82	110.10
1	A	85	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	280	TYR	CA-C-N	5.19	128.61	117.20
1	A	159	TRP	CG-CD1-NE1	-5.13	104.97	110.10
1	A	61	TRP	CB-CG-CD1	-5.09	120.38	127.00
1	A	161	ARG	CA-C-N	5.08	131.32	117.10
1	A	172	TYR	CA-CB-CG	5.08	123.05	113.40
1	A	377	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	161	ARG	CB-CG-CD	5.07	124.77	111.60
1	A	351	TYR	CA-C-N	5.06	128.32	117.20

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	A	125	TYR	Peptide
1	A	140	TYR	Sidechain
1	A	194	ASP	Peptide
1	A	228	GLY	Peptide
1	A	230	PHE	Sidechain
1	A	244	ARG	Sidechain
1	A	259	GLY	Peptide
1	A	272	ARG	Sidechain
1	A	276	TYR	Sidechain
1	A	280	TYR	Sidechain
1	A	332	PHE	Sidechain
1	A	333	PHE	Sidechain
1	A	336	ARG	Sidechain
1	A	356	ALA	Peptide
1	A	362	ARG	Peptide
1	A	44	TYR	Sidechain
1	A	48	GLY	Peptide
1	A	54	GLY	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2898	632	2866	65	0
2	A	10	0	0	0	0
3	A	2	0	0	0	0
4	A	2	0	0	0	0
All	All	2912	632	2866	65	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 11.

All (65) 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:265:LYS:HB3	1:A:269:LYS:HG3	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:THR:HG22	1:A:132:VAL:H	1.45	0.80
1:A:257:HIS:HD2	1:A:258:GLY:O	1.69	0.76
1:A:272:ARG:HH12	1:A:354:THR:HG21	1.55	0.71
1:A:23:SER:OG	1:A:242:THR:HG21	1.91	0.70
1:A:57:THR:HB	1:A:98:GLN:HB3	1.74	0.69
1:A:151:VAL:HA	1:A:154:ASN:ND2	2.09	0.66
1:A:56:ILE:HG23	1:A:58:THR:HG22	1.79	0.63
1:A:354:THR:HG23	1:A:359:HIS:NE2	2.13	0.62
1:A:324:GLN:O	1:A:328:LEU:HD23	2.01	0.61
1:A:244:ARG:O	1:A:246:ILE:HG22	2.03	0.59
1:A:204:GLU:O	1:A:209:PRO:HD3	2.02	0.59
1:A:245:LYS:HB3	1:A:248:VAL:HG13	1.86	0.58
1:A:151:VAL:HA	1:A:154:ASN:HD21	1.68	0.57
1:A:324:GLN:O	1:A:327:LEU:HB3	2.06	0.56
1:A:30:ILE:HD11	1:A:56:ILE:HD11	1.86	0.56
1:A:122:MET:HG3	1:A:274:ALA:HB3	1.89	0.55
1:A:43:THR:H	1:A:242:THR:HG23	1.73	0.53
1:A:328:LEU:HD12	1:A:376:LEU:HG	1.92	0.52
1:A:173:ASP:H	1:A:178:VAL:HG13	1.75	0.51
1:A:144:LEU:HD13	1:A:210:ILE:HG21	1.92	0.50
1:A:266:ASP:OD1	1:A:269:LYS:NZ	2.44	0.50
1:A:6:THR:OG1	1:A:169:THR:HB	2.11	0.50
1:A:223:PHE:HB3	1:A:226:PRO:HG3	1.93	0.49
1:A:147:ARG:HG2	1:A:206:ILE:HA	1.96	0.48
1:A:159:TRP:CE3	1:A:193:ILE:HG21	2.48	0.48
1:A:202:VAL:HG22	1:A:224:ILE:HD13	1.95	0.48
1:A:299:SER:OG	1:A:309:SER:HB3	2.13	0.48
1:A:169:THR:HG23	1:A:182:ALA:HB3	1.96	0.48
1:A:33:GLN:NE2	1:A:62:VAL:HG23	2.30	0.47
1:A:75:ILE:O	1:A:152:ARG:NH2	2.47	0.47
1:A:17:LYS:O	1:A:21:GLN:HG3	2.15	0.47
1:A:130:THR:HG22	1:A:132:VAL:N	2.21	0.47
1:A:12:GLU:HG2	1:A:357:TYR:OH	2.14	0.47
1:A:276:TYR:OH	1:A:359:HIS:HD2	1.98	0.47
1:A:108:ARG:HD2	1:A:113:GLU:O	2.14	0.46
1:A:292:ASP:H	1:A:317:THR:HB	1.79	0.46
1:A:290:LEU:HD23	1:A:325:LEU:CD2	2.45	0.46
1:A:112:LEU:HB3	1:A:336:ARG:NH2	2.31	0.45
1:A:7:SER:HB2	1:A:137:PRO:HB2	1.99	0.45
1:A:17:LYS:HD2	1:A:355:ALA:O	2.17	0.45
1:A:157:LEU:HA	1:A:157:LEU:HD23	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLN:O	1:A:178:VAL:HG22	2.17	0.44
1:A:128:ASN:HA	1:A:133:LEU:HD13	2.00	0.43
1:A:325:LEU:HD23	1:A:325:LEU:HA	1.80	0.43
1:A:130:THR:HB	1:A:134:MET:H	1.82	0.43
1:A:147:ARG:HD3	1:A:210:ILE:HD11	2.00	0.43
1:A:266:ASP:O	1:A:269:LYS:HG2	2.19	0.43
1:A:335:LEU:HA	1:A:340:LEU:CD1	2.48	0.43
1:A:33:GLN:HE22	1:A:62:VAL:HG23	1.84	0.43
1:A:13:GLY:HA2	1:A:18:ILE:HG12	2.01	0.43
1:A:300:TYR:CE1	1:A:307:PRO:HG3	2.54	0.43
1:A:291:ALA:HA	1:A:317:THR:O	2.19	0.42
1:A:157:LEU:HD22	1:A:159:TRP:CZ2	2.54	0.42
1:A:2:LYS:HA	1:A:172:TYR:O	2.20	0.42
1:A:184:VAL:HA	1:A:223:PHE:O	2.20	0.42
1:A:167:GLN:HB3	1:A:184:VAL:HG13	2.03	0.41
1:A:139:THR:O	1:A:143:ARG:HG3	2.20	0.41
1:A:119:GLN:HE21	1:A:119:GLN:HB3	1.76	0.41
1:A:214:GLU:H	1:A:214:GLU:CD	2.23	0.41
1:A:372:LYS:HB2	1:A:372:LYS:HZ2	1.85	0.41
1:A:189:HIS:HD2	1:A:193:ILE:HG23	1.86	0.41
1:A:290:LEU:HD23	1:A:325:LEU:HD21	2.02	0.40
1:A:250:THR:HG22	1:A:251:TYR:N	2.36	0.40
1:A:296:ILE:HD13	1:A:296:ILE:HG21	1.83	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	373/383 (97%)	339 (91%)	32 (9%)	2 (0%)	29 68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	THR
1	A	363	GLU

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	306/311 (98%)	251 (82%)	55 (18%)	1 9

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	31	LEU
1	A	38	ARG
1	A	47	THR
1	A	51	LEU
1	A	52	VAL
1	A	56	ILE
1	A	57	THR
1	A	59	SER
1	A	62	VAL
1	A	81	ASP
1	A	101	ASP
1	A	112	LEU
1	A	119	GLN
1	A	121	LEU
1	A	122	MET
1	A	131	ASP
1	A	144	LEU
1	A	145	VAL
1	A	148	GLN
1	A	154	ASN
1	A	158	PRO
1	A	160	LEU
1	A	169	THR
1	A	184	VAL

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Mol	Chain	Res	Type
1	A	185	LEU
1	A	187	THR
1	A	192	GLU
1	A	196	LYS
1	A	197	SER
1	A	200	GLU
1	A	202	VAL
1	A	230	PHE
1	A	242	THR
1	A	245	LYS
1	A	246	ILE
1	A	248	VAL
1	A	266	ASP
1	A	308	THR
1	A	309	SER
1	A	311	MET
1	A	323	GLU
1	A	326	THR
1	A	327	LEU
1	A	328	LEU
1	A	330	ARG
1	A	331	GLU
1	A	340	LEU
1	A	350	ILE
1	A	354	THR
1	A	366	PRO
1	A	370	THR
1	A	372	LYS
1	A	382	LEU
1	A	383	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	119	GLN
1	A	142	HIS
1	A	148	GLN
1	A	154	ASN
1	A	189	HIS
1	A	257	HIS
1	A	297	GLN

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Mol	Chain	Res	Type
1	A	342	GLN
1	A	348	HIS
1	A	359	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
2	PO4	A	385	3	4,4,4	1.98	2 (50%)	6,6,6	0.38	0
2	PO4	A	384	3	4,4,4	2.31	3 (75%)	6,6,6	1.45	1 (16%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	384	PO4	P-O2	-2.83	1.46	1.54
2	A	384	PO4	P-O4	-2.70	1.46	1.54
2	A	385	PO4	P-O3	-2.60	1.46	1.54
2	A	385	PO4	P-O4	-2.54	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	384	PO4	P-O3	-2.18	1.48	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	384	PO4	O4-P-O1	-2.90	100.29	110.89

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.