



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:07 am BST

PDB ID : 1XRA
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 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) : 2.11

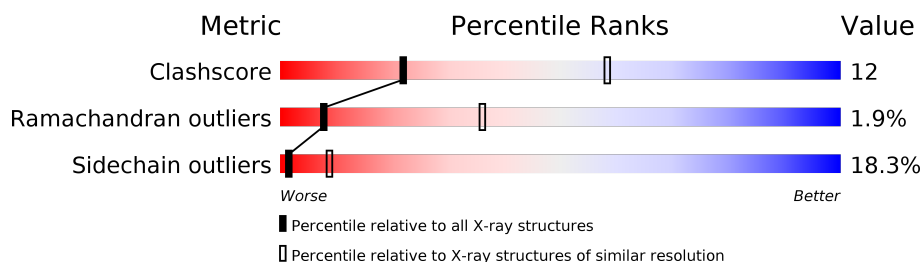
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 on 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	383	

2 Entry composition [i](#)

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
1	A	377	Total	C	H	N	O	S	632	0	0
			3530	1830	632	495	560	13			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

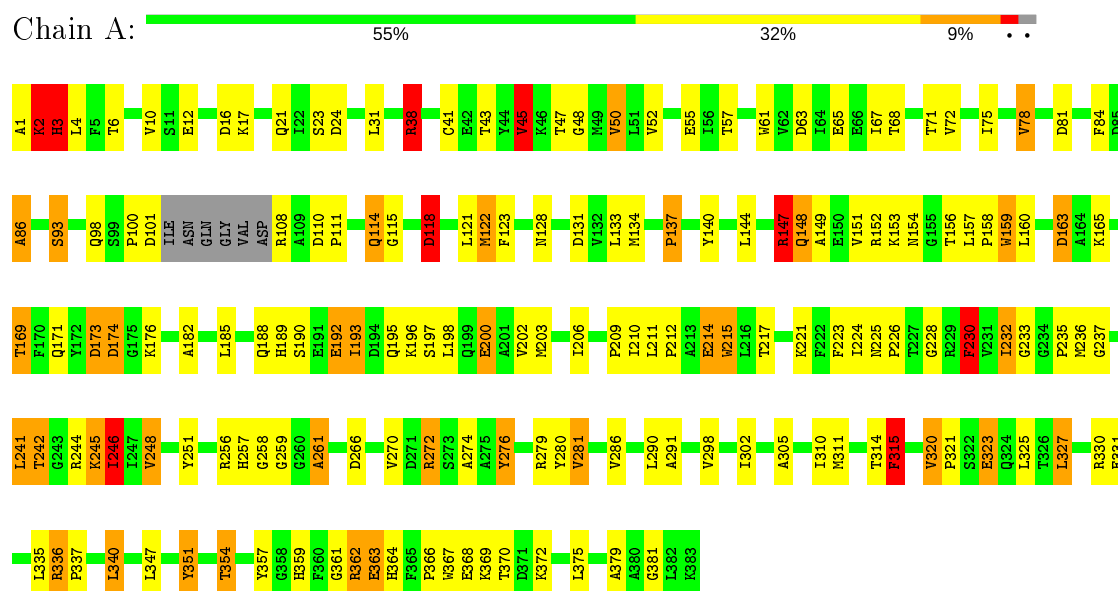
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	K	0	0
			2	2		

3 Residue-property plots [i](#)

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. 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



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 6 ₂ 2 2	Depositor
Cell constants a, b, c, α , β , γ	128.90 Å 128.90 Å 139.80 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.00	Depositor
% Data completeness (in resolution range)	95.7 (10.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.189 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3544	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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: PO4, MG, K

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	1.01	0/2956	1.81	66/4005 (1.6%)

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	15

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	ARG	NE-CZ-NH2	-10.51	115.05	120.30
1	A	159	TRP	CD1-CG-CD2	9.94	114.25	106.30
1	A	61	TRP	CD1-CG-CD2	9.09	113.57	106.30
1	A	354	THR	N-CA-CB	-8.86	93.46	110.30
1	A	215	TRP	CD1-CG-CD2	8.69	113.25	106.30
1	A	159	TRP	CE2-CD2-CG	-8.54	100.47	107.30
1	A	362	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	A	147	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	A	251	TYR	CB-CG-CD2	-8.06	116.16	121.00
1	A	367	TRP	CD1-CG-CD2	7.88	112.60	106.30
1	A	61	TRP	CE2-CD2-CG	-7.79	101.07	107.30
1	A	314	THR	N-CA-C	-7.27	91.37	111.00
1	A	327	LEU	CA-CB-CG	7.00	131.39	115.30
1	A	193	ILE	N-CA-CB	-6.98	94.75	110.80
1	A	50	VAL	CG1-CB-CG2	-6.93	99.81	110.90
1	A	78	VAL	N-CA-CB	-6.88	96.37	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	TYR	CB-CG-CD2	-6.82	116.91	121.00
1	A	367	TRP	CE2-CD2-CG	-6.82	101.84	107.30
1	A	38	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	A	362	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	A	215	TRP	CE2-CD2-CG	-6.78	101.87	107.30
1	A	230	PHE	CB-CG-CD2	-6.77	116.06	120.80
1	A	272	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	24	ASP	CB-CG-OD1	6.52	124.17	118.30
1	A	108	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	A	163	ASP	CB-CG-OD1	6.35	124.02	118.30
1	A	118	ASP	N-CA-CB	6.35	122.03	110.60
1	A	159	TRP	CG-CD2-CE3	6.33	139.59	133.90
1	A	159	TRP	CG-CD1-NE1	-6.30	103.80	110.10
1	A	241	LEU	CB-CG-CD1	-6.22	100.42	111.00
1	A	159	TRP	CB-CG-CD1	-6.19	118.95	127.00
1	A	256	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	215	TRP	CG-CD1-NE1	-5.88	104.22	110.10
1	A	230	PHE	N-CA-CB	-5.88	100.01	110.60
1	A	61	TRP	CG-CD1-NE1	-5.84	104.25	110.10
1	A	232	ILE	O-C-N	-5.81	113.33	123.20
1	A	367	TRP	CG-CD2-CE3	5.74	139.07	133.90
1	A	246	ILE	CA-CB-CG2	5.73	122.37	110.90
1	A	320	VAL	CB-CA-C	-5.73	100.51	111.40
1	A	114	GLN	O-C-N	5.71	132.90	123.20
1	A	261	ALA	CB-CA-C	-5.70	101.55	110.10
1	A	71	THR	CA-CB-OG1	-5.68	97.06	109.00
1	A	45	VAL	CB-CA-C	-5.65	100.66	111.40
1	A	331	GLU	OE1-CD-OE2	-5.64	116.53	123.30
1	A	331	GLU	CA-CB-CG	5.58	125.67	113.40
1	A	61	TRP	CG-CD2-CE3	5.56	138.90	133.90
1	A	163	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	A	281	VAL	N-CA-CB	5.54	123.69	111.50
1	A	185	LEU	CB-CG-CD1	5.51	120.37	111.00
1	A	270	VAL	CA-CB-CG1	-5.51	102.64	110.90
1	A	171	GLN	CA-C-N	-5.45	105.20	117.20
1	A	200	GLU	CA-CB-CG	5.45	125.39	113.40
1	A	367	TRP	CG-CD1-NE1	-5.43	104.67	110.10
1	A	93	SER	CB-CA-C	-5.32	99.99	110.10
1	A	279	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	41	CYS	N-CA-CB	-5.31	101.04	110.60
1	A	110	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	315	PHE	N-CA-C	-5.28	96.75	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	61	TRP	CB-CG-CD1	-5.23	120.20	127.00
1	A	86	ALA	CB-CA-C	-5.23	102.26	110.10
1	A	336	ARG	NH1-CZ-NH2	5.20	125.12	119.40
1	A	351	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	A	147	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	A	251	TYR	CB-CG-CD1	5.07	124.04	121.00
1	A	16	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	PRO	Peptide
1	A	123	PHE	Sidechain
1	A	140	TYR	Sidechain
1	A	173	ASP	Peptide
1	A	192	GLU	Peptide
1	A	228	GLY	Peptide
1	A	230	PHE	Sidechain
1	A	244	ARG	Sidechain
1	A	259	GLY	Peptide
1	A	280	TYR	Sidechain
1	A	336	ARG	Sidechain
1	A	379	ALA	Peptide
1	A	38	ARG	Sidechain
1	A	381	GLY	Peptide
1	A	48	GLY	Peptide

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	2898	632	2866	68	0
2	A	10	0	0	0	0
3	A	2	0	0	0	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2912	632	2866	68	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 12.

All (68) 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:246:ILE:HD11	1:A:261:ALA:HA	1.52	0.90
1:A:351:TYR:O	1:A:354:THR:HB	1.78	0.83
1:A:43:THR:H	1:A:242:THR:HG23	1.59	0.67
1:A:118:ASP:H	1:A:302:ILE:HD13	1.60	0.66
1:A:47:THR:HG22	1:A:237:GLY:H	1.60	0.66
1:A:354:THR:HG23	1:A:359:HIS:CD2	2.31	0.65
1:A:122:MET:HG2	1:A:274:ALA:HB3	1.81	0.61
1:A:223:PHE:HB3	1:A:226:PRO:HG3	1.81	0.61
1:A:347:LEU:HD12	1:A:347:LEU:H	1.66	0.59
1:A:151:VAL:HA	1:A:154:ASN:OD1	2.03	0.59
1:A:321:PRO:HB2	1:A:323:GLU:HG3	1.85	0.58
1:A:347:LEU:N	1:A:347:LEU:HD12	2.20	0.56
1:A:198:LEU:O	1:A:202:VAL:HG23	2.05	0.56
1:A:286:VAL:HG23	1:A:291:ALA:O	2.06	0.56
1:A:151:VAL:HG12	1:A:157:LEU:HB2	1.89	0.55
1:A:206:ILE:O	1:A:209:PRO:HD2	2.06	0.55
1:A:189:HIS:HD2	1:A:190:SER:O	1.90	0.55
1:A:202:VAL:HB	1:A:224:ILE:HD13	1.88	0.54
1:A:375:LEU:HD12	1:A:375:LEU:H	1.72	0.54
1:A:63:ASP:O	1:A:67:ILE:HG12	2.06	0.54
1:A:257:HIS:CD2	1:A:258:GLY:O	2.60	0.54
1:A:147:ARG:HD2	1:A:210:ILE:HD11	1.91	0.52
1:A:173:ASP:O	1:A:176:LYS:HG2	2.10	0.52
1:A:276:TYR:OH	1:A:359:HIS:HD2	1.93	0.52
1:A:57:THR:HA	1:A:98:GLN:O	2.09	0.52
1:A:169:THR:HG23	1:A:182:ALA:HB3	1.93	0.51
1:A:148:GLN:HE21	1:A:149:ALA:N	2.08	0.51
1:A:335:LEU:HA	1:A:340:LEU:CD1	2.41	0.51
1:A:366:PRO:O	1:A:369:LYS:HG2	2.11	0.51
1:A:151:VAL:HG13	1:A:156:THR:HB	1.93	0.50
1:A:10:VAL:HG12	1:A:165:LYS:HG2	1.92	0.50
1:A:272:ARG:HH21	1:A:354:THR:HG21	1.76	0.49
1:A:214:GLU:CD	1:A:214:GLU:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LYS:HG3	1:A:248:VAL:HG11	1.95	0.48
1:A:72:VAL:HG12	1:A:86:ALA:HB2	1.94	0.48
1:A:75:ILE:O	1:A:152:ARG:NH2	2.46	0.48
1:A:115:GLY:HA2	1:A:305:ALA:HB2	1.95	0.47
1:A:163:ASP:H	1:A:188:GLN:HE21	1.63	0.47
1:A:118:ASP:N	1:A:302:ILE:HD13	2.29	0.46
1:A:315:PHE:N	1:A:315:PHE:CD1	2.82	0.46
1:A:6:THR:OG1	1:A:169:THR:HB	2.16	0.46
1:A:45:VAL:HG13	1:A:50:VAL:HG22	1.98	0.45
1:A:12:GLU:HG2	1:A:357:TYR:OH	2.16	0.45
1:A:246:ILE:HG23	1:A:257:HIS:NE2	2.31	0.45
1:A:2:LYS:HA	1:A:173:ASP:HA	1.98	0.44
1:A:211:LEU:HA	1:A:212:PRO:HD3	1.84	0.44
1:A:134:MET:HG3	1:A:361:GLY:HA3	1.98	0.44
1:A:337:PRO:HA	1:A:340:LEU:HD22	1.99	0.43
1:A:257:HIS:HD2	1:A:258:GLY:O	1.99	0.43
1:A:245:LYS:HG3	1:A:248:VAL:CG1	2.49	0.43
1:A:149:ALA:O	1:A:153:LYS:HB2	2.19	0.43
1:A:23:SER:OG	1:A:242:THR:HG21	2.19	0.42
1:A:128:ASN:HA	1:A:133:LEU:HD13	2.02	0.42
1:A:147:ARG:HG2	1:A:206:ILE:HA	2.00	0.42
1:A:50:VAL:HG11	1:A:68:THR:HG23	2.00	0.42
1:A:363:GLU:HA	1:A:368:GLU:HB3	2.00	0.42
1:A:362:ARG:O	1:A:364:HIS:N	2.52	0.42
1:A:84:PHE:CD1	1:A:235:PRO:HG2	2.55	0.42
1:A:290:LEU:N	1:A:290:LEU:HD23	2.35	0.41
1:A:246:ILE:HG23	1:A:257:HIS:CE1	2.55	0.41
1:A:325:LEU:HA	1:A:325:LEU:HD12	1.92	0.41
1:A:1:ALA:H3	1:A:174:ASP:CG	2.24	0.41
1:A:246:ILE:HA	1:A:246:ILE:HD13	1.67	0.41
1:A:157:LEU:HD22	1:A:159:TRP:CZ2	2.55	0.41
1:A:17:LYS:O	1:A:21:GLN:HG3	2.20	0.41
1:A:354:THR:HG23	1:A:359:HIS:NE2	2.36	0.40
1:A:2:LYS:O	1:A:3:HIS:ND1	2.54	0.40
1:A:212:PRO:HG2	1:A:215:TRP:CZ3	2.57	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%)	338 (91%)	28 (8%)	7 (2%)	8 36

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	3	HIS
1	A	118	ASP
1	A	363	GLU
1	A	233	GLY
1	A	137	PRO
1	A	225	ASN

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%)	250 (82%)	56 (18%)	1 9

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	3	HIS
1	A	4	LEU
1	A	31	LEU

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Mol	Chain	Res	Type
1	A	38	ARG
1	A	45	VAL
1	A	52	VAL
1	A	55	GLU
1	A	65	GLU
1	A	78	VAL
1	A	81	ASP
1	A	93	SER
1	A	101	ASP
1	A	111	PRO
1	A	114	GLN
1	A	121	LEU
1	A	122	MET
1	A	131	ASP
1	A	137	PRO
1	A	144	LEU
1	A	147	ARG
1	A	148	GLN
1	A	158	PRO
1	A	160	LEU
1	A	169	THR
1	A	174	ASP
1	A	192	GLU
1	A	193	ILE
1	A	195	GLN
1	A	196	LYS
1	A	197	SER
1	A	200	GLU
1	A	203	MET
1	A	214	GLU
1	A	217	THR
1	A	221	LYS
1	A	230	PHE
1	A	232	ILE
1	A	236	MET
1	A	241	LEU
1	A	242	THR
1	A	245	LYS
1	A	246	ILE
1	A	248	VAL
1	A	266	ASP
1	A	281	VAL

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Mol	Chain	Res	Type
1	A	298	VAL
1	A	310	ILE
1	A	311	MET
1	A	315	PHE
1	A	320	VAL
1	A	323	GLU
1	A	327	LEU
1	A	340	LEU
1	A	370	THR
1	A	372	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	114	GLN
1	A	142	HIS
1	A	148	GLN
1	A	188	GLN
1	A	189	HIS
1	A	257	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 carbohydrates 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	2.26	3 (75%)	6,6,6	1.03	0
2	PO4	A	384	3	4,4,4	2.45	3 (75%)	6,6,6	0.61	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	384	PO4	P-O2	-3.21	1.44	1.54
2	A	384	PO4	P-O4	-2.84	1.46	1.54
2	A	385	PO4	P-O3	-2.69	1.46	1.54
2	A	385	PO4	P-O2	-2.31	1.47	1.54
2	A	385	PO4	P-O4	-2.31	1.47	1.54
2	A	384	PO4	P-O3	-2.26	1.47	1.54

There are no bond angle outliers.

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.