



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:04 PM UTC

PDB ID : 1XRC / pdb_00001xrc
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.

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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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

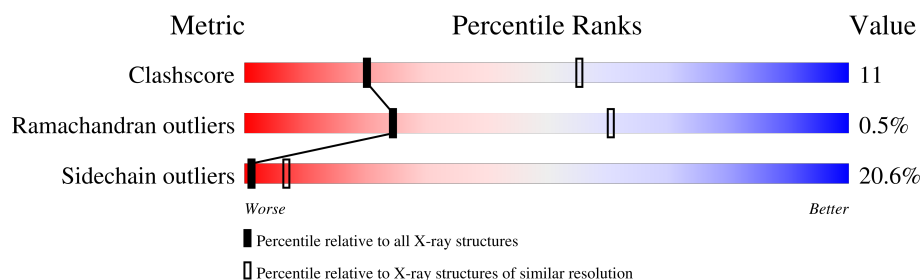
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	383	49% 35% 11% . .

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 [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 (CCD ID: 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 COBALT (II) ION (CCD ID: CO) (formula: Co).

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

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

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

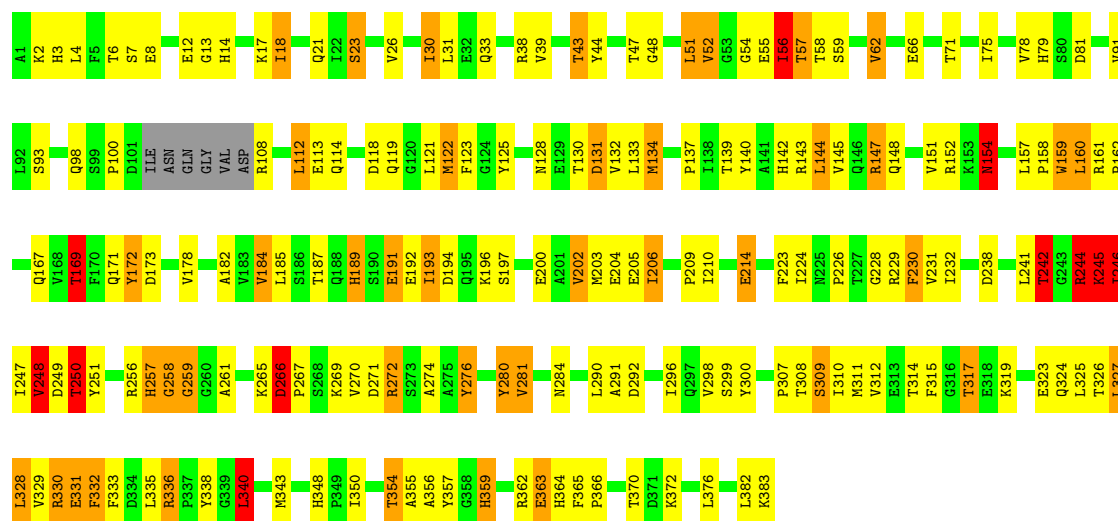
3 Residue-property plots

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

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	1.17	11/2956 (0.4%)	2.00	92/4005 (2.3%)

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	HIS	CD2-NE2	-7.33	1.29	1.37
1	A	364	HIS	CD2-NE2	-7.17	1.29	1.37
1	A	189	HIS	CD2-NE2	-7.04	1.30	1.37
1	A	257	HIS	CD2-NE2	-7.00	1.30	1.37
1	A	348	HIS	CD2-NE2	-6.79	1.30	1.37
1	A	79	HIS	CD2-NE2	-6.54	1.30	1.37
1	A	3	HIS	CD2-NE2	-6.28	1.30	1.37
1	A	14	HIS	CD2-NE2	-6.09	1.31	1.37
1	A	142	HIS	CD2-NE2	-5.93	1.31	1.37
1	A	244	ARG	CA-CB	-5.49	1.44	1.53
1	A	257	HIS	CG-ND1	-5.16	1.32	1.38

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	THR	N-CA-CB	-10.28	93.12	110.49
1	A	281	VAL	N-CA-CB	9.31	122.48	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	THR	CA-CB-CG2	9.23	126.20	110.50
1	A	30	ILE	N-CA-C	-9.18	101.91	110.82
1	A	271	ASP	CA-CB-CG	9.13	121.73	112.60
1	A	314	THR	N-CA-C	-8.83	94.13	108.52
1	A	331	GLU	CB-CG-CD	7.96	126.13	112.60
1	A	359	HIS	CB-CG-CD2	-7.90	120.93	131.20
1	A	8	GLU	CA-CB-CG	7.84	129.78	114.10
1	A	332	PHE	CA-CB-CG	-7.82	105.98	113.80
1	A	131	ASP	CA-CB-CG	7.75	120.35	112.60
1	A	258	GLY	O-C-N	-7.68	115.58	122.88
1	A	270	VAL	N-CA-CB	7.64	120.94	110.54
1	A	284	ASN	OD1-CG-ND2	-7.63	114.97	122.60
1	A	331	GLU	N-CA-CB	7.20	120.70	110.12
1	A	66	GLU	N-CA-C	-7.08	103.49	111.14
1	A	363	GLU	N-CA-C	7.02	125.76	110.80
1	A	159	TRP	CG-CD2-CE3	6.93	140.83	133.90
1	A	78	VAL	N-CA-CB	-6.92	99.81	111.23
1	A	118	ASP	CA-CB-CG	6.89	119.49	112.60
1	A	348	HIS	CB-CG-CD2	-6.70	122.50	131.20
1	A	330	ARG	CA-C-O	-6.67	113.81	120.82
1	A	159	TRP	CB-CG-CD1	-6.48	117.18	126.90
1	A	134	MET	CA-C-O	-6.47	114.00	120.66
1	A	247	ILE	N-CA-C	6.39	116.56	110.42
1	A	18	ILE	N-CA-C	-6.39	104.27	110.72
1	A	242	THR	N-CA-CB	6.26	119.28	109.83
1	A	365	PHE	N-CA-C	-6.24	102.27	110.39
1	A	161	ARG	O-C-N	-6.16	114.24	121.32
1	A	256	ARG	N-CA-CB	-6.12	101.92	110.25
1	A	189	HIS	CB-CG-CD2	-6.10	123.27	131.20
1	A	26	VAL	N-CA-CB	-6.04	101.52	110.58
1	A	14	HIS	CA-C-N	6.04	126.20	119.32
1	A	14	HIS	C-N-CA	6.04	126.20	119.32
1	A	162	PRO	N-CA-C	6.03	121.48	113.40
1	A	14	HIS	CB-CG-CD2	-6.01	123.39	131.20
1	A	56	ILE	O-C-N	-6.01	116.69	123.18
1	A	231	VAL	CB-CA-C	6.00	116.80	110.91
1	A	14	HIS	O-C-N	-6.00	115.96	121.30
1	A	249	ASP	N-CA-C	5.93	118.23	111.11
1	A	114	GLN	O-C-N	5.92	130.11	122.89
1	A	267	PRO	N-CA-C	5.92	121.53	113.84
1	A	193	ILE	N-CA-C	5.90	118.13	109.63
1	A	55	GLU	CB-CG-CD	5.86	122.56	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ARG	CB-CG-CD	5.86	124.77	111.30
1	A	340	LEU	CB-CA-C	-5.84	101.47	110.81
1	A	359	HIS	CB-CG-ND1	5.81	131.41	122.70
1	A	241	LEU	O-C-N	-5.74	116.39	123.33
1	A	284	ASN	CB-CG-ND2	5.71	124.96	116.40
1	A	244	ARG	CA-CB-CG	-5.68	102.73	114.10
1	A	26	VAL	O-C-N	-5.68	115.98	121.83
1	A	250	THR	CA-CB-OG1	-5.63	101.16	109.60
1	A	245	LYS	CB-CG-CD	5.62	124.22	111.30
1	A	248	VAL	N-CA-CB	5.61	117.48	110.47
1	A	363	GLU	O-C-N	-5.57	115.18	122.59
1	A	319	LYS	N-CA-C	-5.56	104.74	112.30
1	A	256	ARG	N-CA-C	5.55	117.07	110.19
1	A	52	VAL	N-CA-C	-5.53	99.68	107.75
1	A	71	THR	CA-CB-OG1	-5.48	101.38	109.60
1	A	189	HIS	CA-C-O	-5.46	115.61	121.45
1	A	160	LEU	N-CA-C	5.45	118.69	109.76
1	A	364	HIS	CB-CG-CD2	-5.44	124.13	131.20
1	A	154	ASN	OD1-CG-ND2	-5.41	117.19	122.60
1	A	330	ARG	N-CA-C	5.41	116.86	111.07
1	A	51	LEU	N-CA-C	-5.40	99.72	108.52
1	A	238	ASP	O-C-N	-5.39	115.42	122.59
1	A	91	VAL	N-CA-C	-5.39	99.88	107.75
1	A	206	ILE	N-CA-C	-5.33	107.41	111.62
1	A	169	THR	OG1-CB-CG2	5.33	119.95	109.30
1	A	280	TYR	CA-C-O	-5.28	115.00	120.92
1	A	147	ARG	N-CA-C	-5.28	105.61	111.36
1	A	250	THR	O-C-N	-5.26	115.59	122.59
1	A	159	TRP	CE2-CD2-CG	-5.24	100.91	107.20
1	A	56	ILE	CA-CB-CG2	5.24	119.40	110.50
1	A	100	PRO	O-C-N	5.24	128.69	122.98
1	A	266	ASP	CA-C-N	5.23	124.89	119.56
1	A	266	ASP	C-N-CA	5.23	124.89	119.56
1	A	259	GLY	CA-C-N	-5.22	117.54	122.66
1	A	259	GLY	C-N-CA	-5.22	117.54	122.66
1	A	244	ARG	N-CA-C	5.21	119.68	112.45
1	A	261	ALA	CB-CA-C	-5.17	101.27	109.80
1	A	205	GLU	N-CA-C	5.16	119.84	113.50
1	A	230	PHE	N-CA-CB	-5.16	102.67	110.35
1	A	93	SER	N-CA-C	5.12	117.60	109.50
1	A	191	GLU	N-CA-C	-5.11	106.30	112.54
1	A	172	TYR	CA-CB-CG	5.08	123.05	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	THR	N-CA-C	5.08	118.35	110.17
1	A	329	VAL	N-CA-C	-5.07	104.96	110.23
1	A	246	ILE	O-C-N	-5.07	116.23	122.57
1	A	23	SER	CB-CA-C	-5.06	102.93	110.88
1	A	229	ARG	CA-C-O	5.05	127.23	121.58
1	A	338	TYR	CA-CB-CG	-5.03	104.85	113.90

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	PHE	Sidechain
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 ⓘ

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:214:GLU:H	1:A:214:GLU:CD	2.23	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
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:343:MET:HB3	1:A:343:MET:HE2	1.85	0.41
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: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

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	373/383 (97%)	339 (91%)	32 (9%)	2 (0%)	24	60

All (2) Ramachandran outliers are listed below:

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

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	306/311 (98%)	243 (79%)	63 (21%)	1	7

All (63) 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	39	VAL
1	A	47	THR
1	A	51	LEU
1	A	52	VAL
1	A	56	ILE
1	A	57	THR

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Mol	Chain	Res	Type
1	A	59	SER
1	A	62	VAL
1	A	81	ASP
1	A	112	LEU
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
1	A	185	LEU
1	A	187	THR
1	A	191	GLU
1	A	192	GLU
1	A	196	LYS
1	A	197	SER
1	A	200	GLU
1	A	202	VAL
1	A	203	MET
1	A	214	GLU
1	A	232	ILE
1	A	242	THR
1	A	245	LYS
1	A	246	ILE
1	A	248	VAL
1	A	266	ASP
1	A	281	VAL
1	A	298	VAL
1	A	308	THR
1	A	309	SER
1	A	310	ILE
1	A	311	MET
1	A	312	VAL
1	A	315	PHE
1	A	317	THR
1	A	323	GLU
1	A	326	THR

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Mol	Chain	Res	Type
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 (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	119	GLN
1	A	148	GLN
1	A	154	ASN
1	A	189	HIS
1	A	257	HIS
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 oligosaccharides 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	2.05	2 (50%)	6,6,6	0.41	0
2	PO4	A	384	3	4,4,4	2.38	3 (75%)	6,6,6	1.52	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	-2.93	1.46	1.54
2	A	384	PO4	P-O4	-2.80	1.46	1.54
2	A	385	PO4	P-O3	-2.69	1.46	1.54
2	A	385	PO4	P-O4	-2.63	1.47	1.54
2	A	384	PO4	P-O3	-2.26	1.48	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	384	PO4	O4-P-O1	-3.02	100.29	110.95

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.