



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:46 AM UTC

PDB ID : 1XRB / pdb_00001xrb
Title : S-adenosylmethionine synthetase (MAT, ATP: L-methionine S-adenosyltransferase, E.C.2.5.1.6) in which MET residues are replaced with selenomethionine residues (MSE)
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	:	4-5-2 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

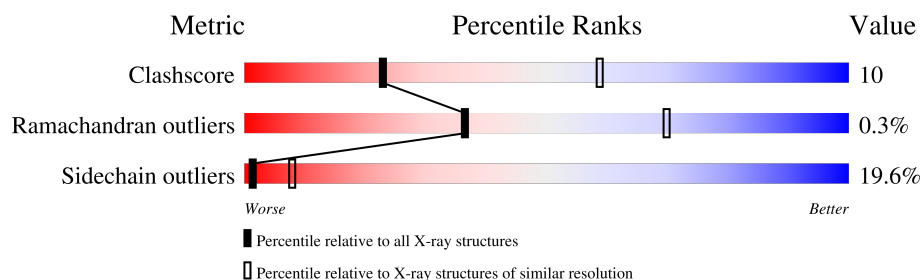
1 Overall quality at a glance

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	55% 32% 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 [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	Se	632	0	0
			3530	1830	632	495	560	4	9			

- 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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

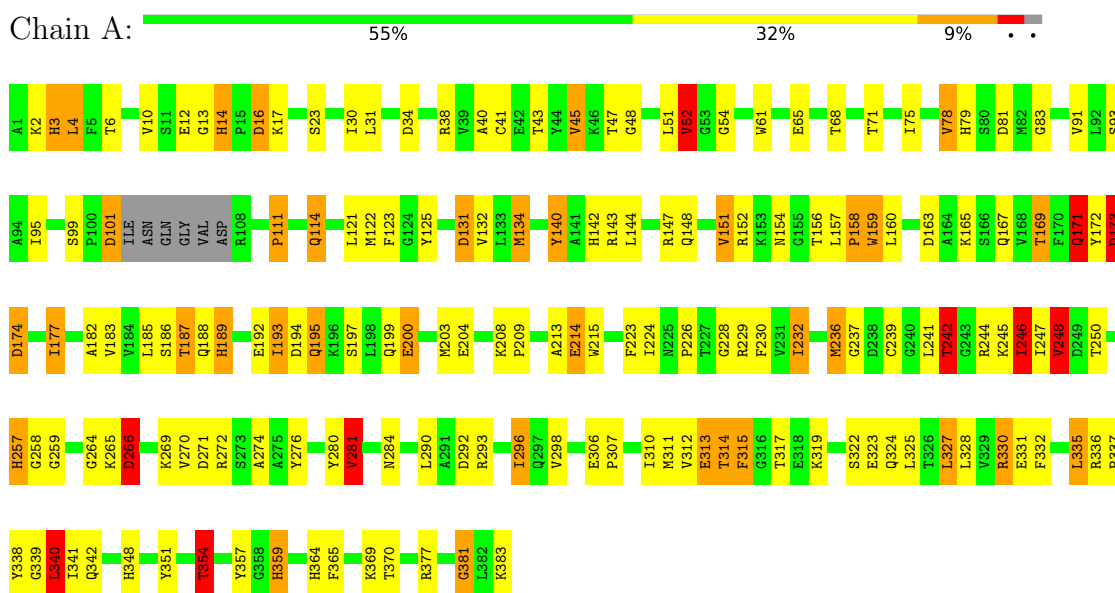
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	K	0	0
			2	2		

3 Residue-property plots [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



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)	97.7 (10.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.188 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3544	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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, PO4, MG

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	1.15	11/2947 (0.4%)	1.94	79/3978 (2.0%)

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	13

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	HIS	CD2-NE2	-8.04	1.29	1.37
1	A	364	HIS	CD2-NE2	-7.18	1.29	1.37
1	A	348	HIS	CD2-NE2	-7.12	1.30	1.37
1	A	79	HIS	CD2-NE2	-7.09	1.30	1.37
1	A	359	HIS	CD2-NE2	-6.99	1.30	1.37
1	A	257	HIS	CD2-NE2	-6.69	1.30	1.37
1	A	142	HIS	CD2-NE2	-6.40	1.30	1.37
1	A	14	HIS	CD2-NE2	-6.18	1.31	1.37
1	A	3	HIS	CD2-NE2	-6.02	1.31	1.37
1	A	142	HIS	CG-ND1	-5.66	1.32	1.38
1	A	79	HIS	CG-ND1	-5.22	1.32	1.38

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	THR	N-CA-C	-10.34	92.53	108.96
1	A	189	HIS	CB-CG-CD2	-10.02	118.17	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	VAL	N-CA-CB	9.97	122.21	110.55
1	A	236	MSE	CA-CB-CG	-9.91	94.28	114.10
1	A	187	THR	CA-CB-OG1	-9.50	95.34	109.60
1	A	354	THR	N-CA-CB	-9.41	95.73	110.22
1	A	271	ASP	CA-CB-CG	9.08	121.68	112.60
1	A	246	ILE	CA-CB-CG2	8.54	125.03	110.50
1	A	359	HIS	CB-CG-CD2	-8.33	120.37	131.20
1	A	174	ASP	N-CA-C	7.87	121.69	109.96
1	A	71	THR	CA-CB-OG1	-7.52	98.33	109.60
1	A	189	HIS	CB-CG-ND1	7.50	133.95	122.70
1	A	78	VAL	N-CA-CB	-7.37	101.40	112.67
1	A	331	GLU	CB-CG-CD	7.28	124.98	112.60
1	A	354	THR	N-CA-C	7.05	119.82	111.71
1	A	332	PHE	CA-CB-CG	-7.03	106.77	113.80
1	A	364	HIS	CB-CG-CD2	-6.85	122.30	131.20
1	A	348	HIS	CB-CG-CD2	-6.84	122.31	131.20
1	A	266	ASP	CA-C-N	6.83	126.53	119.56
1	A	266	ASP	C-N-CA	6.83	126.53	119.56
1	A	248	VAL	N-CA-CB	6.76	118.46	110.55
1	A	14	HIS	CB-CG-CD2	-6.76	122.41	131.20
1	A	232	ILE	CA-C-N	-6.66	117.03	122.16
1	A	232	ILE	C-N-CA	-6.66	117.03	122.16
1	A	313	GLU	CA-C-O	6.56	127.41	120.33
1	A	200	GLU	N-CA-CB	6.51	120.37	110.28
1	A	195	GLN	OE1-CD-NE2	-6.41	116.19	122.60
1	A	188	GLN	N-CA-C	-6.35	101.54	110.50
1	A	41	CYS	N-CA-CB	-6.35	100.62	110.65
1	A	14	HIS	O-C-N	-6.34	115.66	121.30
1	A	359	HIS	CB-CG-ND1	6.24	132.06	122.70
1	A	199	GLN	CA-C-O	-6.20	114.26	120.90
1	A	3	HIS	CB-CG-CD2	-6.19	123.16	131.20
1	A	159	TRP	CG-CD2-CE3	6.18	140.08	133.90
1	A	101	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	16	ASP	N-CA-CB	5.98	119.02	110.16
1	A	134	MSE	CA-C-O	-5.95	115.79	121.08
1	A	365	PHE	N-CA-C	-5.90	101.42	110.32
1	A	159	TRP	CB-CG-CD1	-5.84	118.13	126.90
1	A	250	THR	N-CA-C	5.79	123.14	110.80
1	A	270	VAL	N-CA-CB	5.78	120.54	110.65
1	A	340	LEU	CB-CA-C	-5.68	101.72	110.81
1	A	54	GLY	CA-C-O	-5.68	116.06	121.62
1	A	173	ASP	N-CA-C	-5.67	102.13	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	ASP	CA-CB-CG	5.65	118.25	112.60
1	A	246	ILE	N-CA-C	5.65	116.29	110.36
1	A	140	TYR	CA-CB-CG	-5.62	103.79	113.90
1	A	224	ILE	CA-C-O	-5.61	113.90	121.02
1	A	341	ILE	O-C-N	5.57	127.28	121.87
1	A	242	THR	N-CA-CB	5.51	118.14	110.04
1	A	52	VAL	CB-CA-C	5.47	118.54	110.77
1	A	369	LYS	CA-CB-CG	5.47	125.04	114.10
1	A	167	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	A	213	ALA	N-CA-C	5.44	117.29	111.36
1	A	247	ILE	N-CA-C	5.40	115.60	110.42
1	A	163	ASP	CA-C-O	-5.38	114.73	120.92
1	A	354	THR	CA-CB-CG2	5.38	119.64	110.50
1	A	114	GLN	O-C-N	5.27	129.21	123.04
1	A	34	ASP	O-C-N	-5.26	117.55	121.23
1	A	78	VAL	CA-C-O	5.26	123.56	119.46
1	A	99	SER	N-CA-C	-5.26	101.44	109.64
1	A	45	VAL	CB-CA-C	-5.22	102.71	110.33
1	A	61	TRP	CG-CD2-CE3	5.20	139.10	133.90
1	A	200	GLU	CA-CB-CG	5.20	124.49	114.10
1	A	61	TRP	CE2-CD2-CG	-5.18	100.98	107.20
1	A	257	HIS	CB-CG-CD2	-5.18	124.47	131.20
1	A	159	TRP	CE2-CD2-CG	-5.18	100.99	107.20
1	A	230	PHE	CA-CB-CG	5.18	118.98	113.80
1	A	30	ILE	N-CA-C	-5.15	105.82	110.82
1	A	296	ILE	CA-CB-CG1	5.12	119.11	110.40
1	A	187	THR	CA-CB-CG2	5.12	119.20	110.50
1	A	306	GLU	CA-C-N	5.08	125.36	119.93
1	A	306	GLU	C-N-CA	5.08	125.36	119.93
1	A	340	LEU	N-CA-CB	5.06	117.48	109.94
1	A	270	VAL	CA-C-O	-5.06	115.16	120.57
1	A	246	ILE	CA-CB-CG1	-5.03	101.85	110.40
1	A	284	ASN	CA-CB-CG	-5.01	107.59	112.60
1	A	246	ILE	N-CA-CB	-5.01	104.95	110.51
1	A	171	GLN	CA-CB-CG	5.00	124.10	114.10

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	PHE	Sidechain
1	A	125	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	13	GLY	Peptide
1	A	140	TYR	Sidechain
1	A	173	ASP	Peptide
1	A	194	ASP	Peptide
1	A	228	GLY	Peptide
1	A	244	ARG	Sidechain
1	A	259	GLY	Peptide
1	A	280	TYR	Sidechain
1	A	293	ARG	Sidechain
1	A	336	ARG	Sidechain
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	60	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	60	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 10.

All (60) 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:351:TYR:O	1:A:354:THR:HB	1.78	0.82
1:A:354:THR:HG23	1:A:359:HIS:NE2	2.03	0.73
1:A:354:THR:HG23	1:A:359:HIS:CD2	2.23	0.73
1:A:43:THR:H	1:A:242:THR:HG23	1.54	0.71
1:A:122:MSE:HG2	1:A:274:ALA:HB3	1.73	0.68
1:A:83:GLY:HA2	1:A:236:MSE:HG3	1.78	0.64
1:A:223:PHE:HB3	1:A:226:PRO:HG3	1.80	0.63
1:A:23:SER:OG	1:A:242:THR:HG21	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:LEU:HD23	1:A:325:LEU:HD21	1.85	0.59
1:A:83:GLY:CA	1:A:236:MSE:HG3	2.33	0.58
1:A:189:HIS:HE1	1:A:229:ARG:O	1.87	0.58
1:A:324:GLN:O	1:A:328:LEU:HD12	2.04	0.57
1:A:189:HIS:CE1	1:A:229:ARG:O	2.59	0.56
1:A:339:GLY:O	1:A:342:GLN:HB3	2.05	0.56
1:A:257:HIS:CD2	1:A:258:GLY:O	2.62	0.53
1:A:6:THR:OG1	1:A:169:THR:HB	2.09	0.52
1:A:327:LEU:HA	1:A:330:ARG:HH12	1.74	0.52
1:A:265:LYS:HB3	1:A:269:LYS:HG3	1.90	0.51
1:A:10:VAL:HG12	1:A:165:LYS:HD2	1.93	0.50
1:A:132:VAL:HG23	1:A:134:MSE:HB2	1.94	0.49
1:A:232:ILE:HG12	1:A:236:MSE:HE3	1.95	0.49
1:A:189:HIS:HD2	1:A:193:ILE:CG2	2.26	0.49
1:A:257:HIS:HD2	1:A:258:GLY:O	1.96	0.49
1:A:246:ILE:HG23	1:A:257:HIS:NE2	2.28	0.49
1:A:47:THR:HG22	1:A:237:GLY:H	1.78	0.48
1:A:52:VAL:O	1:A:93:SER:HA	2.13	0.48
1:A:151:VAL:HA	1:A:154:ASN:OD1	2.14	0.48
1:A:266:ASP:OD2	1:A:269:LYS:NZ	2.47	0.48
1:A:169:THR:HG23	1:A:182:ALA:HB3	1.94	0.48
1:A:281:VAL:HG22	1:A:296:ILE:HG13	1.97	0.47
1:A:381:GLY:O	1:A:383:LYS:NZ	2.48	0.46
1:A:298:VAL:HG12	1:A:310:ILE:HG12	1.97	0.46
1:A:245:LYS:HB3	1:A:248:VAL:HG13	1.96	0.46
1:A:2:LYS:NZ	1:A:173:ASP:OD2	2.49	0.45
1:A:68:THR:HG21	1:A:91:VAL:HG13	1.99	0.45
1:A:4:LEU:HD23	1:A:171:GLN:HB2	1.98	0.45
1:A:327:LEU:HA	1:A:330:ARG:NH1	2.32	0.45
1:A:156:THR:O	1:A:158:PRO:HD3	2.17	0.45
1:A:204:GLU:O	1:A:209:PRO:HD3	2.17	0.45
1:A:12:GLU:HG2	1:A:357:TYR:OH	2.17	0.45
1:A:246:ILE:HG23	1:A:257:HIS:CE1	2.52	0.44
1:A:203:MSE:O	1:A:208:LYS:HB2	2.17	0.44
1:A:292:ASP:H	1:A:317:THR:HB	1.81	0.44
1:A:185:LEU:HD13	1:A:186:SER:N	2.33	0.43
1:A:338:TYR:N	1:A:338:TYR:CD1	2.85	0.43
1:A:335:LEU:HA	1:A:340:LEU:CD1	2.49	0.43
1:A:177:ILE:HG13	1:A:215:TRP:CZ2	2.54	0.43
1:A:40:ALA:HA	1:A:264:GLY:O	2.19	0.42
1:A:377:ARG:CZ	1:A:383:LYS:HG3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LEU:HD22	1:A:159:TRP:CZ2	2.54	0.41
1:A:325:LEU:HA	1:A:325:LEU:HD23	1.76	0.41
1:A:75:ILE:O	1:A:152:ARG:NH2	2.53	0.41
1:A:276:TYR:OH	1:A:359:HIS:HD2	2.03	0.41
1:A:324:GLN:O	1:A:327:LEU:HB3	2.21	0.41
1:A:214:GLU:H	1:A:214:GLU:CD	2.28	0.41
1:A:272:ARG:HD2	1:A:276:TYR:CE2	2.55	0.41
1:A:2:LYS:HA	1:A:172:TYR:O	2.21	0.40
1:A:381:GLY:O	1:A:383:LYS:HG2	2.21	0.40
1:A:315:PHE:CD1	1:A:315:PHE:N	2.88	0.40
1:A:111:PRO:O	1:A:114:GLN:HG2	2.22	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%)	342 (92%)	30 (8%)	1 (0%)	36 70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	381	GLY

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	306/302 (101%)	246 (80%)	60 (20%)	1 8

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	4	LEU
1	A	14	HIS
1	A	16	ASP
1	A	17	LYS
1	A	31	LEU
1	A	38	ARG
1	A	45	VAL
1	A	51	LEU
1	A	52	VAL
1	A	65	GLU
1	A	78	VAL
1	A	81	ASP
1	A	95	ILE
1	A	101	ASP
1	A	111	PRO
1	A	121	LEU
1	A	131	ASP
1	A	143	ARG
1	A	144	LEU
1	A	147	ARG
1	A	148	GLN
1	A	151	VAL
1	A	158	PRO
1	A	160	LEU
1	A	169	THR
1	A	171	GLN
1	A	174	ASP
1	A	177	ILE
1	A	183	VAL
1	A	187	THR
1	A	192	GLU
1	A	193	ILE
1	A	195	GLN
1	A	197	SER
1	A	200	GLU
1	A	214	GLU
1	A	239	CYS

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Mol	Chain	Res	Type
1	A	241	LEU
1	A	242	THR
1	A	246	ILE
1	A	248	VAL
1	A	266	ASP
1	A	281	VAL
1	A	307	PRO
1	A	311	MSE
1	A	312	VAL
1	A	313	GLU
1	A	314	THR
1	A	315	PHE
1	A	319	LYS
1	A	322	SER
1	A	323	GLU
1	A	327	LEU
1	A	330	ARG
1	A	335	LEU
1	A	337	PRO
1	A	340	LEU
1	A	354	THR
1	A	370	THR

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	21	GLN
1	A	114	GLN
1	A	142	HIS
1	A	171	GLN
1	A	189	HIS
1	A	257	HIS
1	A	297	GLN
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 [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	384	3	4,4,4	2.36	3 (75%)	6,6,6	1.31	1 (16%)
2	PO4	A	385	3	4,4,4	1.81	2 (50%)	6,6,6	1.15	0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	384	PO4	P-O3	-2.91	1.46	1.54
2	A	384	PO4	P-O4	-2.74	1.46	1.54
2	A	384	PO4	P-O2	-2.51	1.47	1.54
2	A	385	PO4	P-O3	-2.25	1.48	1.54
2	A	385	PO4	P-O4	-2.08	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-O3	-2.34	100.64	107.91

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.