



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 07:40 pm BST

PDB ID : 1INP
Title : CRYSTAL STRUCTURE OF INOSITOL POLYPHOSPHATE 1-PHOSPHATASE AT 2.3 ANGSTROMS RESOLUTION
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Deposited on : 1994-10-04
Resolution : 2.30 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
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

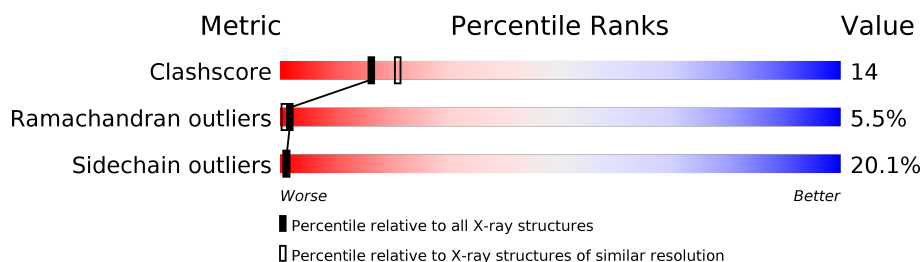
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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	400	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3985 atoms, of which 825 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 INOSITOL POLYPHOSPHATE 1-PHOSPHATASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	400	Total	C	H	N	O	S	0	0	0
			3773	1951	685	525	598	14			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is water.

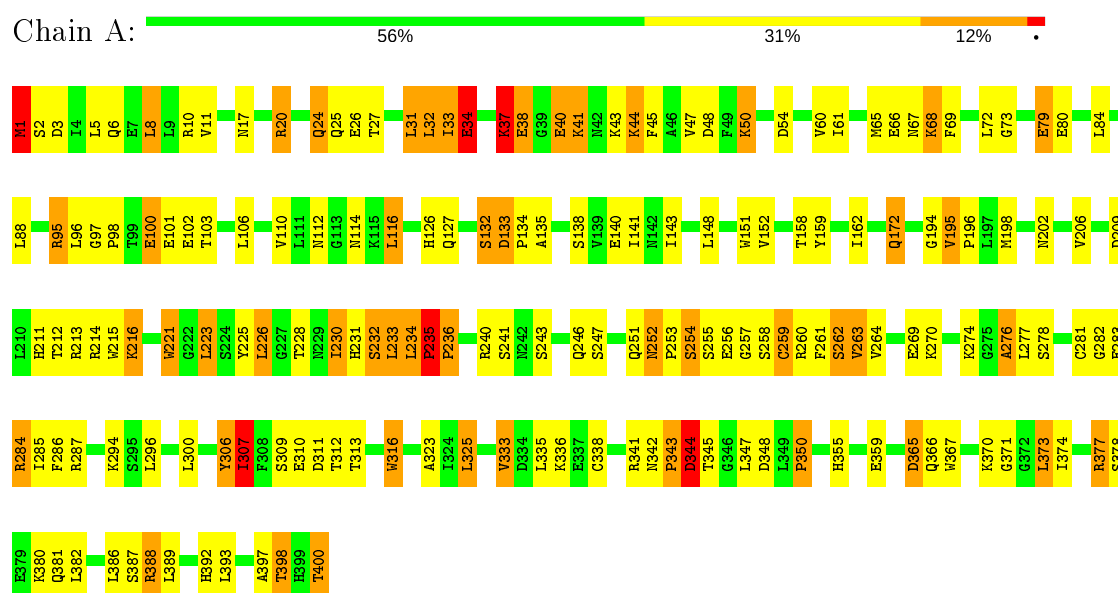
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	70	Total	H	O	0	0
			210	140	70		

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. 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: INOSITOL POLYPHOSPHATE 1-PHOSPHATASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	51.64 Å 51.64 Å 143.33 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	99.3 (8.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3985	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: 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	0.97	9/3143 (0.3%)	1.81	67/4254 (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	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	GLY	C-N	-16.19	0.96	1.34
1	A	344	ASP	N-CA	10.89	1.68	1.46
1	A	234	LEU	N-CA	-10.34	1.25	1.46
1	A	235	PRO	C-N	8.51	1.50	1.34
1	A	235	PRO	CA-C	7.83	1.68	1.52
1	A	236	PRO	N-CA	6.63	1.58	1.47
1	A	233	LEU	CA-C	-6.56	1.35	1.52
1	A	235	PRO	N-CA	5.94	1.57	1.47
1	A	233	LEU	C-N	-5.04	1.22	1.34

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	GLY	C-N-CA	16.51	162.98	121.70
1	A	343	PRO	O-C-N	-15.62	97.70	122.70
1	A	20	ARG	NE-CZ-NH2	-15.16	112.72	120.30
1	A	194	GLY	O-C-N	-14.59	99.36	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	GLY	CA-C-N	13.73	147.41	117.20
1	A	20	ARG	NE-CZ-NH1	12.64	126.62	120.30
1	A	234	LEU	O-C-N	-10.68	100.81	121.10
1	A	343	PRO	CA-C-N	9.79	138.74	117.20
1	A	151	TRP	CD1-CG-CD2	9.33	113.76	106.30
1	A	215	TRP	CD1-CG-CD2	9.32	113.76	106.30
1	A	234	LEU	CB-CA-C	-9.25	92.62	110.20
1	A	233	LEU	O-C-N	9.24	137.49	122.70
1	A	151	TRP	CE2-CD2-CG	-8.12	100.81	107.30
1	A	221	TRP	CE2-CD2-CG	-8.01	100.89	107.30
1	A	221	TRP	CD1-CG-CD2	8.00	112.70	106.30
1	A	215	TRP	CE2-CD2-CG	-7.96	100.93	107.30
1	A	367	TRP	CD1-CG-CD2	7.79	112.54	106.30
1	A	215	TRP	CG-CD2-CE3	7.76	140.88	133.90
1	A	367	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	A	287	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	A	373	LEU	CA-CB-CG	7.28	132.05	115.30
1	A	284	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	A	198	MET	CG-SD-CE	-7.13	88.79	100.20
1	A	233	LEU	CA-C-N	-7.04	101.70	117.20
1	A	316	TRP	CD1-CG-CD2	6.74	111.69	106.30
1	A	234	LEU	CA-C-N	6.72	135.91	117.10
1	A	215	TRP	CB-CG-CD1	-6.70	118.29	127.00
1	A	221	TRP	CB-CG-CD1	-6.42	118.65	127.00
1	A	31	LEU	CA-CB-CG	6.41	130.03	115.30
1	A	343	PRO	C-N-CA	-6.39	105.72	121.70
1	A	101	GLU	N-CA-C	-6.39	93.75	111.00
1	A	274	LYS	CA-CB-CG	6.30	127.27	113.40
1	A	221	TRP	CG-CD2-CE3	6.30	139.57	133.90
1	A	38	GLU	N-CA-C	6.28	127.95	111.00
1	A	316	TRP	CE2-CD2-CG	-6.20	102.34	107.30
1	A	37	LYS	N-CA-C	6.16	127.64	111.00
1	A	10	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	3	ASP	CA-C-N	-6.01	103.98	117.20
1	A	215	TRP	CG-CD1-NE1	-5.99	104.11	110.10
1	A	41	LYS	CA-CB-CG	5.94	126.47	113.40
1	A	234	LEU	N-CA-C	5.92	127.00	111.00
1	A	367	TRP	CG-CD2-CE3	5.91	139.22	133.90
1	A	223	LEU	CA-CB-CG	5.82	128.68	115.30
1	A	350	PRO	CA-N-CD	-5.78	103.41	111.50
1	A	1	MET	N-CA-C	-5.68	95.65	111.00
1	A	206	VAL	CG1-CB-CG2	-5.67	101.82	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	CYS	CA-CB-SG	5.63	124.13	114.00
1	A	151	TRP	CG-CD1-NE1	-5.54	104.56	110.10
1	A	367	TRP	CB-CG-CD1	-5.47	119.89	127.00
1	A	195	VAL	O-C-N	-5.46	110.73	121.10
1	A	230	ILE	CA-CB-CG2	-5.45	100.00	110.90
1	A	60	VAL	CG1-CB-CG2	-5.41	102.25	110.90
1	A	159	TYR	CB-CG-CD1	-5.39	117.76	121.00
1	A	44	LYS	CA-C-N	-5.34	105.44	117.20
1	A	261	PHE	N-CA-C	5.34	125.41	111.00
1	A	287	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	365	ASP	CA-C-N	-5.32	105.51	117.20
1	A	132	SER	N-CA-C	5.31	125.33	111.00
1	A	40	GLU	N-CA-C	5.27	125.22	111.00
1	A	388	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	307	ILE	CB-CA-C	-5.20	101.20	111.60
1	A	325	LEU	CA-CB-CG	5.11	127.06	115.30
1	A	377	ARG	CB-CG-CD	-5.11	98.32	111.60
1	A	211	HIS	CA-CB-CG	-5.10	104.93	113.60
1	A	34	GLU	CA-CB-CG	5.09	124.61	113.40
1	A	240	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	95	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195	VAL	Mainchain

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	3088	685	3090	89	0
2	A	2	0	0	0	0
3	A	70	140	0	12	0
All	All	3160	825	3090	89	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 14.

All (89) 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:344:ASP:N	1:A:344:ASP:CA	1.68	1.55
1:A:343:PRO:O	1:A:344:ASP:CA	2.02	1.08
1:A:343:PRO:O	1:A:344:ASP:HA	1.63	0.95
1:A:343:PRO:C	1:A:344:ASP:CA	2.37	0.92
1:A:234:LEU:HD12	1:A:234:LEU:O	1.71	0.89
1:A:97:GLY:HA3	3:A:462:HOH:O	1.84	0.77
1:A:47:VAL:HG23	1:A:50:LYS:HD3	1.72	0.72
1:A:234:LEU:CD1	1:A:234:LEU:O	2.39	0.69
1:A:152:VAL:HG21	3:A:440:HOH:O	1.94	0.67
1:A:69:PHE:HB2	1:A:72:LEU:HD22	1.78	0.66
1:A:348:ASP:HA	3:A:411:HOH:O	1.96	0.64
1:A:212:THR:HG22	1:A:214:ARG:HD2	1.79	0.64
1:A:135:ALA:HB3	3:A:407:HOH:O	1.97	0.64
1:A:37:LYS:HE2	1:A:50:LYS:HD2	1.79	0.64
1:A:172:GLN:HG2	1:A:284:ARG:HH22	1.62	0.64
1:A:264:VAL:HG22	1:A:284:ARG:NE	2.15	0.61
1:A:79:GLU:HB3	1:A:316:TRP:CE2	2.34	0.61
1:A:382:LEU:O	1:A:386:LEU:HG	2.00	0.60
1:A:226:LEU:HD11	3:A:410:HOH:O	2.02	0.58
1:A:134:PRO:HD2	1:A:221:TRP:HE1	1.68	0.58
1:A:344:ASP:N	1:A:344:ASP:CB	2.62	0.55
1:A:172:GLN:HG2	1:A:284:ARG:NH2	2.22	0.55
1:A:344:ASP:N	1:A:344:ASP:C	2.53	0.55
1:A:196:PRO:HB2	1:A:323:ALA:HB2	1.89	0.54
1:A:148:LEU:HB2	3:A:437:HOH:O	2.07	0.54
1:A:103:THR:OG1	1:A:126:HIS:HE1	1.92	0.53
1:A:343:PRO:HG3	1:A:386:LEU:HD22	1.90	0.53
1:A:66:GLU:HG2	1:A:73:GLY:HA3	1.91	0.53
1:A:66:GLU:CG	1:A:73:GLY:HA3	2.39	0.52
1:A:264:VAL:HG13	1:A:286:PHE:HE1	1.74	0.52
1:A:342:ASN:CG	1:A:343:PRO:HD2	2.30	0.52
1:A:294:LYS:HE2	1:A:306:TYR:CE1	2.44	0.52
1:A:65:MET:HB3	1:A:72:LEU:HD23	1.92	0.51
1:A:54:ASP:HB3	1:A:80:GLU:HG3	1.91	0.51
1:A:226:LEU:HD23	1:A:226:LEU:N	2.25	0.51
1:A:262:SER:HA	1:A:281:CYS:HB2	1.94	0.50
1:A:344:ASP:N	1:A:345:THR:N	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:VAL:HG11	1:A:61:ILE:HG23	1.94	0.49
1:A:381:GLN:HG3	3:A:467:HOH:O	2.11	0.49
1:A:11:VAL:CG1	1:A:61:ILE:HG23	2.43	0.49
1:A:158:THR:O	1:A:162:ILE:HB	2.12	0.49
1:A:342:ASN:O	1:A:343:PRO:C	2.51	0.49
1:A:214:ARG:O	1:A:216:LYS:HE2	2.12	0.48
1:A:313:THR:HB	3:A:412:HOH:O	2.13	0.48
1:A:262:SER:HA	1:A:281:CYS:O	2.14	0.48
1:A:32:LEU:O	1:A:33:ILE:HG23	2.13	0.48
1:A:347:LEU:O	1:A:350:PRO:HD2	2.14	0.48
1:A:252:ASN:O	1:A:256:GLU:HG2	2.13	0.47
1:A:1:MET:N	1:A:141:ILE:O	2.47	0.47
1:A:343:PRO:CG	1:A:386:LEU:HD13	2.44	0.47
1:A:231:HIS:HD2	1:A:233:LEU:HD23	1.77	0.47
1:A:276:ALA:O	1:A:277:LEU:HD12	2.14	0.47
1:A:143:ILE:HG21	1:A:148:LEU:HD21	1.95	0.47
1:A:232:SER:O	1:A:234:LEU:HG	2.15	0.47
1:A:263:VAL:HG13	3:A:439:HOH:O	2.14	0.47
1:A:263:VAL:HG23	1:A:281:CYS:SG	2.55	0.47
1:A:333:VAL:CG1	1:A:338:CYS:SG	3.04	0.46
1:A:100:GLU:HA	3:A:462:HOH:O	2.14	0.46
1:A:20:ARG:O	1:A:24:GLN:HG2	2.16	0.46
1:A:336:LYS:HE2	1:A:371:GLY:HA3	1.98	0.45
1:A:133:ASP:OD1	1:A:134:PRO:HA	2.17	0.45
1:A:307:ILE:HG23	1:A:374:ILE:HG12	1.99	0.44
1:A:343:PRO:HG2	1:A:386:LEU:HD13	1.99	0.44
1:A:84:LEU:HD13	1:A:110:VAL:HG11	2.00	0.44
1:A:365:ASP:HA	3:A:450:HOH:O	2.19	0.43
1:A:1:MET:SD	1:A:2:SER:N	2.92	0.43
1:A:135:ALA:HA	1:A:138:SER:OG	2.18	0.42
1:A:95:ARG:O	1:A:106:LEU:HD22	2.19	0.42
1:A:278:SER:HA	1:A:282:GLY:O	2.19	0.42
1:A:8:LEU:HD13	1:A:65:MET:CE	2.49	0.42
1:A:225:TYR:C	1:A:226:LEU:HG	2.40	0.42
1:A:341:ARG:NH2	1:A:350:PRO:HG3	2.35	0.42
1:A:37:LYS:CE	1:A:50:LYS:HD2	2.48	0.42
1:A:264:VAL:HG13	1:A:284:ARG:HE	1.84	0.42
1:A:309:SER:HA	1:A:335:LEU:HD23	2.01	0.42
1:A:17:ASN:HD22	1:A:20:ARG:HH11	1.68	0.42
1:A:33:ILE:HD11	1:A:162:ILE:HG13	2.02	0.42
1:A:235:PRO:CD	1:A:300:LEU:HD22	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ILE:HG21	1:A:47:VAL:HB	2.03	0.41
1:A:100:GLU:HG2	1:A:102:GLU:HA	2.03	0.41
1:A:252:ASN:C	1:A:256:GLU:HG2	2.41	0.41
1:A:33:ILE:HB	1:A:34:GLU:H	1.77	0.41
1:A:254:SER:HA	1:A:377:ARG:HH22	1.86	0.41
1:A:398:THR:HG22	1:A:400:THR:O	2.21	0.41
1:A:68:LYS:HG3	1:A:69:PHE:CE2	2.56	0.40
1:A:45:PHE:HD1	3:A:455:HOH:O	2.03	0.40
1:A:209:ASP:O	1:A:213:ARG:N	2.55	0.40
1:A:344:ASP:N	1:A:345:THR:H	2.19	0.40
1:A:162:ILE:HA	1:A:162:ILE:HD13	2.01	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	398/400 (100%)	320 (80%)	56 (14%)	22 (6%)	2 1

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ILE
1	A	37	LYS
1	A	43	LYS
1	A	98	PRO
1	A	114	ASN
1	A	116	LEU
1	A	255	SER
1	A	258	SER
1	A	397	ALA
1	A	48	ASP

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Mol	Chain	Res	Type
1	A	257	GLY
1	A	260	ARG
1	A	243	SER
1	A	276	ALA
1	A	247	SER
1	A	283	GLU
1	A	370	LYS
1	A	387	SER
1	A	26	GLU
1	A	252	ASN
1	A	259	CYS
1	A	236	PRO

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	339/339 (100%)	271 (80%)	68 (20%)	1 1

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	LEU
1	A	6	GLN
1	A	8	LEU
1	A	24	GLN
1	A	25	GLN
1	A	27	THR
1	A	31	LEU
1	A	32	LEU
1	A	34	GLU
1	A	37	LYS
1	A	38	GLU
1	A	40	GLU
1	A	41	LYS

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Mol	Chain	Res	Type
1	A	44	LYS
1	A	50	LYS
1	A	67	ASN
1	A	68	LYS
1	A	79	GLU
1	A	88	LEU
1	A	96	LEU
1	A	100	GLU
1	A	112	ASN
1	A	116	LEU
1	A	127	GLN
1	A	132	SER
1	A	133	ASP
1	A	140	GLU
1	A	172	GLN
1	A	202	ASN
1	A	216	LYS
1	A	223	LEU
1	A	226	LEU
1	A	228	THR
1	A	230	ILE
1	A	232	SER
1	A	235	PRO
1	A	241	SER
1	A	246	GLN
1	A	251	GLN
1	A	253	PRO
1	A	254	SER
1	A	262	SER
1	A	263	VAL
1	A	269	GLU
1	A	270	LYS
1	A	285	ILE
1	A	296	LEU
1	A	306	TYR
1	A	307	ILE
1	A	310	GLU
1	A	311	ASP
1	A	312	THR
1	A	325	LEU
1	A	333	VAL
1	A	344	ASP

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Mol	Chain	Res	Type
1	A	355	HIS
1	A	359	GLU
1	A	366	GLN
1	A	373	LEU
1	A	378	SER
1	A	380	LYS
1	A	388	ARG
1	A	389	LEU
1	A	392	HIS
1	A	393	LEU
1	A	398	THR
1	A	400	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	24	GLN
1	A	126	HIS
1	A	202	ASN
1	A	208	GLN
1	A	369	ASN

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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	194:GLY	C	195:VAL	N	0.96

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.