



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:11 PM UTC

PDB ID : 1INP / pdb_00001inp
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 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
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

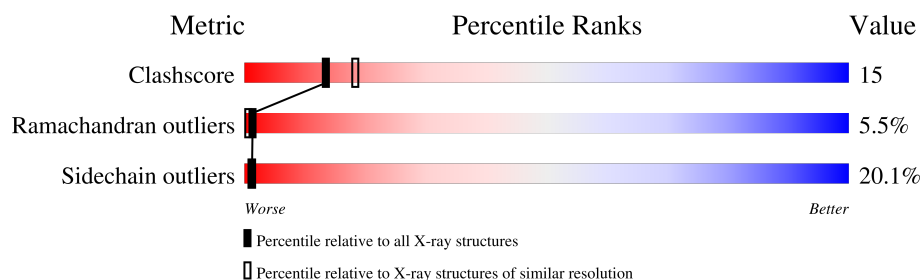
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 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	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 (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is water.

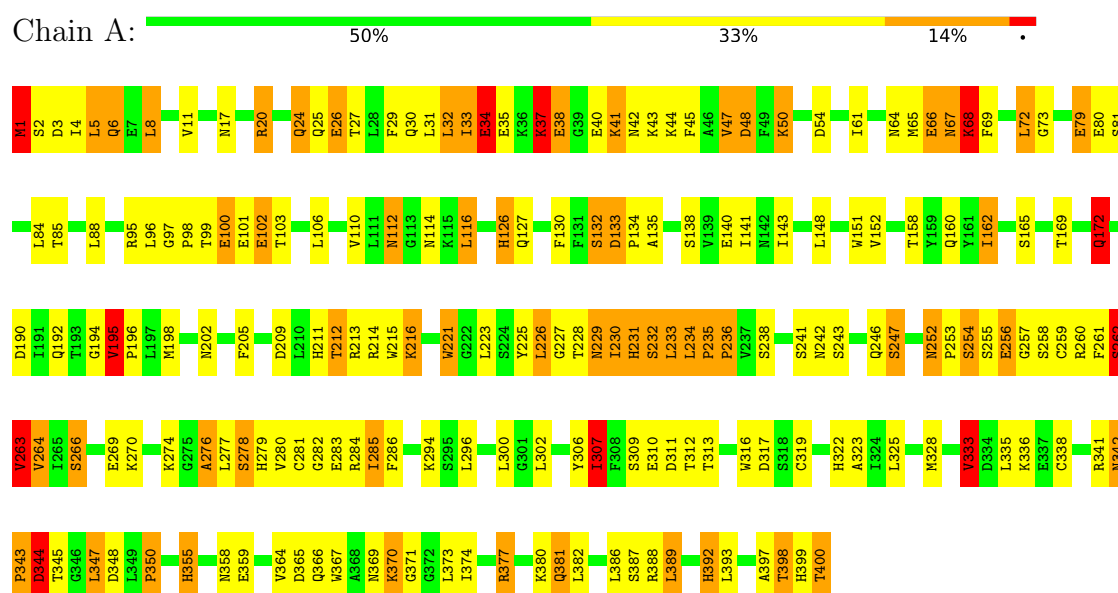
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	70	Total	H	O	0	0
			210	140	70		

3 Residue-property plots

These plots are drawn for all protein, RNA, 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: 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	51.64Å 51.64Å 143.33Å 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 [i](#)

5.1 Standard geometry [i](#)

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	1.46	22/3143 (0.7%)	2.49	111/4254 (2.6%)

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 (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	GLY	C-N	-37.56	0.96	1.33
1	A	235	PRO	CA-C	24.42	1.68	1.52
1	A	344	ASP	N-CA	20.23	1.68	1.46
1	A	234	LEU	N-CA	-14.51	1.25	1.46
1	A	233	LEU	CA-C	-13.13	1.35	1.52
1	A	236	PRO	N-CA	8.75	1.58	1.47
1	A	235	PRO	N-CA	7.83	1.57	1.46
1	A	211	HIS	CD2-NE2	-7.44	1.29	1.37
1	A	235	PRO	C-N	7.09	1.50	1.33
1	A	126	HIS	CD2-NE2	-6.68	1.30	1.37
1	A	399	HIS	CD2-NE2	-6.46	1.30	1.37
1	A	235	PRO	CA-CB	-6.44	1.48	1.54
1	A	355	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	322	HIS	CD2-NE2	-6.03	1.31	1.37
1	A	392	HIS	CD2-NE2	-5.75	1.31	1.37
1	A	279	HIS	CD2-NE2	-5.72	1.31	1.37
1	A	211	HIS	CG-ND1	-5.63	1.32	1.38
1	A	231	HIS	CD2-NE2	-5.63	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	195	VAL	C-N	-5.61	1.26	1.33
1	A	285	ILE	CA-CB	5.60	1.60	1.54
1	A	233	LEU	C-N	-5.36	1.22	1.33
1	A	342	ASN	CA-C	-5.34	1.47	1.53

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	GLY	CA-C-N	56.10	162.98	122.59
1	A	194	GLY	C-N-CA	56.10	162.98	122.59
1	A	235	PRO	O-C-N	-18.83	112.30	121.15
1	A	343	PRO	O-C-N	-18.47	97.70	122.64
1	A	194	GLY	O-C-N	-18.16	99.36	122.43
1	A	234	LEU	O-C-N	-17.83	100.81	121.32
1	A	195	VAL	O-C-N	-12.46	110.73	121.57
1	A	38	GLU	N-CA-C	12.42	127.95	110.68
1	A	280	VAL	N-CA-C	-10.98	100.75	110.74
1	A	317	ASP	CA-CB-CG	10.94	123.54	112.60
1	A	132	SER	N-CA-C	10.92	125.33	107.32
1	A	233	LEU	O-C-N	10.90	137.49	122.77
1	A	343	PRO	CA-C-N	-9.84	105.72	122.14
1	A	343	PRO	C-N-CA	-9.84	105.72	122.14
1	A	261	PHE	N-CA-C	9.78	125.41	113.38
1	A	48	ASP	CA-CB-CG	9.74	122.34	112.60
1	A	278	SER	N-CA-C	9.53	122.64	111.02
1	A	47	VAL	N-CA-C	9.33	121.06	106.88
1	A	101	GLU	N-CA-C	-9.11	93.75	108.41
1	A	234	LEU	CB-CA-C	-8.91	92.62	110.17
1	A	211	HIS	CA-CB-CG	-8.87	104.93	113.80
1	A	100	GLU	N-CA-C	8.71	123.63	110.14
1	A	44	LYS	N-CA-C	8.67	124.21	108.17
1	A	4	ILE	N-CA-C	-8.63	101.81	110.62
1	A	40	GLU	N-CA-C	8.40	125.22	111.37
1	A	42	ASN	CA-CB-CG	8.39	121.00	112.60
1	A	235	PRO	CB-CA-C	-8.36	103.31	111.17
1	A	231	HIS	CA-CB-CG	8.16	121.96	113.80
1	A	369	ASN	OD1-CG-ND2	-8.15	114.44	122.60
1	A	242	ASN	CA-CB-CG	8.12	120.72	112.60
1	A	37	LYS	N-CA-C	7.91	127.64	110.80
1	A	234	LEU	N-CA-C	7.78	127.00	109.81
1	A	30	GLN	N-CA-C	7.76	120.64	111.71
1	A	235	PRO	N-CA-C	7.76	118.88	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	HIS	CA-CB-CG	7.72	121.52	113.80
1	A	355	HIS	CB-CG-CD2	-7.57	121.36	131.20
1	A	3	ASP	CA-C-O	7.55	128.89	120.43
1	A	67	ASN	CA-CB-CG	7.51	120.11	112.60
1	A	256	GLU	N-CA-C	7.29	121.24	110.30
1	A	262	SER	N-CA-C	7.24	121.52	108.48
1	A	20	ARG	NE-CZ-NH2	-7.20	112.72	119.20
1	A	192	GLN	OE1-CD-NE2	-7.01	115.59	122.60
1	A	215	TRP	CG-CD2-CE3	6.98	140.88	133.90
1	A	355	HIS	CB-CG-ND1	6.98	133.17	122.70
1	A	99	THR	N-CA-C	-6.88	99.25	109.15
1	A	229	ASN	CA-CB-CG	-6.75	105.85	112.60
1	A	311	ASP	CA-CB-CG	6.65	119.25	112.60
1	A	274	LYS	CA-CB-CG	6.58	127.27	114.10
1	A	42	ASN	OD1-CG-ND2	-6.55	116.05	122.60
1	A	72	LEU	N-CA-C	6.51	118.04	111.07
1	A	227	GLY	N-CA-C	-6.48	102.73	111.54
1	A	347	LEU	N-CA-C	6.42	124.47	110.80
1	A	130	PHE	N-CA-C	-6.41	98.45	108.90
1	A	381	GLN	OE1-CD-NE2	-6.39	116.21	122.60
1	A	307	ILE	CB-CA-C	-6.32	101.20	110.62
1	A	64	ASN	OD1-CG-ND2	-6.27	116.33	122.60
1	A	41	LYS	CA-CB-CG	6.19	126.47	114.10
1	A	230	ILE	CA-CB-CG2	-6.18	100.00	110.50
1	A	350	PRO	CA-N-CD	-6.14	103.41	112.00
1	A	42	ASN	N-CA-C	-6.04	97.84	108.23
1	A	319	CYS	N-CA-C	6.03	117.52	111.07
1	A	266	SER	CA-CB-OG	5.92	122.94	111.10
1	A	190	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	234	LEU	CA-C-N	-5.87	115.44	119.66
1	A	234	LEU	C-N-CA	-5.87	115.44	119.66
1	A	112	ASN	OD1-CG-ND2	-5.82	116.78	122.60
1	A	6	GLN	OE1-CD-NE2	-5.81	116.79	122.60
1	A	227	GLY	O-C-N	-5.77	116.89	122.84
1	A	344	ASP	N-CA-C	-5.76	104.46	112.30
1	A	215	TRP	CB-CG-CD1	-5.74	118.29	126.90
1	A	35	GLU	N-CA-C	5.72	118.89	109.85
1	A	221	TRP	CG-CD2-CE3	5.67	139.57	133.90
1	A	333	VAL	N-CA-CB	-5.66	101.53	111.39
1	A	263	VAL	CB-CA-C	-5.65	103.90	110.91
1	A	377	ARG	CB-CG-CD	-5.64	98.32	111.30
1	A	81	SER	N-CA-C	-5.64	102.41	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	GLN	OE1-CD-NE2	-5.63	116.97	122.60
1	A	264	VAL	O-C-N	-5.61	117.29	123.18
1	A	169	THR	CA-C-O	-5.57	115.01	120.19
1	A	230	ILE	CA-CB-CG1	5.51	119.77	110.40
1	A	198	MET	CG-SD-CE	-5.50	88.79	100.90
1	A	221	TRP	CB-CG-CD1	-5.50	118.65	126.90
1	A	205	PHE	CA-CB-CG	5.48	119.28	113.80
1	A	68	LYS	CB-CG-CD	5.48	123.91	111.30
1	A	1	MET	N-CA-C	-5.48	95.65	111.00
1	A	230	ILE	CA-C-N	5.40	128.52	120.90
1	A	230	ILE	C-N-CA	5.40	128.52	120.90
1	A	165	SER	N-CA-C	5.36	117.47	109.59
1	A	370	LYS	N-CA-C	5.35	122.19	110.80
1	A	151	TRP	CE2-CD2-CG	-5.33	100.81	107.20
1	A	102	GLU	N-CA-C	5.33	122.14	110.80
1	A	44	LYS	CA-C-O	5.32	127.89	121.66
1	A	367	TRP	CG-CD2-CE3	5.32	139.22	133.90
1	A	212	THR	N-CA-CB	-5.30	102.14	110.46
1	A	5	LEU	CA-C-O	-5.29	115.27	120.82
1	A	221	TRP	CE2-CD2-CG	-5.26	100.89	107.20
1	A	34	GLU	CA-CB-CG	5.25	124.61	114.10
1	A	302	LEU	N-CA-C	-5.23	105.66	111.36
1	A	215	TRP	CE2-CD2-CG	-5.22	100.93	107.20
1	A	194	GLY	CA-C-O	-5.21	113.22	119.06
1	A	358	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	A	342	ASN	CB-CA-C	5.17	118.03	109.56
1	A	85	THR	N-CA-C	-5.16	100.83	109.24
1	A	160	GLN	OE1-CD-NE2	-5.16	117.44	122.60
1	A	264	VAL	N-CA-C	-5.15	100.96	108.17
1	A	20	ARG	NE-CZ-NH1	5.12	126.62	121.50
1	A	263	VAL	N-CA-CB	5.09	116.27	110.72
1	A	389	LEU	N-CA-C	5.09	116.77	108.63
1	A	342	ASN	O-C-N	-5.06	116.36	121.27
1	A	66	GLU	CB-CG-CD	5.05	121.18	112.60
1	A	29	PHE	CA-CB-CG	5.03	118.83	113.80

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	91	0
2	A	2	0	0	0	0
3	A	70	140	0	12	0
All	All	3160	825	3090	91	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 15.

All (91) 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:C	1:A:344:ASP:CA	2.37	0.96
1:A:343:PRO:O	1:A:344:ASP:HA	1.63	0.95
1:A:234:LEU:O	1:A:234:LEU:HD12	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:O	1:A:234:LEU:CD1	2.39	0.69
1:A:152:VAL:HG21	3:A:440:HOH:O	1.94	0.67
1:A:344:ASP:N	1:A:344:ASP:C	2.53	0.66
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:79:GLU:HB3	1:A:316:TRP:CE2	2.34	0.61
1:A:264:VAL:HG22	1:A:284:ARG:NE	2.15	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:342:ASN:CG	1:A:343:PRO:HD2	2.30	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:PRO:HB2	1:A:323:ALA:HB2	1.89	0.54
1:A:8:LEU:HD13	1:A:65:MET:HE2	1.89	0.54
1:A:148:LEU:HB2	3:A:437:HOH:O	2.07	0.54
1:A:342:ASN:O	1:A:343:PRO:C	2.51	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: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
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: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:328:MET:HE3	1:A:377:ARG:HG3	1.95	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:225:TYR:C	1:A:226:LEU:HG	2.40	0.47
1:A:333:VAL:CG1	1:A:338:CYS:SG	3.04	0.46
1:A:20:ARG:O	1:A:24:GLN:HG2	2.16	0.46
1:A:100:GLU:HA	3:A:462:HOH:O	2.14	0.46
1:A:252:ASN:C	1:A:256:GLU:HG2	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:8:LEU:HD13	1:A:65:MET:CE	2.49	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:37:LYS:CE	1:A:50:LYS:HD2	2.48	0.42
1:A:341:ARG:NH2	1:A:350:PRO:HG3	2.35	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
1:A:33:ILE:HG21	1:A:47:VAL:HB	2.03	0.41
1:A:33:ILE:HB	1:A:34:GLU:H	1.77	0.41
1:A:100:GLU:HG2	1:A:102:GLU:HA	2.03	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:HD13	1:A:162:ILE:HA	2.01	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	398/400 (100%)	320 (80%)	56 (14%)	22 (6%)	1 0

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
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	26	GLU
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	41	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	112	ASN
1	A	116	LEU
1	A	127	GLN
1	A	132	SER
1	A	133	ASP
1	A	140	GLU
1	A	162	ILE
1	A	172	GLN
1	A	195	VAL
1	A	202	ASN
1	A	216	LYS
1	A	223	LEU
1	A	226	LEU
1	A	228	THR
1	A	229	ASN
1	A	230	ILE
1	A	232	SER
1	A	238	SER
1	A	241	SER
1	A	246	GLN
1	A	247	SER
1	A	253	PRO
1	A	254	SER

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Mol	Chain	Res	Type
1	A	262	SER
1	A	263	VAL
1	A	266	SER
1	A	269	GLU
1	A	270	LYS
1	A	285	ILE
1	A	296	LEU
1	A	307	ILE
1	A	310	GLU
1	A	312	THR
1	A	325	LEU
1	A	333	VAL
1	A	344	ASP
1	A	355	HIS
1	A	359	GLU
1	A	364	VAL
1	A	366	GLN
1	A	373	LEU
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	112	ASN
1	A	126	HIS
1	A	171	ASN
1	A	203	GLN
1	A	208	GLN
1	A	218	GLN
1	A	242	ASN
1	A	369	ASN
1	A	392	HIS

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 oligosaccharides 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.