



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:19 AM UTC

PDB ID : 1BT9 / pdb_00001bt9
Title : OMPF PORIN MUTANT D74A
Authors : Philippsen, A.; Schirmer, T.
Deposited on : 1998-09-01
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
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

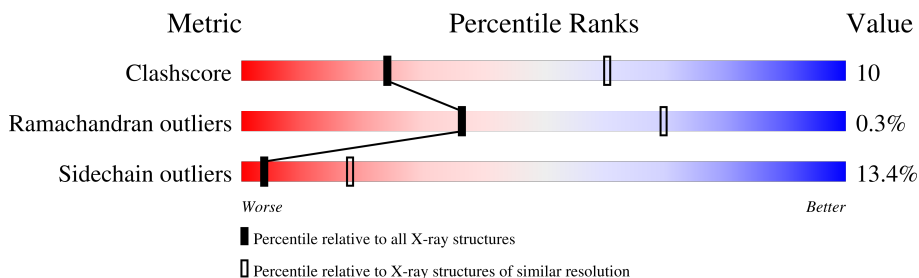
1 Overall quality at a glance

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	340	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2640 atoms, of which 0 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 PROTEIN (MATRIX PORIN OUTER MEMBRANE PROTEIN F).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	41	0	0
			2624	1653	438	530	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ALA	ASP	engineered mutation	UNP P02931

- Molecule 2 is water.

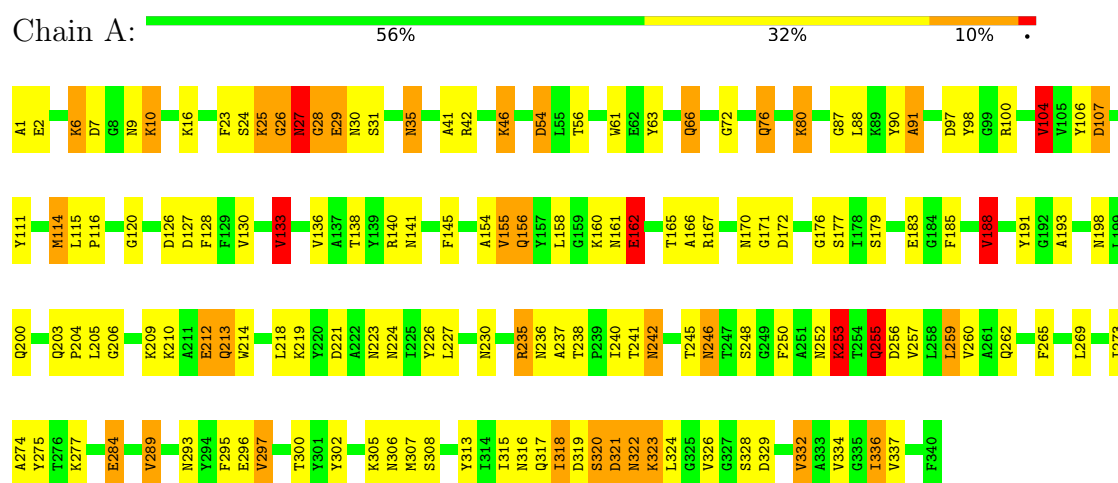
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	16	Total	O	0	0
			16	16		

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: PROTEIN (MATRIX PORIN OUTER MEMBRANE PROTEIN F)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.50Å 118.50Å 52.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	91.0 (20.00-3.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.191 , 0.269	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2640	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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	1.91	10/2680 (0.4%)	2.35	117/3624 (3.2%)

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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	GLU	CA-CB	84.60	2.70	1.53
1	A	28	GLY	CA-C	-21.63	1.21	1.51
1	A	25	LYS	CA-C	-17.16	1.31	1.52
1	A	29	GLU	C-O	15.01	1.46	1.23
1	A	28	GLY	C-O	9.03	1.36	1.23
1	A	162	GLU	CG-CD	7.56	1.71	1.52
1	A	305	LYS	CB-CG	5.85	1.70	1.52
1	A	183	GLU	CB-CG	5.53	1.69	1.52
1	A	27	ASN	C-N	5.50	1.41	1.33
1	A	10	LYS	CG-CD	5.30	1.68	1.52

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	GLY	O-C-N	-34.06	78.42	122.70
1	A	27	ASN	O-C-N	-30.49	74.63	121.89
1	A	25	LYS	CA-CB-CG	21.05	156.21	114.10
1	A	29	GLU	CB-CA-C	-20.01	79.96	111.18
1	A	25	LYS	CB-CG-CD	16.39	148.99	111.30
1	A	29	GLU	N-CA-CB	-16.10	88.19	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	GLU	CA-C-O	-13.69	104.38	120.53
1	A	10	LYS	CG-CD-CE	12.40	139.81	111.30
1	A	319	ASP	CA-C-N	12.13	137.75	120.28
1	A	319	ASP	C-N-CA	12.13	137.75	120.28
1	A	221	ASP	CA-CB-CG	11.05	123.65	112.60
1	A	28	GLY	CA-C-O	10.78	139.33	120.57
1	A	25	LYS	CB-CA-C	10.58	133.19	110.45
1	A	162	GLU	CG-CD-OE1	9.82	140.99	118.40
1	A	162	GLU	CG-CD-OE2	-9.72	96.03	118.40
1	A	7	ASP	CA-CB-CG	-9.65	102.95	112.60
1	A	100	ARG	NE-CZ-NH2	9.50	127.75	119.20
1	A	80	LYS	CA-C-O	9.43	131.37	121.28
1	A	133	VAL	CB-CA-C	-9.35	98.38	111.19
1	A	262	GLN	OE1-CD-NE2	8.53	131.13	122.60
1	A	29	GLU	O-C-N	8.46	133.53	122.19
1	A	183	GLU	CA-CB-CG	-8.44	97.21	114.10
1	A	76	GLN	OE1-CD-NE2	8.40	131.00	122.60
1	A	227	LEU	CA-C-O	-8.38	111.65	120.70
1	A	161	ASN	OD1-CG-ND2	-7.70	114.90	122.60
1	A	320	SER	N-CA-C	7.66	120.52	111.71
1	A	306	ASN	CA-CB-CG	-7.60	105.00	112.60
1	A	10	LYS	CB-CA-C	7.59	123.45	109.70
1	A	161	ASN	CA-CB-CG	7.59	120.19	112.60
1	A	133	VAL	CA-C-O	-7.56	113.66	121.67
1	A	133	VAL	CA-C-N	-7.46	115.35	122.66
1	A	133	VAL	C-N-CA	-7.46	115.35	122.66
1	A	26	GLY	O-C-N	7.38	132.29	122.70
1	A	80	LYS	O-C-N	-7.34	115.94	123.29
1	A	337	VAL	N-CA-C	7.28	118.30	108.11
1	A	223	ASN	CA-CB-CG	-7.03	105.57	112.60
1	A	256	ASP	CA-CB-CG	6.92	119.52	112.60
1	A	72	GLY	CA-C-N	6.86	130.16	120.28
1	A	72	GLY	C-N-CA	6.86	130.16	120.28
1	A	213	GLN	OE1-CD-NE2	-6.78	115.82	122.60
1	A	188	VAL	CB-CA-C	-6.71	98.70	110.71
1	A	35	ASN	N-CA-C	6.70	120.53	108.48
1	A	295	PHE	CA-C-O	-6.67	113.49	121.56
1	A	295	PHE	N-CA-C	-6.59	99.92	110.14
1	A	120	GLY	O-C-N	-6.53	117.22	122.51
1	A	104	VAL	CA-C-O	-6.51	114.18	120.95
1	A	332	VAL	CA-C-O	-6.43	113.15	120.67
1	A	136	VAL	O-C-N	-6.40	116.15	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	ARG	NH1-CZ-NH2	-6.36	111.03	119.30
1	A	269	LEU	CA-C-O	6.35	128.22	120.92
1	A	255	GLN	CA-C-O	-6.30	113.56	120.36
1	A	35	ASN	N-CA-CB	-6.28	100.29	110.71
1	A	297	VAL	CA-C-O	-6.23	113.69	120.67
1	A	255	GLN	N-CA-C	-6.22	98.75	108.90
1	A	29	GLU	CA-CB-CG	6.22	126.53	114.10
1	A	308	SER	O-C-N	-6.18	116.81	123.42
1	A	2	GLU	CA-C-O	-6.12	113.98	121.02
1	A	274	ALA	CA-C-O	-6.12	114.72	121.33
1	A	316	ASN	OD1-CG-ND2	6.10	128.70	122.60
1	A	265	PHE	N-CA-C	-6.09	101.91	110.50
1	A	98	TYR	CA-C-O	-6.08	114.00	121.11
1	A	255	GLN	N-CA-CB	6.07	120.87	110.68
1	A	104	VAL	N-CA-CB	6.02	118.73	110.54
1	A	226	TYR	CA-C-N	-5.99	113.95	122.94
1	A	226	TYR	C-N-CA	-5.99	113.95	122.94
1	A	23	PHE	CA-C-O	5.97	126.89	120.32
1	A	9	ASN	CA-CB-CG	-5.97	106.63	112.60
1	A	336	ILE	CB-CA-C	5.91	118.40	110.42
1	A	321	ASP	CA-CB-CG	-5.90	106.70	112.60
1	A	230	ASN	OD1-CG-ND2	-5.88	116.72	122.60
1	A	253	LYS	CA-CB-CG	5.84	125.78	114.10
1	A	141	ASN	CA-C-O	-5.83	114.40	120.70
1	A	295	PHE	N-CA-CB	5.78	119.75	110.85
1	A	35	ASN	O-C-N	-5.76	116.35	123.44
1	A	326	VAL	CA-C-N	5.74	125.56	120.10
1	A	326	VAL	C-N-CA	5.74	125.56	120.10
1	A	224	ASN	CA-CB-CG	-5.67	106.93	112.60
1	A	66	GLN	CG-CD-NE2	5.67	124.90	116.40
1	A	155	VAL	CB-CA-C	5.63	119.50	110.82
1	A	336	ILE	CA-C-O	5.60	125.92	120.27
1	A	127	ASP	CA-CB-CG	-5.56	107.04	112.60
1	A	23	PHE	CA-C-N	5.54	130.43	122.23
1	A	23	PHE	C-N-CA	5.54	130.43	122.23
1	A	145	PHE	CA-CB-CG	-5.48	108.32	113.80
1	A	80	LYS	N-CA-C	5.41	116.36	108.14
1	A	212	GLU	CB-CG-CD	-5.37	103.47	112.60
1	A	100	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	A	322	ASN	CA-CB-CG	5.33	117.94	112.60
1	A	128	PHE	CA-C-O	-5.31	112.92	120.51
1	A	166	ALA	CA-C-O	-5.31	114.92	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	LYS	N-CA-C	-5.29	101.02	109.07
1	A	227	LEU	O-C-N	5.28	130.10	123.23
1	A	126	ASP	CA-C-O	-5.27	115.86	122.03
1	A	165	THR	N-CA-CB	-5.27	101.83	110.68
1	A	9	ASN	OD1-CG-ND2	5.26	127.86	122.60
1	A	107	ASP	CA-C-O	-5.25	114.99	120.55
1	A	260	VAL	CA-CB-CG2	5.22	119.27	110.40
1	A	104	VAL	CB-CA-C	-5.21	105.11	112.14
1	A	257	VAL	CB-CA-C	-5.21	102.48	110.50
1	A	46	LYS	CA-CB-CG	5.21	124.52	114.10
1	A	223	ASN	OD1-CG-ND2	5.20	127.80	122.60
1	A	177	SER	CA-C-O	-5.20	114.14	120.54
1	A	316	ASN	N-CA-CB	-5.18	101.73	109.71
1	A	156	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	A	6	LYS	CB-CA-C	5.17	119.16	109.86
1	A	27	ASN	CA-C-N	5.14	131.49	121.41
1	A	27	ASN	C-N-CA	5.14	131.49	121.41
1	A	242	ASN	CA-C-O	-5.14	115.29	120.84
1	A	170	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	A	171	GLY	N-CA-C	-5.12	104.72	112.41
1	A	107	ASP	N-CA-C	-5.10	105.72	111.28
1	A	167	ARG	CB-CG-CD	5.09	123.01	111.30
1	A	334	VAL	CA-C-O	-5.08	115.05	120.39
1	A	136	VAL	CA-C-N	5.07	129.51	122.77
1	A	136	VAL	C-N-CA	5.07	129.51	122.77
1	A	140	ARG	NE-CZ-NH1	-5.07	116.43	121.50
1	A	140	ARG	CA-C-O	-5.05	114.71	120.32

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ALA	Mainchain
1	A	133	VAL	Mainchain
1	A	162	GLU	Sidechain
1	A	185	PHE	Mainchain
1	A	188	VAL	Mainchain
1	A	236	ASN	Mainchain
1	A	26	GLY	Mainchain
1	A	27	ASN	Peptide,Mainchain
1	A	28	GLY	Mainchain
1	A	29	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	A	307	MET	Mainchain
1	A	54	ASP	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	2624	0	2445	50	0
2	A	16	0	0	0	0
All	All	2640	0	2445	50	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 (50) 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:235:ARG:HE	1:A:253:LYS:HD2	1.31	0.93
1:A:205:LEU:HD23	1:A:284:GLU:HG2	1.64	0.78
1:A:31:SER:HA	1:A:329:ASP:HB2	1.72	0.71
1:A:138:THR:OG1	1:A:156:GLN:HG3	1.93	0.68
1:A:259:LEU:HD12	1:A:275:TYR:HD2	1.62	0.64
1:A:115:LEU:HB3	1:A:116:PRO:HD2	1.79	0.62
1:A:24:SER:HB2	1:A:35:ASN:HB2	1.81	0.62
1:A:235:ARG:NE	1:A:253:LYS:HD2	2.09	0.62
1:A:313:TYR:CD1	1:A:332:VAL:HG22	2.36	0.60
1:A:138:THR:HG1	1:A:156:GLN:HG3	1.66	0.60
1:A:206:GLY:H	1:A:284:GLU:CD	2.09	0.60
1:A:321:ASP:O	1:A:322:ASN:C	2.47	0.57
1:A:179:SER:CB	1:A:188:VAL:HG13	2.36	0.56
1:A:115:LEU:HD13	1:A:296:GLU:HG3	1.89	0.54
1:A:293:ASN:HB3	1:A:318:ILE:HG12	1.90	0.53
1:A:213:GLN:HE21	1:A:237:ALA:HB1	1.73	0.53
1:A:179:SER:HB3	1:A:188:VAL:HG13	1.92	0.52
1:A:61:TRP:CZ2	1:A:63:TYR:HB2	2.45	0.51
1:A:90:TYR:O	1:A:91:ALA:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:THR:O	1:A:246:ASN:HB2	2.11	0.49
1:A:104:VAL:O	1:A:107:ASP:HB2	2.13	0.48
1:A:87:GLY:HA3	1:A:97:ASP:HB3	1.95	0.47
1:A:205:LEU:HD13	1:A:240:ILE:HD11	1.96	0.47
1:A:111:TYR:CZ	1:A:188:VAL:HG22	2.50	0.47
1:A:241:THR:HG23	1:A:248:SER:OG	2.14	0.46
1:A:255:GLN:HE21	1:A:255:GLN:HB3	1.60	0.46
1:A:30:ASN:ND2	1:A:328:SER:OG	2.47	0.46
1:A:42:ARG:HH11	1:A:42:ARG:HG3	1.80	0.46
1:A:193:ALA:HB2	1:A:212:GLU:HG2	1.98	0.46
1:A:54:ASP:HB3	1:A:91:ALA:HB2	1.99	0.45
1:A:179:SER:HB2	1:A:188:VAL:HG13	1.97	0.45
1:A:205:LEU:HD13	1:A:240:ILE:CD1	2.47	0.45
1:A:200:GLN:O	1:A:203:GLN:HG2	2.17	0.45
1:A:205:LEU:HD13	1:A:240:ILE:HG13	1.99	0.45
1:A:154:ALA:O	1:A:176:GLY:HA2	2.17	0.44
1:A:191:TYR:HD1	1:A:214:TRP:HB3	1.83	0.43
1:A:203:GLN:HA	1:A:204:PRO:HD3	1.88	0.43
1:A:315:ILE:HG22	1:A:317:GLN:NE2	2.32	0.43
1:A:289:VAL:HG21	1:A:324:LEU:HG	2.01	0.42
1:A:238:THR:O	1:A:250:PHE:HA	2.20	0.42
1:A:242:ASN:O	1:A:246:ASN:N	2.49	0.42
1:A:106:TYR:HB2	1:A:130:VAL:O	2.20	0.42
1:A:245:THR:O	1:A:246:ASN:CB	2.68	0.41
1:A:300:THR:HG21	1:A:302:TYR:CZ	2.55	0.41
1:A:273:ILE:HD11	1:A:297:VAL:HG13	2.02	0.41
1:A:158:LEU:O	1:A:172:ASP:HA	2.20	0.41
1:A:273:ILE:HD13	1:A:273:ILE:HA	1.93	0.41
1:A:321:ASP:O	1:A:323:LYS:NZ	2.40	0.41
1:A:114:MET:HE3	1:A:114:MET:HB3	1.90	0.40
1:A:16:LYS:O	1:A:41:ALA:HA	2.22	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	338/340 (99%)	316 (94%)	21 (6%)	1 (0%)	36 70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	ALA

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	262/262 (100%)	227 (87%)	35 (13%)	4 18

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	10	LYS
1	A	25	LYS
1	A	27	ASN
1	A	46	LYS
1	A	56	THR
1	A	66	GLN
1	A	76	GLN
1	A	80	LYS
1	A	88	LEU
1	A	104	VAL
1	A	114	MET
1	A	133	VAL
1	A	155	VAL
1	A	160	LYS
1	A	162	GLU
1	A	188	VAL
1	A	198	ASN

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Mol	Chain	Res	Type
1	A	209	LYS
1	A	210	LYS
1	A	218	LEU
1	A	219	LYS
1	A	235	ARG
1	A	246	ASN
1	A	252	ASN
1	A	253	LYS
1	A	255	GLN
1	A	259	LEU
1	A	277	LYS
1	A	284	GLU
1	A	289	VAL
1	A	318	ILE
1	A	320	SER
1	A	323	LYS
1	A	336	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	ASN
1	A	236	ASN
1	A	255	GLN

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

There are no ligands in this entry.

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.