



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:31 PM GMT

PDB ID : 1PFO
Title : PERFRINGOLYSIN O
Authors : Rossjohn, J.; Parker, M.W.
Deposited on : 1997-07-31
Resolution : 2.20 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

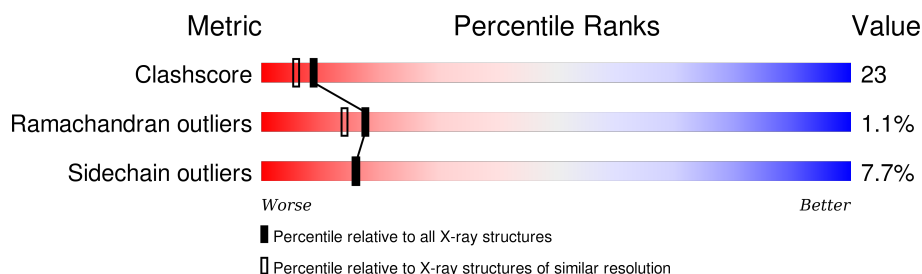
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	500	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4035 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 PERFRINGOLYSIN O.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3705	2332	622	746	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	114	LEU	PHE	CONFLICT	UNP P19995

- Molecule 2 is water.

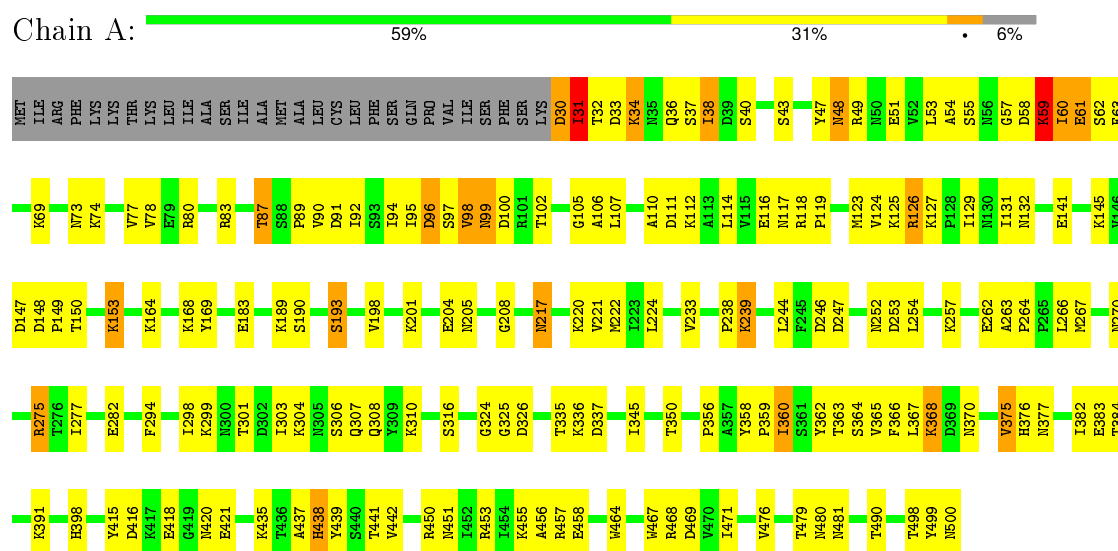
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	330	Total	O	0	0
			330	330		

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: PERFRINGOLYSIN O



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	46.99 Å 178.29 Å 174.21 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	86.0 (20.00-2.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.211 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4035	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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	0.38	0/3776	0.68	2/5127 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	GLU	N-CA-C	6.83	129.44	111.00
1	A	59	LYS	N-CA-C	-5.46	96.27	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3705	0	3656	172	0
2	A	330	0	0	31	0
All	All	4035	0	3656	172	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 23.

All (172) 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:30:ASP:HA	1:A:36:GLN:HB3	1.43	0.97
1:A:239:LYS:O	1:A:239:LYS:HE3	1.75	0.87
1:A:335:THR:HG22	1:A:337:ASP:H	1.40	0.85
1:A:78:VAL:HG13	1:A:384:THR:HG23	1.61	0.80
1:A:266:LEU:HD23	1:A:366:PHE:HA	1.60	0.80
1:A:31:ILE:HG22	1:A:32:THR:H	1.45	0.79
1:A:335:THR:HG22	1:A:336:LYS:H	1.47	0.79
1:A:30:ASP:HA	1:A:36:GLN:CB	2.13	0.77
1:A:294:PHE:O	2:A:593:HOH:O	2.03	0.76
1:A:148:ASP:HB3	1:A:153:LYS:HD2	1.68	0.75
1:A:310:LYS:HE3	2:A:681:HOH:O	1.87	0.73
1:A:30:ASP:CA	1:A:36:GLN:HB3	2.17	0.73
1:A:457:ARG:HD2	1:A:469:ASP:OD1	1.89	0.72
1:A:464:TRP:HA	1:A:467:TRP:CE3	2.25	0.71
1:A:59:LYS:O	1:A:60:ILE:HD12	1.91	0.70
1:A:77:VAL:HG21	2:A:687:HOH:O	1.92	0.69
1:A:127:LYS:HE3	2:A:568:HOH:O	1.94	0.68
1:A:30:ASP:CG	1:A:36:GLN:HB3	2.13	0.68
1:A:304:LYS:O	1:A:310:LYS:HE2	1.93	0.67
1:A:47:TYR:CE2	1:A:264:PRO:HB3	2.30	0.67
1:A:335:THR:HG22	1:A:336:LYS:N	2.10	0.66
1:A:33:ASP:C	1:A:34:LYS:HG3	2.14	0.66
1:A:224:LEU:HD11	1:A:298:ILE:HD11	1.77	0.66
1:A:150:THR:OG1	1:A:153:LYS:HB2	1.95	0.66
1:A:441:THR:HG22	1:A:442:VAL:N	2.10	0.66
1:A:33:ASP:O	1:A:34:LYS:HE2	1.95	0.66
1:A:80:ARG:HD3	1:A:382:ILE:HG21	1.78	0.65
1:A:148:ASP:HB3	1:A:153:LYS:CD	2.28	0.64
1:A:59:LYS:HG3	2:A:694:HOH:O	1.98	0.63
1:A:32:THR:HG22	1:A:32:THR:O	1.97	0.63
1:A:398:HIS:O	1:A:438:HIS:HA	1.98	0.63
1:A:451:ASN:N	2:A:514:HOH:O	2.33	0.61
1:A:90:VAL:O	1:A:363:THR:HG22	2.00	0.61
1:A:54:ALA:HB2	1:A:376:HIS:HB2	1.82	0.61
1:A:114:LEU:HD11	1:A:362:TYR:OH	2.01	0.61
1:A:441:THR:CG2	1:A:442:VAL:N	2.63	0.61
1:A:239:LYS:HD3	2:A:543:HOH:O	2.01	0.60
1:A:73:ASN:HA	1:A:391:LYS:HE3	1.83	0.60
1:A:87:THR:HG22	1:A:89:PRO:HD3	1.83	0.60
1:A:153:LYS:HD3	2:A:672:HOH:O	2.02	0.59
1:A:298:ILE:HD12	2:A:593:HOH:O	2.01	0.59
1:A:31:ILE:C	1:A:33:ASP:H	2.05	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:LEU:HD13	1:A:119:PRO:HB3	1.84	0.59
1:A:37:SER:HG	1:A:40:SER:HB3	1.67	0.59
1:A:34:LYS:H	1:A:36:GLN:HE21	1.51	0.59
1:A:263:ALA:N	1:A:264:PRO:HD3	2.18	0.58
1:A:127:LYS:HE2	1:A:246:ASP:HA	1.86	0.58
1:A:30:ASP:HA	1:A:36:GLN:CG	2.34	0.57
1:A:498:THR:HG22	1:A:499:TYR:N	2.19	0.57
1:A:275:ARG:NH2	1:A:350:THR:O	2.36	0.57
1:A:480:ASN:HB2	1:A:500:ASN:O	2.05	0.57
1:A:126:ARG:HH21	1:A:244:LEU:HD22	1.70	0.57
1:A:453:ARG:HH11	1:A:453:ARG:HG2	1.69	0.57
1:A:107:LEU:HG	1:A:126:ARG:NH1	2.20	0.56
1:A:126:ARG:HG2	1:A:244:LEU:O	2.05	0.56
1:A:189:LYS:O	1:A:193:SER:OG	2.22	0.56
1:A:456:ALA:HB3	1:A:471:ILE:HG22	1.86	0.56
1:A:110:ALA:HB2	1:A:266:LEU:HD11	1.88	0.55
1:A:73:ASN:HB3	2:A:728:HOH:O	2.07	0.55
1:A:33:ASP:O	1:A:34:LYS:CE	2.54	0.55
1:A:277:ILE:HD13	1:A:345:ILE:HA	1.89	0.55
1:A:37:SER:OG	1:A:40:SER:HB3	2.07	0.54
1:A:222:MET:HE1	1:A:224:LEU:HD21	1.90	0.54
1:A:221:VAL:HG22	1:A:282:GLU:HG3	1.90	0.54
1:A:34:LYS:HA	1:A:36:GLN:NE2	2.23	0.54
1:A:364:SER:HB2	2:A:802:HOH:O	2.08	0.54
1:A:94:ILE:HD13	1:A:359:PRO:HB2	1.90	0.53
1:A:217:ASN:OD1	1:A:384:THR:HG21	2.09	0.53
1:A:224:LEU:HD11	1:A:298:ILE:CD1	2.39	0.53
1:A:131:ILE:HG21	2:A:616:HOH:O	2.08	0.53
1:A:303:ILE:HG13	2:A:575:HOH:O	2.08	0.53
1:A:458:GLU:OE2	1:A:490:THR:HG23	2.09	0.52
1:A:201:LYS:O	1:A:205:ASN:HB2	2.09	0.52
1:A:498:THR:HG22	1:A:499:TYR:H	1.74	0.52
1:A:148:ASP:HB3	1:A:153:LYS:NZ	2.25	0.52
1:A:457:ARG:HG3	1:A:468:ARG:O	2.10	0.51
1:A:365:VAL:HG11	1:A:370:ASN:OD1	2.10	0.51
1:A:95:ILE:HG12	1:A:117:ASN:HB3	1.92	0.51
1:A:114:LEU:HD12	2:A:637:HOH:O	2.11	0.51
1:A:238:PRO:HG3	1:A:244:LEU:HG	1.93	0.51
1:A:450:ARG:NH2	2:A:687:HOH:O	2.44	0.50
1:A:453:ARG:NH1	1:A:453:ARG:HG2	2.25	0.50
1:A:98:VAL:HG13	2:A:678:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:GLY:CA	1:A:358:TYR:HD2	2.24	0.50
1:A:222:MET:CE	1:A:224:LEU:HD21	2.42	0.50
1:A:54:ALA:CB	1:A:376:HIS:HB2	2.42	0.50
1:A:476:VAL:O	2:A:818:HOH:O	2.19	0.50
1:A:125:LYS:HE3	1:A:246:ASP:OD2	2.12	0.50
1:A:59:LYS:O	1:A:59:LYS:HG2	2.12	0.49
1:A:415:TYR:HA	1:A:420:ASN:O	2.13	0.49
1:A:298:ILE:CG1	2:A:593:HOH:O	2.61	0.49
1:A:78:VAL:HG13	1:A:384:THR:CG2	2.37	0.49
1:A:335:THR:CG2	1:A:337:ASP:H	2.18	0.48
1:A:481:ASN:HB2	1:A:500:ASN:HB2	1.96	0.48
1:A:325:GLY:HA2	1:A:358:TYR:HD2	1.78	0.48
1:A:111:ASP:HB2	2:A:679:HOH:O	2.12	0.48
1:A:89:PRO:HD2	1:A:375:VAL:O	2.14	0.48
1:A:61:GLU:CG	1:A:61:GLU:O	2.61	0.48
1:A:246:ASP:OD1	1:A:247:ASP:N	2.46	0.47
1:A:141:GLU:O	1:A:164:LYS:HD3	2.14	0.47
1:A:34:LYS:N	1:A:36:GLN:HE21	2.11	0.47
1:A:53:LEU:O	1:A:375:VAL:HG12	2.15	0.47
1:A:147:ASP:O	1:A:149:PRO:HD3	2.15	0.47
1:A:37:SER:OG	1:A:40:SER:CB	2.63	0.47
1:A:498:THR:HG21	2:A:677:HOH:O	2.14	0.47
1:A:105:GLY:O	1:A:126:ARG:CZ	2.63	0.47
1:A:30:ASP:O	1:A:31:ILE:O	2.33	0.46
1:A:94:ILE:CD1	1:A:359:PRO:HB2	2.44	0.46
1:A:356:PRO:HG2	2:A:822:HOH:O	2.15	0.46
1:A:87:THR:HG21	2:A:756:HOH:O	2.14	0.46
1:A:98:VAL:O	1:A:99:ASN:CG	2.55	0.46
1:A:204:GLU:O	1:A:208:GLY:HA2	2.15	0.46
1:A:40:SER:HA	1:A:43:SER:OG	2.15	0.46
1:A:97:SER:OG	1:A:324:GLY:HA2	2.16	0.46
1:A:148:ASP:O	1:A:153:LYS:HD2	2.16	0.46
1:A:415:TYR:CE2	1:A:421:GLU:HG2	2.50	0.46
1:A:125:LYS:HB3	1:A:246:ASP:HB3	1.99	0.45
1:A:325:GLY:O	1:A:326:ASP:HB2	2.17	0.45
1:A:114:LEU:CD1	1:A:362:TYR:OH	2.64	0.45
1:A:105:GLY:O	1:A:126:ARG:NH1	2.49	0.45
1:A:441:THR:CG2	1:A:442:VAL:H	2.28	0.45
1:A:183:GLU:HG3	1:A:222:MET:HE2	1.98	0.45
1:A:126:ARG:HB3	1:A:149:PRO:HG2	1.99	0.45
1:A:60:ILE:HG23	1:A:61:GLU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ASN:HB2	2:A:663:HOH:O	2.16	0.45
1:A:282:GLU:O	1:A:316:SER:HA	2.17	0.45
1:A:91:ASP:HA	1:A:363:THR:HG22	1.99	0.44
1:A:418:GLU:HB2	1:A:420:ASN:ND2	2.32	0.44
1:A:57:GLY:O	1:A:58:ASP:C	2.55	0.44
1:A:98:VAL:O	1:A:99:ASN:ND2	2.51	0.44
1:A:74:LYS:HG3	2:A:663:HOH:O	2.16	0.44
1:A:105:GLY:O	1:A:126:ARG:NH2	2.50	0.44
1:A:366:PHE:O	1:A:370:ASN:HA	2.18	0.44
1:A:59:LYS:HE3	1:A:59:LYS:HB2	1.87	0.44
1:A:325:GLY:HA2	1:A:358:TYR:CD2	2.53	0.44
1:A:131:ILE:HG23	1:A:233:VAL:CG1	2.48	0.43
1:A:106:ALA:O	1:A:267:MET:HA	2.18	0.43
1:A:335:THR:CG2	1:A:336:LYS:H	2.24	0.43
1:A:83:ARG:HG3	1:A:383:GLU:HB2	2.00	0.43
1:A:55:SER:O	1:A:377:ASN:HA	2.18	0.43
1:A:96:ASP:HB3	1:A:99:ASN:HB2	2.00	0.43
1:A:69:LYS:NZ	2:A:705:HOH:O	2.51	0.43
1:A:238:PRO:HG3	1:A:244:LEU:CG	2.49	0.43
1:A:435:LYS:HE3	1:A:439:TYR:CZ	2.53	0.43
1:A:34:LYS:HB2	1:A:34:LYS:HE3	1.70	0.43
1:A:31:ILE:O	1:A:36:GLN:NE2	2.52	0.43
1:A:418:GLU:HB2	1:A:420:ASN:HD22	1.84	0.43
1:A:116:GLU:OE1	1:A:118:ARG:NH1	2.52	0.42
1:A:263:ALA:N	1:A:264:PRO:CD	2.82	0.42
1:A:47:TYR:OH	1:A:368:LYS:HB2	2.18	0.42
1:A:38:ILE:HD11	1:A:254:LEU:HD11	2.01	0.42
1:A:416:ASP:OD2	1:A:420:ASN:HB2	2.19	0.42
1:A:123:MET:O	1:A:124:VAL:HG13	2.19	0.42
1:A:30:ASP:OD1	1:A:36:GLN:HB3	2.19	0.42
1:A:98:VAL:HG12	1:A:358:TYR:CE1	2.55	0.42
1:A:239:LYS:HA	1:A:239:LYS:HD2	1.55	0.41
1:A:306:SER:HA	2:A:793:HOH:O	2.20	0.41
1:A:61:GLU:HG2	1:A:61:GLU:O	2.21	0.41
1:A:270:ASN:O	1:A:362:TYR:HB2	2.20	0.41
1:A:360:ILE:CD1	2:A:513:HOH:O	2.69	0.41
1:A:198:VAL:CG1	2:A:651:HOH:O	2.67	0.41
1:A:49:ARG:HD3	2:A:634:HOH:O	2.20	0.41
1:A:92:ILE:HD12	2:A:802:HOH:O	2.21	0.41
1:A:299:LYS:HB3	1:A:301:THR:HG23	2.03	0.41
1:A:87:THR:CG2	1:A:89:PRO:HD3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ASP:CG	1:A:102:THR:HG1	2.24	0.41
1:A:220:LYS:HE2	2:A:727:HOH:O	2.21	0.41
1:A:168:LYS:HD3	1:A:169:TYR:CE2	2.56	0.40
1:A:63:PHE:C	1:A:63:PHE:CD1	2.94	0.40
1:A:37:SER:O	1:A:38:ILE:C	2.58	0.40
1:A:48:ASN:HB3	1:A:51:GLU:HB2	2.04	0.40
1:A:455:LYS:HB2	1:A:455:LYS:HE3	1.84	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	469/500 (94%)	438 (93%)	26 (6%)	5 (1%)	17 14

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	ILE
1	A	368	LYS
1	A	99	ASN
1	A	437	ALA
1	A	438	HIS

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	418/444 (94%)	386 (92%)	32 (8%)	16	16

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ASP
1	A	31	ILE
1	A	34	LYS
1	A	38	ILE
1	A	48	ASN
1	A	59	LYS
1	A	60	ILE
1	A	62	SER
1	A	87	THR
1	A	96	ASP
1	A	98	VAL
1	A	112	LYS
1	A	126	ARG
1	A	129	ILE
1	A	132	ASN
1	A	145	LYS
1	A	153	LYS
1	A	190	SER
1	A	193	SER
1	A	217	ASN
1	A	239	LYS
1	A	252	ASN
1	A	253	ASP
1	A	257	LYS
1	A	262	GLU
1	A	275	ARG
1	A	307	GLN
1	A	308	GLN
1	A	360	ILE
1	A	367	LEU
1	A	375	VAL
1	A	479	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN

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Mol	Chain	Res	Type
1	A	50	ASN
1	A	99	ASN
1	A	132	ASN
1	A	197	ASN
1	A	228	GLN
1	A	307	GLN
1	A	395	ASN
1	A	420	ASN
1	A	451	ASN
1	A	483	ASN
1	A	500	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](#)

There are no ligands in this entry.

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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.