



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:08 AM UTC

PDB ID : 1PBH / pdb_00001pbh
Title : CRYSTAL STRUCTURE OF HUMAN RECOMBINANT PROCATHEPSIN
B AT 3.2 ANGSTROM RESOLUTION
Authors : Podobnik, M.; Turk, D.
Deposited on : 1997-02-14
Resolution : 3.20 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

<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

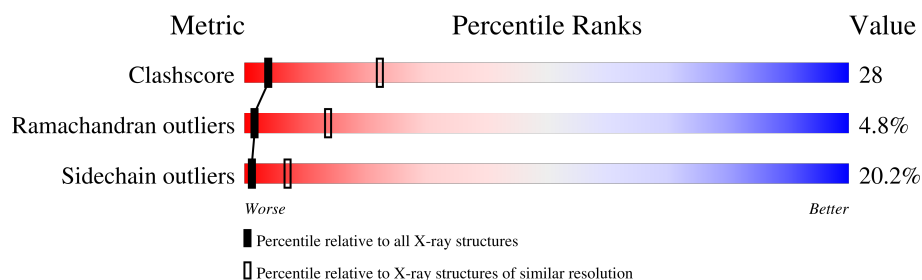
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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 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	317	44% 41% 14% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3015 atoms, of which 545 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 PROCATHEPSIN B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	317	Total	C	H	N	O	S	632	0	0
			3015	1552	545	428	468	22			

There is a discrepancy between the modelled and reference sequences:

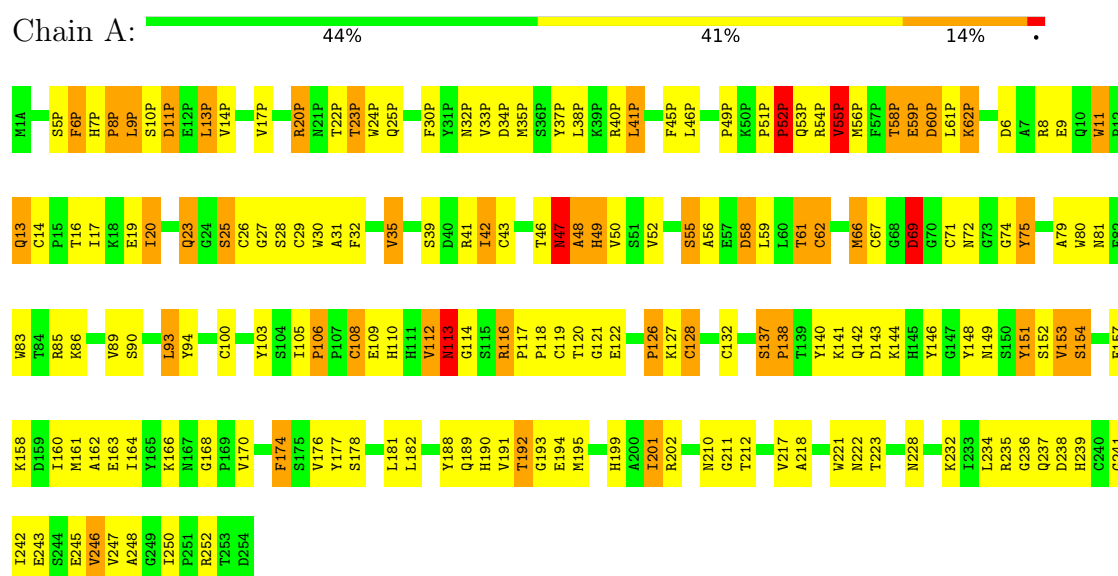
Chain	Residue	Modelled	Actual	Comment	Reference
A	9P	LEU	VAL	conflict	UNP P07858

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: PROCATHEPSIN B



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.95Å 77.10Å 97.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-3.20)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	0.12	Depositor
Refinement program	MAIN	Depositor
R, R_{free}	0.216 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3015	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.64	1/2545 (0.0%)	1.19	27/3457 (0.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	MET	SD-CE	6.34	1.95	1.79

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	CYS	CA-C-N	10.73	130.50	119.56
1	A	14	CYS	C-N-CA	10.73	130.50	119.56
1	A	69	ASP	N-CA-C	7.27	123.01	111.81
1	A	46(P)	LEU	N-CA-C	6.73	119.71	108.20
1	A	42	ILE	N-CA-C	-6.45	104.36	110.42
1	A	59(P)	GLU	N-CA-C	-6.41	97.14	110.80
1	A	113	ASN	N-CA-C	6.38	124.39	110.80
1	A	106	PRO	CA-C-N	6.04	126.23	120.31
1	A	106	PRO	C-N-CA	6.04	126.23	120.31
1	A	61	THR	N-CA-C	5.87	120.59	112.90
1	A	137	SER	C-N-CD	-5.78	107.89	120.60
1	A	11	TRP	CA-C-N	5.69	125.31	119.56
1	A	11	TRP	C-N-CA	5.69	125.31	119.56
1	A	11(P)	ASP	N-CA-C	-5.69	104.55	112.45
1	A	153	VAL	N-CA-C	-5.68	100.23	108.87
1	A	151	TYR	N-CA-C	5.62	117.39	108.79
1	A	47	ASN	N-CA-C	-5.61	98.86	110.80
1	A	75	TYR	CA-C-N	5.56	125.66	119.32
1	A	75	TYR	C-N-CA	5.56	125.66	119.32
1	A	201	ILE	N-CA-C	5.41	115.97	108.23
1	A	250	ILE	CA-C-N	5.41	125.38	120.03
1	A	250	ILE	C-N-CA	5.41	125.38	120.03
1	A	19	GLU	N-CA-C	5.14	117.75	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	ASP	N-CA-C	5.12	119.16	113.01
1	A	56	ALA	N-CA-C	-5.11	106.88	113.01
1	A	7(P)	HIS	CA-C-N	5.07	126.17	119.84
1	A	7(P)	HIS	C-N-CA	5.07	126.17	119.84

There are no chirality outliers.

There are no planarity outliers.

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	2470	545	2305	129	3
All	All	2470	545	2305	129	3

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 28.

All (129) 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:13:GLN:NE2	1:A:48:ALA:HB1	1.83	0.93
1:A:32(P):ASN:HD22	1:A:114:GLY:HA2	1.36	0.89
1:A:54(P):ARG:HG3	1:A:56(P):MET:SD	2.13	0.88
1:A:34(P):ASP:HB3	1:A:120:THR:HA	1.57	0.86
1:A:37(P):TYR:HA	1:A:121:GLY:HA3	1.60	0.83
1:A:46:THR:HG21	1:A:50:VAL:HG22	1.61	0.83
1:A:158:LYS:HD2	1:A:158:LYS:H	1.54	0.73
1:A:32(P):ASN:ND2	1:A:114:GLY:HA2	2.04	0.73
1:A:46:THR:HG23	1:A:50:VAL:HG13	1.73	0.69
1:A:13:GLN:HE21	1:A:48:ALA:HB1	1.55	0.67
1:A:37(P):TYR:HA	1:A:121:GLY:CA	2.24	0.67
1:A:20(P):ARG:NH1	1:A:191:VAL:HG13	2.10	0.66
1:A:33(P):VAL:HG12	1:A:119:CYS:HB2	1.76	0.66
1:A:109:GLU:HB3	1:A:112:VAL:HG23	1.79	0.64
1:A:93:LEU:H	1:A:93:LEU:HD12	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ASN:O	1:A:49:HIS:N	2.31	0.62
1:A:58(P):THR:HA	1:A:61(P):LEU:HD22	1.80	0.62
1:A:43:CYS:O	1:A:48:ALA:HA	1.99	0.62
1:A:190:HIS:H	1:A:239:HIS:CE1	2.18	0.62
1:A:8:ARG:HG3	1:A:17:ILE:HG22	1.83	0.61
1:A:146:TYR:HB2	1:A:252:ARG:HH11	1.66	0.60
1:A:81:ASN:O	1:A:85:ARG:HB2	2.02	0.60
1:A:16:THR:HG21	1:A:39:SER:HB3	1.82	0.60
1:A:178:SER:HB3	1:A:194:GLU:HG2	1.83	0.60
1:A:46:THR:O	1:A:47:ASN:HB2	2.02	0.60
1:A:132:CYS:SG	1:A:140:TYR:HA	2.43	0.59
1:A:61:THR:HG21	1:A:126:PRO:HB2	1.83	0.59
1:A:30(P):PHE:HB3	1:A:33(P):VAL:HG21	1.86	0.58
1:A:189:GLN:NE2	1:A:234:LEU:HD13	2.19	0.57
1:A:8:ARG:CG	1:A:17:ILE:HG22	2.34	0.57
1:A:37(P):TYR:CA	1:A:121:GLY:HA3	2.33	0.57
1:A:148:TYR:HD2	1:A:149:ASN:ND2	2.01	0.57
1:A:100:CYS:O	1:A:132:CYS:HA	2.05	0.57
1:A:20(P):ARG:O	1:A:20(P):ARG:HG3	2.05	0.55
1:A:32(P):ASN:O	1:A:116:ARG:NH2	2.40	0.55
1:A:189:GLN:HA	1:A:239:HIS:CE1	2.42	0.55
1:A:33(P):VAL:HG11	1:A:110:HIS:HB2	1.87	0.54
1:A:51(P):PRO:HB2	1:A:151:TYR:HA	1.88	0.54
1:A:59:LEU:HD21	1:A:79:ALA:HB1	1.88	0.54
1:A:54(P):ARG:HB2	1:A:151:TYR:CD1	2.42	0.54
1:A:109:GLU:O	1:A:112:VAL:HG23	2.08	0.54
1:A:32(P):ASN:OD1	1:A:118:PRO:HA	2.07	0.54
1:A:109:GLU:O	1:A:116:ARG:NH1	2.40	0.54
1:A:14(P):VAL:HG22	1:A:182:LEU:HD13	1.91	0.53
1:A:54(P):ARG:CG	1:A:56(P):MET:SD	2.93	0.53
1:A:29:CYS:HA	1:A:32:PHE:HB2	1.91	0.53
1:A:178:SER:OG	1:A:193:GLY:HA2	2.09	0.53
1:A:190:HIS:H	1:A:239:HIS:HE1	1.56	0.53
1:A:38(P):LEU:H	1:A:38(P):LEU:CD1	2.23	0.52
1:A:22(P):THR:HG23	1:A:24(P):TRP:H	1.74	0.52
1:A:162:ALA:HB1	1:A:166:LYS:HE3	1.90	0.52
1:A:52(P):PRO:O	1:A:53(P):GLN:HG2	2.10	0.52
1:A:151:TYR:CE1	1:A:248:ALA:HB3	2.45	0.52
1:A:112:VAL:O	1:A:116:ARG:NH1	2.43	0.51
1:A:189:GLN:HE21	1:A:234:LEU:HD13	1.75	0.51
1:A:38(P):LEU:N	1:A:38(P):LEU:HD12	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ALA:O	1:A:35:VAL:HG13	2.09	0.51
1:A:242:ILE:HG23	1:A:243:GLU:HG3	1.93	0.51
1:A:38(P):LEU:H	1:A:38(P):LEU:HD12	1.75	0.51
1:A:40(P):ARG:O	1:A:27:GLY:HA2	2.10	0.51
1:A:37(P):TYR:HB2	1:A:119:CYS:O	2.11	0.51
1:A:112:VAL:HB	1:A:113:ASN:HD22	1.76	0.50
1:A:37(P):TYR:CZ	1:A:108:CYS:SG	3.05	0.50
1:A:55:SER:HB2	1:A:90:SER:O	2.11	0.50
1:A:25:SER:HB3	1:A:121:GLY:HA2	1.93	0.50
1:A:14(P):VAL:CG2	1:A:182:LEU:HD13	2.41	0.50
1:A:177:TYR:HA	1:A:194:GLU:O	2.12	0.50
1:A:55(P):VAL:HG22	1:A:55(P):VAL:O	2.11	0.50
1:A:26:CYS:SG	1:A:28:SER:HB3	2.52	0.50
1:A:100:CYS:SG	1:A:140:TYR:HD1	2.35	0.49
1:A:113:ASN:OD1	1:A:116:ARG:HG2	2.11	0.49
1:A:41(P):LEU:HG	1:A:221:TRP:CE2	2.47	0.49
1:A:46:THR:HG23	1:A:46:THR:O	2.11	0.49
1:A:153:VAL:HB	1:A:246:VAL:CG2	2.42	0.49
1:A:238:ASP:OD2	1:A:241:GLY:HA2	2.13	0.49
1:A:33(P):VAL:CG1	1:A:110:HIS:HB2	2.43	0.48
1:A:164:ILE:HA	1:A:168:GLY:O	2.12	0.48
1:A:30:TRP:CZ3	1:A:67:CYS:HB3	2.49	0.48
1:A:66:MET:HE1	1:A:85:ARG:HG2	1.94	0.48
1:A:9(P):LEU:HD12	1:A:9(P):LEU:H	1.79	0.48
1:A:46:THR:CG2	1:A:50:VAL:HG22	2.35	0.47
1:A:41(P):LEU:HD12	1:A:41(P):LEU:HA	1.71	0.47
1:A:13:GLN:HG3	1:A:48:ALA:O	2.13	0.47
1:A:148:TYR:CD2	1:A:149:ASN:ND2	2.82	0.47
1:A:17(P):VAL:HG11	1:A:24(P):TRP:CH2	2.49	0.47
1:A:94:TYR:CZ	1:A:106:PRO:HB3	2.50	0.47
1:A:42:ILE:O	1:A:46:THR:HG22	2.15	0.47
1:A:61:THR:O	1:A:128:CYS:HB2	2.14	0.47
1:A:61:THR:CG2	1:A:126:PRO:HB2	2.44	0.47
1:A:90:SER:HB2	1:A:100:CYS:H	1.81	0.46
1:A:8(P):PRO:HB2	1:A:9(P):LEU:HD12	1.96	0.46
1:A:45(P):PHE:HD2	1:A:75:TYR:CZ	2.33	0.46
1:A:113:ASN:CG	1:A:116:ARG:HG2	2.40	0.46
1:A:138:PRO:HB2	1:A:142:GLN:HB2	1.97	0.46
1:A:41(P):LEU:HG	1:A:221:TRP:NE1	2.30	0.46
1:A:45(P):PHE:HD2	1:A:75:TYR:CE2	2.34	0.46
1:A:157:GLU:O	1:A:161:MET:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ARG:HG3	1:A:236:GLY:N	2.30	0.46
1:A:89:VAL:HG11	1:A:140:TYR:CD1	2.51	0.45
1:A:235:ARG:CG	1:A:236:GLY:N	2.80	0.45
1:A:26:CYS:HA	1:A:71:CYS:HB3	1.99	0.44
1:A:190:HIS:CE1	1:A:192:THR:O	2.70	0.44
1:A:58:ASP:CG	1:A:89:VAL:HG22	2.42	0.44
1:A:69:ASP:HB3	1:A:72:ASN:HB2	2.00	0.44
1:A:153:VAL:HG11	1:A:160:ILE:HA	2.00	0.44
1:A:13(P):LEU:HD23	1:A:13(P):LEU:HA	1.78	0.43
1:A:30:TRP:CE2	1:A:74:GLY:HA3	2.54	0.43
1:A:9(P):LEU:CD2	1:A:181:LEU:HB2	2.50	0.42
1:A:20:ILE:CD1	1:A:218:ALA:HB1	2.49	0.42
1:A:137:SER:HA	1:A:138:PRO:O	2.20	0.42
1:A:23(P):THR:HG21	1:A:212:THR:HG21	2.02	0.42
1:A:176:VAL:CG2	1:A:199:HIS:HB3	2.49	0.41
1:A:51(P):PRO:O	1:A:152:SER:N	2.53	0.41
1:A:116:ARG:HB2	1:A:117:PRO:CD	2.49	0.41
1:A:40(P):ARG:HD3	1:A:25:SER:O	2.20	0.41
1:A:23:GLN:O	1:A:26:CYS:HB3	2.20	0.41
1:A:113:ASN:HD22	1:A:113:ASN:N	2.18	0.41
1:A:58:ASP:O	1:A:62:CYS:HB2	2.20	0.41
1:A:161:MET:HE3	1:A:235:ARG:HD2	2.03	0.41
1:A:51(P):PRO:O	1:A:52(P):PRO:C	2.63	0.41
1:A:93:LEU:H	1:A:93:LEU:CD1	2.28	0.41
1:A:170:VAL:HG12	1:A:248:ALA:HB2	2.03	0.41
1:A:58(P):THR:HA	1:A:61(P):LEU:CD2	2.46	0.40
1:A:89:VAL:HG13	1:A:144:LYS:HG3	2.03	0.40
1:A:105:ILE:HA	1:A:106:PRO:HD2	1.98	0.40
1:A:174:PHE:N	1:A:174:PHE:CD1	2.89	0.40
1:A:94:TYR:HA	1:A:103:TYR:O	2.22	0.40
1:A:188:TYR:OH	1:A:190:HIS:HB2	2.21	0.40
1:A:80:TRP:O	1:A:83:TRP:HB3	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60(P):ASP:OD1	1:A:228:ASN:ND2[4_555]	1.69	0.51
1:A:47:ASN:ND2	1:A:211:GLY:O[4_555]	2.06	0.14
1:A:62(P):LYS:O	1:A:148:TYR:CE1[4_455]	2.08	0.12

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	315/317 (99%)	258 (82%)	42 (13%)	15 (5%)	2 14

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8(P)	PRO
1	A	49(P)	PRO
1	A	52(P)	PRO
1	A	59(P)	GLU
1	A	48	ALA
1	A	113	ASN
1	A	10(P)	SER
1	A	128	CYS
1	A	49	HIS
1	A	5(P)	SER
1	A	60(P)	ASP
1	A	154	SER
1	A	6(P)	PHE
1	A	55(P)	VAL
1	A	138	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	267/267 (100%)	213 (80%)	54 (20%)	1 7

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6(P)	PHE
1	A	9(P)	LEU
1	A	11(P)	ASP
1	A	13(P)	LEU
1	A	20(P)	ARG
1	A	23(P)	THR
1	A	25(P)	GLN
1	A	35(P)	MET
1	A	41(P)	LEU
1	A	52(P)	PRO
1	A	55(P)	VAL
1	A	58(P)	THR
1	A	62(P)	LYS
1	A	6	ASP
1	A	9	GLU
1	A	11	TRP
1	A	13	GLN
1	A	20	ILE
1	A	23	GLN
1	A	25	SER
1	A	35	VAL
1	A	41	ARG
1	A	47	ASN
1	A	52	VAL
1	A	55	SER
1	A	58	ASP
1	A	62	CYS
1	A	69	ASP
1	A	86	LYS
1	A	93	LEU
1	A	108	CYS
1	A	112	VAL
1	A	113	ASN
1	A	116	ARG
1	A	122	GLU
1	A	126	PRO
1	A	127	LYS
1	A	141	LYS
1	A	154	SER
1	A	163	GLU
1	A	174	PHE
1	A	192	THR

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Mol	Chain	Res	Type
1	A	195	MET
1	A	201	ILE
1	A	202	ARG
1	A	210	ASN
1	A	217	VAL
1	A	222	ASN
1	A	223	THR
1	A	232	LYS
1	A	237	GLN
1	A	245	GLU
1	A	246	VAL
1	A	247	VAL

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	25(P)	GLN
1	A	113	ASN
1	A	155	ASN
1	A	167	ASN
1	A	189	GLN
1	A	222	ASN
1	A	237	GLN
1	A	239	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

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.