



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:37 pm GMT

PDB ID : 1NBZ
Title : Crystal Structure of HyHEL-63 complexed with HEL mutant K97A
Authors : Mariuzza, R.A.; Li, Y.; Urrutia, M.; Smith-Gill, S.J.
Deposited on : 2002-12-04
Resolution : 1.85 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

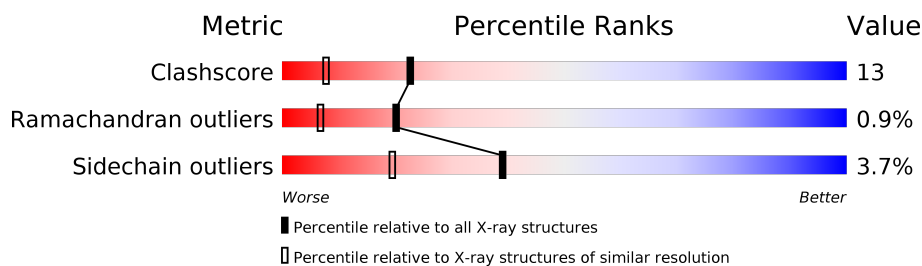
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	112137	2083 (1.86-1.86)
Ramachandran outliers	110173	2060 (1.86-1.86)
Sidechain outliers	110143	2060 (1.86-1.86)

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	214	
2	B	210	
3	C	129	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4732 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 antibody kappa light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1645	1016	280	342	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ASP	GLU	CLONING ARTIFACT	UNP 13359425
A	2	ILE	LEU	CLONING ARTIFACT	UNP 13359425
A	4	LEU	MET	CLONING ARTIFACT	UNP 13359425

- Molecule 2 is a protein called immunoglobulin gamma 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	0	0
			1580	996	253	325	6			

- Molecule 3 is a protein called Lysozyme C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	129	Total	C	N	O	S	0	0	0
			990	604	192	184	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	697	ALA	LYS	ENGINEERED	UNP P00698

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	228	Total	O	0	0
			228	228		

Continued on next page...

Continued from previous page...


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	224	Total 224	O 224	0	0
4	C	65	Total 65	O 65	0	0

3 Residue-property plots [i](#)

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 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.

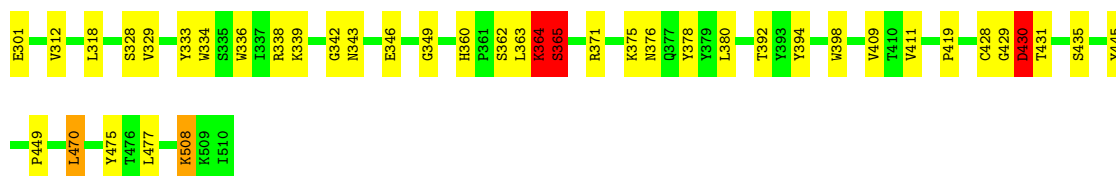
- Molecule 1: antibody kappa light chain

Chain A: 



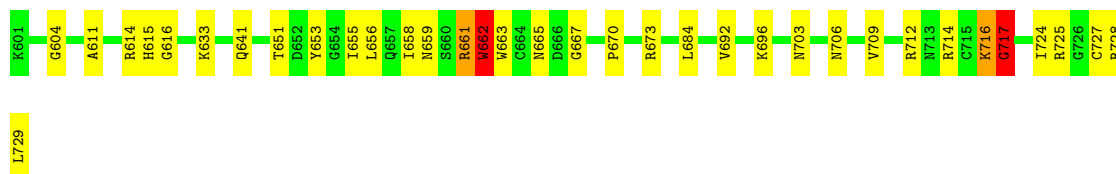
- Molecule 2: immunoglobulin gamma 1 chain

Chain B: 



- Molecule 3: Lysozyme C

Chain C: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	90.90Å 90.90Å 151.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.90 – 1.85	Depositor
% Data completeness (in resolution range)	78.0 (34.90-1.85)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.229 , 0.229	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4732	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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	0.74	4/1683 (0.2%)	1.13	12/2288 (0.5%)
2	B	0.96	3/1622 (0.2%)	0.85	7/2226 (0.3%)
3	C	0.70	4/1010 (0.4%)	1.28	8/1368 (0.6%)
All	All	0.82	11/4315 (0.3%)	1.07	27/5882 (0.5%)

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	1	2
2	B	0	2
3	C	0	1
All	All	1	5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	364	LYS	C-N	-30.27	0.64	1.34
1	A	213	GLU	C-N	20.88	1.82	1.34
2	B	365	SER	C-N	-16.30	0.96	1.34
3	C	716	LYS	C-N	-11.97	1.11	1.33
2	B	429	GLY	C-N	-11.35	1.07	1.34
1	A	42	GLU	C-N	11.06	1.59	1.34
3	C	662	TRP	C-N	-10.76	1.09	1.34
3	C	717	GLY	C-N	10.54	1.58	1.34
1	A	40	SER	C-N	8.74	1.54	1.34
1	A	41	HIS	C-N	-8.04	1.15	1.34
3	C	661	ARG	C-N	5.21	1.46	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	GLU	CB-CA-C	24.82	160.04	110.40
3	C	716	LYS	O-C-N	-23.33	83.54	123.20
3	C	716	LYS	C-N-CA	22.41	169.37	122.30
3	C	716	LYS	CA-C-N	19.20	154.61	116.20
1	A	213	GLU	N-CA-C	-17.24	64.44	111.00
2	B	364	LYS	O-C-N	-15.78	97.46	122.70
1	A	213	GLU	C-N-CA	14.39	157.66	121.70
1	A	213	GLU	CA-C-N	-13.43	87.66	117.20
1	A	41	HIS	O-C-N	12.92	143.38	122.70
3	C	717	GLY	CA-C-N	-12.26	90.24	117.20
2	B	365	SER	O-C-N	-11.10	104.94	122.70
1	A	212	ASN	C-N-CA	10.41	147.72	121.70
1	A	213	GLU	O-C-N	10.20	139.02	122.70
1	A	41	HIS	CA-C-N	-9.31	96.72	117.20
3	C	717	GLY	C-N-CA	7.62	140.76	121.70
1	A	212	ASN	O-C-N	-6.87	111.71	122.70
2	B	430	ASP	O-C-N	6.63	133.31	122.70
2	B	430	ASP	CA-C-N	-6.26	103.42	117.20
1	A	40	SER	C-N-CA	-6.25	106.07	121.70
1	A	39	LYS	CA-C-N	-5.59	104.89	117.20
2	B	365	SER	CA-C-N	5.56	129.44	117.20
3	C	661	ARG	O-C-N	5.56	131.59	122.70
1	A	40	SER	O-C-N	5.38	131.32	122.70
2	B	364	LYS	C-N-CA	5.34	135.06	121.70
3	C	604	GLY	N-CA-C	-5.30	99.84	113.10
3	C	717	GLY	O-C-N	5.26	131.12	122.70
2	B	429	GLY	O-C-N	-5.25	114.31	122.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	213	GLU	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	212	ASN	Mainchain
1	A	39	LYS	Mainchain
2	B	364	LYS	Mainchain
2	B	365	SER	Mainchain
3	C	717	GLY	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	1645	0	1514	49	0
2	B	1580	0	1500	31	1
3	C	990	0	916	37	0
4	A	228	0	0	4	0
4	B	224	0	0	1	1
4	C	65	0	0	3	1
All	All	4732	0	3930	106	2

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 13.

All (106) 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:213:GLU:C	1:A:214:CYS:N	1.82	1.30
3:C:662:TRP:CD1	3:C:673:ARG:HD2	1.73	1.23
3:C:662:TRP:HE1	3:C:673:ARG:CZ	1.81	0.92
3:C:662:TRP:HD1	3:C:673:ARG:HD2	1.24	0.91
1:A:213:GLU:HG2	1:A:214:CYS:SG	2.12	0.90
1:A:213:GLU:CA	1:A:214:CYS:N	2.37	0.88
1:A:39:LYS:O	1:A:40:SER:CB	2.26	0.83
1:A:105:GLU:HG2	1:A:106:ILE:N	1.90	0.82
2:B:360:HIS:HD2	2:B:362:SER:H	1.25	0.82
3:C:641:GLN:NE2	3:C:684:LEU:O	2.20	0.74
1:A:41:HIS:O	4:A:317:HOH:O	2.07	0.73
1:A:211:ARG:O	1:A:213:GLU:HB2	1.89	0.72
3:C:662:TRP:NE1	3:C:673:ARG:HD2	2.05	0.71
1:A:39:LYS:O	1:A:40:SER:HB3	1.89	0.71
3:C:662:TRP:CD1	3:C:673:ARG:CD	2.66	0.70
2:B:334:TRP:HB3	2:B:378:TYR:CZ	2.28	0.68
3:C:724:ILE:HG23	3:C:729:LEU:HD22	1.76	0.67
1:A:103:LYS:HE2	4:A:437:HOH:O	1.93	0.66
2:B:329:VAL:H	2:B:376:ASN:HD21	1.41	0.66
3:C:662:TRP:HE1	3:C:673:ARG:NE	1.93	0.66
2:B:301:GLU:HG2	2:B:301:GLU:O	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:GLU:OE1	1:A:173:TYR:OH	2.15	0.65
3:C:641:GLN:NE2	4:C:390:HOH:O	2.30	0.65
2:B:329:VAL:H	2:B:376:ASN:ND2	1.95	0.64
2:B:333:TYR:HB2	2:B:398:TRP:CB	2.27	0.64
1:A:38:GLN:HG3	1:A:42:GLU:O	1.97	0.64
1:A:41:HIS:CD2	2:B:339:LYS:HD3	2.34	0.63
3:C:659:ASN:OD1	3:C:661:ARG:HB3	1.99	0.63
1:A:147:LYS:HE3	1:A:154:GLU:OE1	1.98	0.62
2:B:419:PRO:HB3	2:B:445:TYR:HB3	1.81	0.62
2:B:338:ARG:HD3	2:B:346:GLU:OE1	2.00	0.61
1:A:39:LYS:O	1:A:40:SER:OG	2.18	0.61
2:B:360:HIS:CD2	2:B:362:SER:H	2.13	0.61
3:C:662:TRP:HE1	3:C:673:ARG:NH1	2.00	0.59
1:A:41:HIS:O	2:B:394:TYR:OH	2.20	0.59
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.85	0.57
1:A:213:GLU:HA	1:A:214:CYS:N	2.20	0.56
1:A:12:SER:OG	1:A:105:GLU:OE2	2.18	0.56
1:A:31:ASN:HD21	3:C:696:LYS:HZ3	1.54	0.55
2:B:364:LYS:HD3	2:B:364:LYS:N	2.23	0.54
2:B:508:LYS:NZ	2:B:508:LYS:HB2	2.21	0.54
2:B:363:LEU:O	2:B:365:SER:N	2.41	0.54
1:A:32:ASN:HD21	3:C:696:LYS:NZ	2.05	0.54
3:C:712:ARG:HA	3:C:716:LYS:HB2	1.89	0.54
1:A:38:GLN:NE2	1:A:42:GLU:O	2.35	0.54
3:C:611:ALA:HA	3:C:614:ARG:NH2	2.23	0.53
2:B:342:GLY:O	2:B:343:ASN:HB2	2.09	0.53
3:C:728:ARG:C	3:C:729:LEU:HD12	2.28	0.53
1:A:213:GLU:HG2	2:B:428:CYS:SG	2.49	0.53
1:A:211:ARG:C	1:A:213:GLU:HB2	2.30	0.52
3:C:659:ASN:OD1	3:C:661:ARG:N	2.34	0.52
2:B:333:TYR:HB2	2:B:398:TRP:HB3	1.91	0.52
2:B:329:VAL:N	2:B:376:ASN:HD21	2.07	0.52
1:A:213:GLU:HA	1:A:214:CYS:SG	2.50	0.52
3:C:615:HIS:HD2	4:C:8:HOH:O	1.92	0.51
1:A:213:GLU:CG	1:A:214:CYS:SG	2.93	0.51
1:A:94:TRP:CD2	1:A:95:PRO:HA	2.46	0.51
1:A:31:ASN:ND2	3:C:616:GLY:HA3	2.26	0.51
1:A:31:ASN:HD21	3:C:696:LYS:NZ	2.08	0.50
2:B:328:SER:HA	2:B:376:ASN:HD21	1.76	0.49
3:C:662:TRP:NE1	3:C:673:ARG:NH1	2.61	0.49
2:B:333:TYR:HB2	2:B:398:TRP:HB2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LYS:HB3	4:A:278:HOH:O	2.13	0.49
3:C:662:TRP:NE1	3:C:673:ARG:CD	2.74	0.48
2:B:375:LYS:HE2	4:B:565:HOH:O	2.14	0.47
3:C:615:HIS:HB3	3:C:692:VAL:HG11	1.96	0.47
3:C:665:ASN:HA	4:C:336:HOH:O	2.12	0.47
1:A:189:HIS:O	1:A:211:ARG:HD3	2.15	0.47
3:C:658:ILE:HG22	3:C:663:TRP:HB2	1.95	0.47
1:A:94:TRP:CH2	2:B:349:GLY:HA2	2.50	0.47
3:C:655:ILE:HG23	3:C:656:LEU:HG	1.97	0.47
2:B:371:ARG:HA	2:B:378:TYR:HA	1.96	0.47
2:B:470:LEU:HD13	2:B:475:TYR:CE1	2.49	0.47
1:A:94:TRP:HH2	2:B:349:GLY:HA2	1.79	0.47
3:C:633:LYS:HD3	3:C:633:LYS:C	2.35	0.46
3:C:661:ARG:NH2	3:C:670:PRO:O	2.48	0.46
3:C:703:ASN:O	3:C:706:ASN:HB2	2.15	0.46
3:C:651:THR:HB	3:C:653:TYR:CE1	2.50	0.45
1:A:76:ASN:O	1:A:77:SER:HB2	2.17	0.45
1:A:105:GLU:HG3	1:A:166:GLN:OE1	2.16	0.45
3:C:709:VAL:HA	3:C:712:ARG:NH2	2.32	0.44
3:C:709:VAL:HG22	3:C:712:ARG:HH22	1.82	0.44
2:B:318:LEU:HD23	2:B:318:LEU:C	2.38	0.44
2:B:318:LEU:CD1	2:B:409:VAL:HG11	2.48	0.44
1:A:41:HIS:HB3	4:A:337:HOH:O	2.18	0.43
1:A:39:LYS:C	1:A:40:SER:OG	2.55	0.43
1:A:113:PRO:HB3	1:A:139:PHE:HB3	2.00	0.43
1:A:103:LYS:HB3	1:A:103:LYS:HE3	1.88	0.43
1:A:41:HIS:CE1	2:B:392:THR:HG1	2.36	0.43
3:C:665:ASN:OD1	3:C:667:GLY:N	2.50	0.43
3:C:727:CYS:HB2	3:C:729:LEU:HD13	2.01	0.43
1:A:31:ASN:C	1:A:31:ASN:ND2	2.72	0.42
1:A:105:GLU:CG	1:A:106:ILE:N	2.71	0.42
2:B:336:TRP:CE2	2:B:380:LEU:HB2	2.54	0.42
1:A:105:GLU:HG3	1:A:173:TYR:OH	2.20	0.42
1:A:12:SER:CB	1:A:105:GLU:OE2	2.68	0.41
2:B:312:VAL:O	2:B:411:VAL:HA	2.19	0.41
1:A:147:LYS:HE2	1:A:149:LYS:HE3	2.01	0.41
3:C:662:TRP:HE1	3:C:673:ARG:CD	2.33	0.41
1:A:21:LEU:HD22	1:A:102:THR:HG21	2.01	0.41
1:A:13:VAL:HG11	1:A:19:VAL:HG11	2.02	0.41
3:C:727:CYS:CB	3:C:729:LEU:HD13	2.49	0.41
1:A:147:LYS:HE2	1:A:149:LYS:CE	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ASN:H	1:A:31:ASN:HD22	1.68	0.41
2:B:364:LYS:CD	2:B:364:LYS:N	2.83	0.41
1:A:30:SER:HB3	3:C:616:GLY:HA2	2.03	0.41

All (2) 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)
2:B:430:ASP:OD1	4:C:366:HOH:O[1_455]	1.67	0.53
4:B:610:HOH:O	4:B:610:HOH:O[2_765]	2.16	0.04

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	212/214 (99%)	204 (96%)	7 (3%)	1 (0%)	32	16
2	B	208/210 (99%)	197 (95%)	8 (4%)	3 (1%)	13	3
3	C	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	22	8
All	All	547/553 (99%)	520 (95%)	22 (4%)	5 (1%)	20	7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	SER
2	B	364	LYS
2	B	365	SER
2	B	431	THR
3	C	717	GLY

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	182/193 (94%)	174 (96%)	8 (4%)	33	14
2	B	180/186 (97%)	174 (97%)	6 (3%)	43	24
3	C	98/104 (94%)	95 (97%)	3 (3%)	45	27
All	All	460/483 (95%)	443 (96%)	17 (4%)	39	19

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	31	ASN
1	A	39	LYS
1	A	41	HIS
1	A	54	SER
1	A	104	LEU
1	A	105	GLU
1	A	203	SER
2	B	430	ASP
2	B	435	SER
2	B	449	PRO
2	B	470	LEU
2	B	477	LEU
2	B	508	LYS
3	C	662	TRP
3	C	714	ARG
3	C	725	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	32	ASN
1	A	53	GLN
1	A	92	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	145	ASN
1	A	189	HIS
2	B	305	GLN
2	B	360	HIS
2	B	376	ASN
2	B	471	GLN
3	C	615	HIS
3	C	693	ASN
3	C	713	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 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.