Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 11:30 AM EDT

PDB ID	:	3C8K
Title	:	The crystal structure of Ly49C bound to H-2Kb
Authors	:	Deng, L.; Mariuzza, R.A.
Deposited on	:	2008-02-12
Resolution	:	2.90 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:

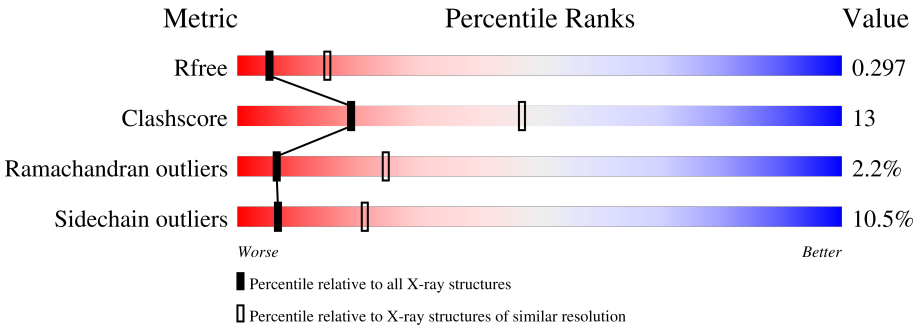
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	274	66% 28% 5%
2	B	99	73% 16% 11%
3	P	8	62% 38%
4	D	125	67% 24% 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4229 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 H-2 class I histocompatibility antigen, K-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2232	1408	393	422	9			

- Molecule 2 is a protein called beta-2 microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			818	523	138	150	7			

- Molecule 3 is a protein called Ovalbumin peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	8	Total	C	N	O	0	0	0
			68	45	10	13			

- Molecule 4 is a protein called Natural killer cell receptor Ly-49C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	125	Total	C	N	O	S	0	0	0
			1046	682	173	180	11			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	171	GLY	SER	engineered mutation	UNP Q61198
D	193	GLY	GLU	engineered mutation	UNP Q61198
D	223	LYS	ARG	engineered mutation	UNP Q61198

- Molecule 5 is water.

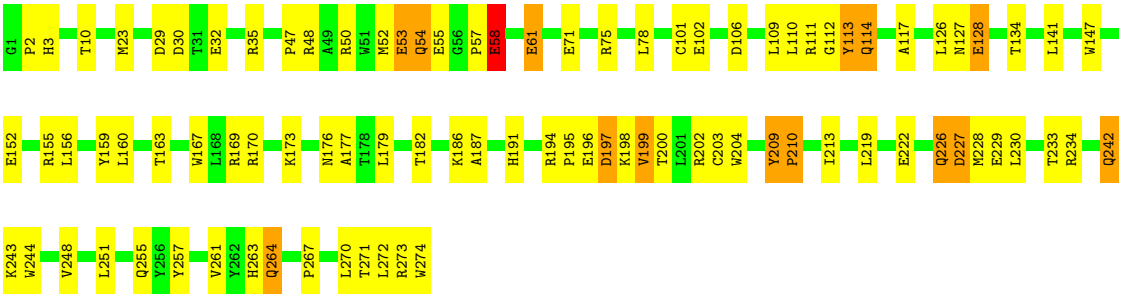
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	26	Total O 26 26	0	0
5	B	21	Total O 21 21	0	0
5	P	2	Total O 2 2	0	0
5	D	16	Total O 16 16	0	0

3 Residue-property plots (i)

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.

• Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain

Chain A:

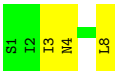


• Molecule 2: beta-2 microglobulin

Chain B:

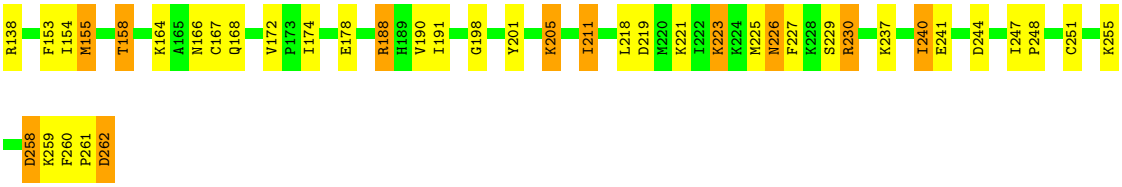
• Molecule 3: Ovalbumin peptide

Chain P:



• Molecule 4: Natural killer cell receptor Ly-49C

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	152.01Å 152.01Å 64.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.81 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.6 (30.00-2.90) 95.6 (29.81-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.42 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.199 , 0.263 0.258 , 0.297	Depositor DCC
R_{free} test set	665 reflections (3.94%)	wwPDB-VP
Wilson B-factor (Å^2)	68.9	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	4229	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	1.10	9/2293 (0.4%)	0.80	5/3113 (0.2%)
2	B	0.60	0/844	0.67	0/1144
3	P	0.57	0/68	0.73	0/88
4	D	0.83	3/1077 (0.3%)	0.76	2/1445 (0.1%)
All	All	0.95	12/4282 (0.3%)	0.77	7/5790 (0.1%)

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
2	B	0	1
All	All	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	GLU	CD-OE1	27.51	1.55	1.25
1	A	58	GLU	CG-CD	20.99	1.83	1.51
4	D	205	LYS	CD-CE	15.18	1.89	1.51
1	A	55	GLU	CD-OE2	13.41	1.40	1.25
1	A	58	GLU	CD-OE2	13.24	1.40	1.25
1	A	58	GLU	CB-CG	11.50	1.74	1.52
1	A	57	PRO	C-N	11.42	1.60	1.34
1	A	55	GLU	CD-OE1	8.80	1.35	1.25
4	D	262	ASP	C-OXT	5.48	1.33	1.23
1	A	53	GLU	CD-OE2	5.15	1.31	1.25
4	D	205	LYS	CG-CD	5.05	1.69	1.52
1	A	203	CYS	CB-SG	-5.04	1.73	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	58	GLU	OE1-CD-OE2	-13.39	107.23	123.30
1	A	58	GLU	CG-CD-OE2	10.44	139.19	118.30
1	A	209	TYR	C-N-CD	-7.68	103.71	120.60
1	A	55	GLU	OE1-CD-OE2	7.01	131.72	123.30
4	D	205	LYS	CD-CE-NZ	-6.16	97.54	111.70
4	D	205	LYS	CG-CD-CE	-5.55	95.25	111.90
1	A	57	PRO	CA-C-N	-5.53	105.03	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	TYR	Peptide
2	B	31	HIS	Peptide

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	2232	0	2123	55	0
2	B	818	0	797	24	0
3	P	68	0	74	3	0
4	D	1046	0	1033	33	0
5	A	26	0	0	0	0
5	B	21	0	0	0	0
5	D	16	0	0	0	0
5	P	2	0	0	0	0
All	All	4229	0	4027	107	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 13.

All (107) 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)
4:D:205:LYS:CD	4:D:205:LYS:CE	1.89	1.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLU:CD	1:A:58:GLU:CG	1.83	1.44
2:B:32:PRO:HD2	2:B:84:HIS:NE2	1.94	0.83
4:D:188:ARG:HG3	4:D:188:ARG:HH11	1.43	0.82
4:D:190:VAL:O	4:D:237:LYS:HE2	1.81	0.81
1:A:126:LEU:HD22	1:A:156:LEU:HD23	1.63	0.81
4:D:167:CYS:HB3	4:D:172:VAL:O	1.83	0.78
2:B:3:LYS:HD3	2:B:31:HIS:HB3	1.66	0.77
1:A:191:HIS:NE2	1:A:199:VAL:HG11	2.00	0.76
1:A:213:ILE:H	4:D:230:ARG:HH21	1.30	0.76
4:D:205:LYS:CE	4:D:205:LYS:CG	2.65	0.75
4:D:188:ARG:HH11	4:D:188:ARG:CG	2.00	0.75
4:D:240:ILE:HD13	4:D:240:ILE:N	2.04	0.72
2:B:32:PRO:HD2	2:B:84:HIS:HE2	1.56	0.70
2:B:32:PRO:HD3	2:B:84:HIS:CE1	2.27	0.69
1:A:210:PRO:HD2	1:A:263:HIS:NE2	2.08	0.69
2:B:74:GLU:HG2	2:B:75:THR:HG23	1.75	0.68
2:B:32:PRO:CD	2:B:84:HIS:CE1	2.79	0.65
4:D:172:VAL:HG13	4:D:255:LYS:HB2	1.79	0.65
1:A:35:ARG:HB3	1:A:48:ARG:HD2	1.79	0.64
4:D:153:PHE:HB3	4:D:155:MET:CE	2.29	0.63
1:A:23:MET:CE	1:A:35:ARG:HE	2.12	0.62
1:A:155:ARG:NH2	3:P:4:ASN:O	2.32	0.61
4:D:154:ILE:HB	4:D:251:CYS:HB3	1.82	0.61
4:D:164:LYS:HE3	4:D:211:ILE:HD11	1.82	0.60
1:A:110:LEU:HD13	4:D:226:ASN:HD21	1.66	0.60
4:D:205:LYS:CD	4:D:205:LYS:NZ	2.63	0.60
1:A:202:ARG:NH1	1:A:244:TRP:CZ3	2.70	0.59
1:A:234:ARG:HE	1:A:242:GLN:HG3	1.68	0.59
2:B:73:THR:HB	2:B:76:ASP:OD2	2.04	0.57
1:A:114:GLN:HG3	1:A:156:LEU:HD21	1.87	0.56
2:B:58:LYS:NZ	4:D:241:GLU:HG3	2.20	0.55
1:A:61:GLU:OE2	1:A:61:GLU:HA	2.06	0.55
2:B:10:TYR:CD1	2:B:10:TYR:N	2.73	0.55
4:D:153:PHE:HB3	4:D:155:MET:HE3	1.87	0.55
1:A:261:VAL:HB	1:A:270:LEU:HB2	1.89	0.55
2:B:2:GLN:HA	2:B:31:HIS:O	2.06	0.55
1:A:127:ASN:OD1	1:A:134:THR:HG23	2.08	0.54
1:A:47:PRO:O	1:A:48:ARG:HG2	2.09	0.53
1:A:58:GLU:CD	1:A:58:GLU:CB	2.77	0.53
1:A:229:GLU:HG2	1:A:230:LEU:H	1.75	0.52
1:A:52:MET:C	1:A:54:GLN:N	2.63	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.44	0.51
1:A:226:GLN:HG2	1:A:227:ASP:N	2.24	0.51
1:A:196:GLU:O	1:A:198:LYS:HG3	2.10	0.51
1:A:226:GLN:O	1:A:228:MET:N	2.43	0.51
2:B:32:PRO:CD	2:B:84:HIS:NE2	2.68	0.51
4:D:260:PHE:O	4:D:262:ASP:N	2.42	0.51
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.46	0.50
2:B:32:PRO:HD2	2:B:84:HIS:CE1	2.44	0.50
4:D:244:ASP:HB3	4:D:247:ILE:HG13	1.92	0.50
4:D:153:PHE:HB3	4:D:155:MET:HE1	1.95	0.49
1:A:3:HIS:ND1	1:A:29:ASP:OD2	2.45	0.49
1:A:255:GLN:OE1	1:A:273:ARG:NH1	2.44	0.49
4:D:154:ILE:HD13	4:D:166:ASN:HD22	1.77	0.49
1:A:112:GLY:HA3	1:A:160:LEU:HD13	1.95	0.49
4:D:225:MET:HB3	4:D:227:PHE:CE1	2.47	0.48
1:A:219:LEU:HD13	1:A:257:TYR:CZ	2.49	0.48
1:A:210:PRO:CD	1:A:263:HIS:NE2	2.77	0.48
1:A:52:MET:C	1:A:54:GLN:H	2.16	0.47
4:D:158:THR:O	4:D:248:PRO:HA	2.15	0.47
1:A:147:TRP:HB3	1:A:152:GLU:HB2	1.97	0.47
4:D:219:ASP:O	4:D:223:LYS:HB2	2.15	0.47
1:A:177:ALA:C	1:A:179:LEU:H	2.18	0.46
1:A:271:THR:C	1:A:272:LEU:HD12	2.36	0.46
4:D:201:TYR:CZ	4:D:229:SER:HB3	2.50	0.46
1:A:47:PRO:C	1:A:48:ARG:HG2	2.36	0.46
2:B:58:LYS:HZ2	4:D:241:GLU:HG3	1.81	0.46
1:A:202:ARG:HD2	1:A:204:TRP:CZ2	2.51	0.45
1:A:226:GLN:HG2	1:A:227:ASP:HB2	1.98	0.45
1:A:255:GLN:NE2	1:A:274:TRP:O	2.50	0.45
1:A:264:GLN:C	1:A:264:GLN:HE21	2.20	0.45
1:A:187:ALA:HA	1:A:204:TRP:O	2.18	0.44
4:D:174:ILE:HG12	4:D:198:GLY:N	2.32	0.44
1:A:128:GLU:H	1:A:128:GLU:CD	2.21	0.44
4:D:164:LYS:O	4:D:168:GLN:HG2	2.17	0.44
1:A:102:GLU:O	1:A:109:LEU:HD12	2.18	0.43
4:D:240:ILE:HD13	4:D:240:ILE:H	1.83	0.43
4:D:188:ARG:HG3	4:D:188:ARG:NH1	2.23	0.43
1:A:71:GLU:HG2	1:A:75:ARG:NH2	2.34	0.43
2:B:59:ASP:OD1	2:B:59:ASP:C	2.57	0.43
2:B:69:GLU:CD	2:B:69:GLU:H	2.22	0.43
1:A:101:CYS:HB2	1:A:109:LEU:HD13	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LYS:HA	1:A:176:ASN:HD21	1.83	0.43
1:A:194:ARG:HB3	1:A:195:PRO:HD2	2.00	0.43
1:A:233:THR:OG1	1:A:243:LYS:HD2	2.19	0.43
4:D:190:VAL:HG13	4:D:191:ILE:O	2.19	0.43
4:D:258:ASP:C	4:D:259:LYS:HG2	2.39	0.42
1:A:113:TYR:CD1	1:A:113:TYR:N	2.86	0.42
1:A:106:ASP:OD1	1:A:106:ASP:N	2.53	0.42
2:B:29:GLN:HA	2:B:61:SER:HB2	2.02	0.42
1:A:117:ALA:HB2	2:B:60:TRP:CZ2	2.54	0.42
4:D:247:ILE:HA	4:D:248:PRO:HD3	1.88	0.42
3:P:3:ILE:CG1	3:P:4:ASN:N	2.83	0.42
1:A:23:MET:HE1	1:A:35:ARG:HE	1.83	0.41
1:A:163:THR:HG22	1:A:167:TRP:HD1	1.85	0.41
1:A:50:ARG:O	1:A:53:GLU:HG2	2.21	0.41
2:B:32:PRO:HD3	2:B:84:HIS:HE1	1.82	0.41
1:A:191:HIS:CD2	1:A:199:VAL:HG11	2.54	0.41
4:D:190:VAL:O	4:D:237:LYS:CE	2.60	0.41
1:A:32:GLU:OE2	1:A:48:ARG:HD3	2.21	0.41
2:B:76:ASP:OD2	2:B:76:ASP:N	2.53	0.41
1:A:159:TYR:CG	3:P:3:ILE:HD12	2.56	0.41
2:B:19:LYS:HE2	2:B:21:ASN:ND2	2.36	0.41
1:A:110:LEU:HD23	1:A:110:LEU:HA	1.90	0.41
2:B:14:PRO:HA	2:B:15:PRO:HD3	1.92	0.40
2:B:39:MET:HG3	2:B:49:VAL:HG11	2.03	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	272/274 (99%)	243 (89%)	24 (9%)	5 (2%)	8 29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	97/99 (98%)	87 (90%)	5 (5%)	5 (5%)	2 6
3	P	6/8 (75%)	5 (83%)	1 (17%)	0	100 100
4	D	123/125 (98%)	113 (92%)	9 (7%)	1 (1%)	19 51
All	All	498/506 (98%)	448 (90%)	39 (8%)	11 (2%)	6 24

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	58	LYS
1	A	197	ASP
1	A	267	PRO
2	B	60	TRP
4	D	261	PRO
1	A	210	PRO
1	A	227	ASP
2	B	32	PRO
1	A	226	GLN
2	B	48	LYS
2	B	43	GLY

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	232/232 (100%)	208 (90%)	24 (10%)	7 22
2	B	93/93 (100%)	84 (90%)	9 (10%)	8 25
3	P	8/8 (100%)	7 (88%)	1 (12%)	4 14
4	D	114/114 (100%)	101 (89%)	13 (11%)	5 17
All	All	447/447 (100%)	400 (90%)	47 (10%)	7 21

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
1	A	10	THR
1	A	30	ASP
1	A	54	GLN
1	A	58	GLU
1	A	61	GLU
1	A	78	LEU
1	A	111	ARG
1	A	113	TYR
1	A	114	GLN
1	A	128	GLU
1	A	141	LEU
1	A	169	ARG
1	A	170	ARG
1	A	182	THR
1	A	186	LYS
1	A	197	ASP
1	A	199	VAL
1	A	200	THR
1	A	222	GLU
1	A	242	GLN
1	A	248	VAL
1	A	251	LEU
1	A	264	GLN
2	B	2	GLN
2	B	3	LYS
2	B	16	GLU
2	B	19	LYS
2	B	48	LYS
2	B	70	PHE
2	B	73	THR
2	B	74	GLU
2	B	77	THR
3	P	8	LEU
4	D	138	ARG
4	D	155	MET
4	D	158	THR
4	D	178	GLU
4	D	188	ARG
4	D	211	ILE
4	D	218	LEU
4	D	221	LYS
4	D	223	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	226	ASN
4	D	230	ARG
4	D	240	ILE
4	D	258	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	ASN
1	A	264	GLN
2	B	31	HIS
4	D	166	ASN
4	D	194	ASN
4	D	226	ASN

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 monosaccharides 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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.