



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 03:04 pm GMT

PDB ID : 1FDL
Title : CRYSTALLOGRAPHIC REFINEMENT OF THE THREE-DIMENSIONAL
STRUCTURE OF THE FAB D1.3-LYSOZYME COMPLEX AT 2.5-
ANGSTROMS RESOLUTION
Authors : Fischmann, T.O.; Poljak, R.J.
Deposited on : 1990-08-27
Resolution : 2.50 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

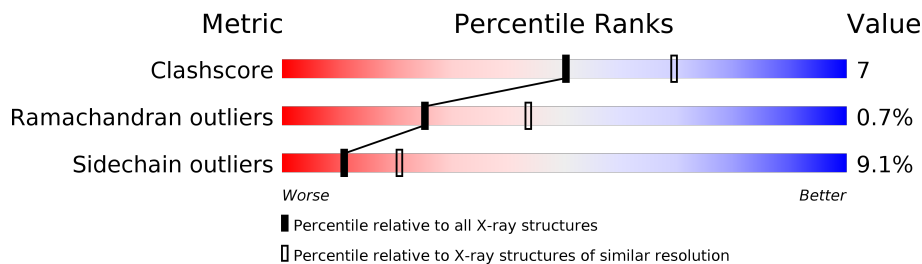
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)

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	L	214	
2	H	218	
3	Y	129	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4309 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 IGG1-KAPPA D1.3 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1665	1037	282	339	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	50	TYR	ASN	CONFLICT	GB 2072141
L	51	THR	ALA	CONFLICT	GB 2072141
L	52	THR	LYS	CONFLICT	GB 2072141
L	85	SER	THR	CONFLICT	GB 2072141
L	89	GLN	HIS	CONFLICT	GB 2072141
L	96	ARG	TRP	CONFLICT	GB 2072141
L	106	ILE	VAL	CONFLICT	GB 2072141
L	118	PHE	LEU	CONFLICT	GB 2072141

- Molecule 2 is a protein called IGG1-KAPPA D1.3 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1643	1030	279	326	8			

- Molecule 3 is a protein called HEN EGG WHITE LYSOZYME.

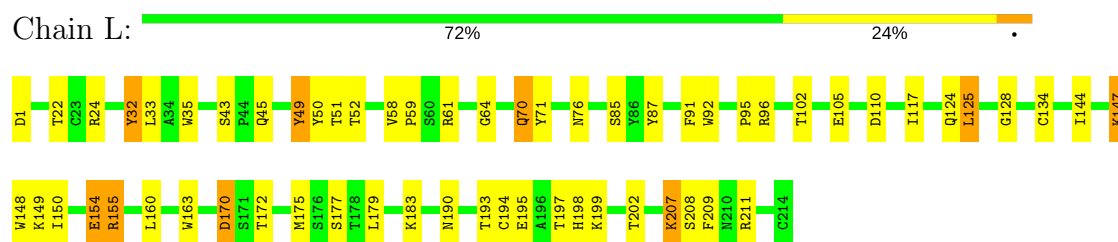
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	129	Total	C	N	O	S	0	0	0
			1001	613	193	185	10			

3 Residue-property plots [i](#)

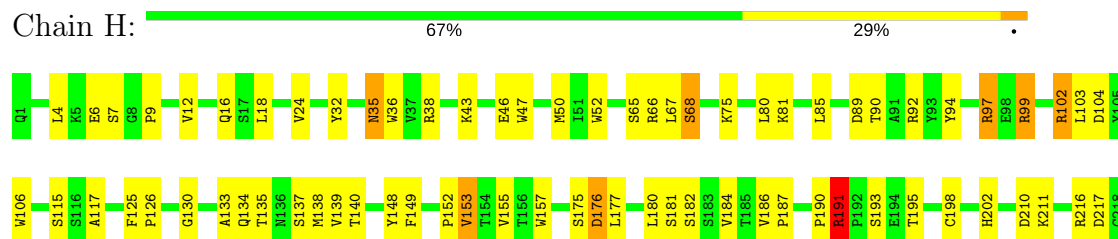
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

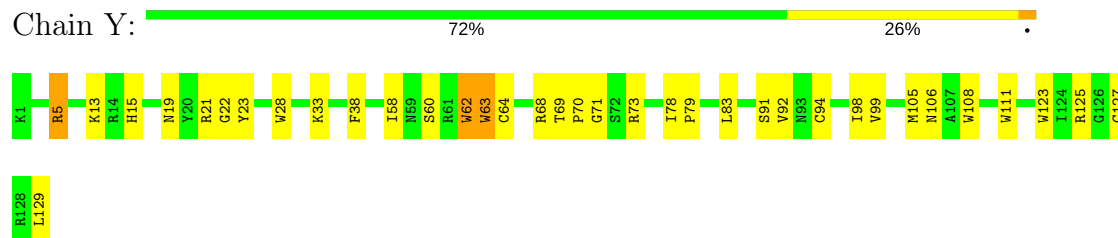
• Molecule 1: IGG1-KAPPA D1.3 FAB (LIGHT CHAIN)



• Molecule 2: IGG1-KAPPA D1.3 FAB (HEAVY CHAIN)



• Molecule 3: HEN EGG WHITE LYSOZYME



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.00Å 143.50Å 49.30Å 90.00° 120.40° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.184 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4309	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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	L	0.80	0/1705	1.54	26/2315 (1.1%)
2	H	0.88	0/1684	1.83	34/2300 (1.5%)
3	Y	0.91	0/1021	1.77	25/1379 (1.8%)
All	All	0.85	0/4410	1.71	85/5994 (1.4%)

There are no bond length outliers.

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	66	ARG	NE-CZ-NH2	-19.60	110.50	120.30
2	H	191	ARG	NE-CZ-NH1	13.71	127.16	120.30
2	H	97	ARG	NE-CZ-NH2	-11.53	114.53	120.30
1	L	163	TRP	CD1-CG-CD2	10.21	114.47	106.30
2	H	52	TRP	CD1-CG-CD2	9.68	114.04	106.30
2	H	191	ARG	NE-CZ-NH2	-9.45	115.58	120.30
2	H	36	TRP	CD1-CG-CD2	9.41	113.83	106.30
3	Y	108	TRP	CD1-CG-CD2	9.41	113.83	106.30
1	L	148	TRP	CD1-CG-CD2	8.81	113.35	106.30
2	H	66	ARG	NE-CZ-NH1	8.73	124.67	120.30
3	Y	123	TRP	CD1-CG-CD2	8.71	113.27	106.30
3	Y	62	TRP	CD1-CG-CD2	8.71	113.26	106.30
3	Y	108	TRP	CB-CG-CD1	-8.65	115.76	127.00
2	H	157	TRP	CD1-CG-CD2	8.61	113.19	106.30
3	Y	108	TRP	CG-CD2-CE3	8.60	141.64	133.90
3	Y	28	TRP	CD1-CG-CD2	8.32	112.96	106.30
2	H	99	ARG	NE-CZ-NH2	-8.29	116.15	120.30
3	Y	108	TRP	CE2-CD2-CG	-8.25	100.70	107.30
1	L	92	TRP	CD1-CG-CD2	8.18	112.84	106.30
1	L	163	TRP	CE2-CD2-CG	-8.16	100.77	107.30
1	L	35	TRP	CD1-CG-CD2	8.14	112.81	106.30
3	Y	28	TRP	CE2-CD2-CG	-7.93	100.95	107.30
2	H	52	TRP	CE2-CD2-CG	-7.89	100.99	107.30
3	Y	111	TRP	CD1-CG-CD2	7.84	112.58	106.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	123	TRP	CE2-CD2-CG	-7.62	101.20	107.30
3	Y	62	TRP	CE2-CD2-CG	-7.62	101.21	107.30
1	L	35	TRP	CE2-CD2-CG	-7.57	101.25	107.30
1	L	148	TRP	CE2-CD2-CG	-7.53	101.27	107.30
2	H	157	TRP	CE2-CD2-CG	-7.50	101.30	107.30
2	H	47	TRP	CD1-CG-CD2	7.46	112.27	106.30
2	H	36	TRP	CE2-CD2-CG	-7.28	101.48	107.30
3	Y	125	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	L	35	TRP	CG-CD2-CE3	7.17	140.35	133.90
2	H	47	TRP	CE2-CD2-CG	-7.13	101.59	107.30
1	L	92	TRP	CE2-CD2-CG	-7.03	101.68	107.30
2	H	106	TRP	CD1-CG-CD2	6.81	111.75	106.30
3	Y	63	TRP	CE2-CD2-CG	-6.74	101.91	107.30
2	H	104	ASP	CB-CG-OD1	6.71	124.34	118.30
3	Y	63	TRP	CD1-CG-CD2	6.71	111.67	106.30
3	Y	111	TRP	CE2-CD2-CG	-6.64	101.98	107.30
1	L	35	TRP	CB-CG-CD1	-6.64	118.37	127.00
3	Y	21	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	L	87	TYR	CB-CG-CD2	-6.55	117.07	121.00
1	L	163	TRP	CG-CD1-NE1	-6.35	103.75	110.10
2	H	148	TYR	CB-CG-CD2	-6.34	117.19	121.00
1	L	24	ARG	NE-CZ-NH1	6.16	123.38	120.30
2	H	36	TRP	CG-CD1-NE1	-6.07	104.03	110.10
2	H	52	TRP	CB-CG-CD1	-6.01	119.19	127.00
2	H	97	ARG	NE-CZ-NH1	5.98	123.29	120.30
3	Y	108	TRP	CG-CD1-NE1	-5.97	104.13	110.10
1	L	211	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	L	32	TYR	CB-CG-CD2	-5.95	117.43	121.00
2	H	52	TRP	CG-CD1-NE1	-5.93	104.17	110.10
1	L	49	TYR	CB-CG-CD2	-5.92	117.45	121.00
1	L	92	TRP	CG-CD1-NE1	-5.87	104.23	110.10
2	H	52	TRP	CG-CD2-CE3	5.76	139.08	133.90
1	L	50	TYR	CB-CG-CD1	-5.64	117.61	121.00
2	H	92	ARG	NE-CZ-NH1	5.64	123.12	120.30
2	H	90	THR	N-CA-C	-5.60	95.88	111.00
2	H	106	TRP	CE2-CD2-CG	-5.56	102.85	107.30
2	H	157	TRP	CG-CD1-NE1	-5.56	104.54	110.10
3	Y	105	MET	CA-CB-CG	-5.54	103.88	113.30
1	L	134	CYS	CA-CB-SG	-5.52	104.06	114.00
1	L	175	MET	CG-SD-CE	-5.50	91.40	100.20
3	Y	68	ARG	NE-CZ-NH1	5.50	123.05	120.30
3	Y	5	ARG	NE-CZ-NH1	5.48	123.04	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	211	ARG	NE-CZ-NH1	5.46	123.03	120.30
2	H	191	ARG	CA-CB-CG	5.40	125.27	113.40
1	L	35	TRP	CG-CD1-NE1	-5.36	104.74	110.10
2	H	94	TYR	CB-CA-C	-5.31	99.78	110.40
2	H	68	SER	N-CA-CB	-5.28	102.58	110.50
1	L	148	TRP	CG-CD1-NE1	-5.25	104.85	110.10
3	Y	68	ARG	CA-CB-CG	5.25	124.96	113.40
3	Y	21	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	L	155	ARG	NE-CZ-NH1	5.17	122.89	120.30
2	H	176	ASP	CB-CA-C	-5.16	100.07	110.40
3	Y	62	TRP	CG-CD1-NE1	-5.16	104.94	110.10
3	Y	23	TYR	CB-CG-CD1	-5.13	117.92	121.00
3	Y	111	TRP	CG-CD1-NE1	-5.10	105.00	110.10
2	H	6	GLU	CA-CB-CG	5.09	124.59	113.40
1	L	32	TYR	CG-CD2-CE2	-5.07	117.25	121.30
2	H	115	SER	CA-C-N	-5.06	106.08	117.20
2	H	104	ASP	CB-CG-OD2	-5.05	113.75	118.30
2	H	38	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	L	194	CYS	N-CA-C	-5.01	97.48	111.00

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	L	1665	0	1583	20	0
2	H	1643	0	1611	24	0
3	Y	1001	0	959	15	0
All	All	4309	0	4153	56	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 7.

All (56) 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)
2:H:191:ARG:HG2	2:H:191:ARG:HH11	1.31	0.94
2:H:191:ARG:HG2	2:H:191:ARG:NH1	1.97	0.75
1:L:61:ARG:HB2	1:L:76:ASN:O	1.95	0.67
1:L:144:ILE:HG13	1:L:198:HIS:HB2	1.78	0.66
1:L:155:ARG:HH11	1:L:179:LEU:HD11	1.62	0.63
2:H:130:GLY:HA2	2:H:216:ARG:HD2	1.82	0.62
2:H:117:ALA:HB2	2:H:176:ASP:HB3	1.86	0.56
3:Y:15:HIS:HB3	3:Y:92:VAL:HG11	1.87	0.56
1:L:32:TYR:HB3	1:L:91:PHE:HB2	1.87	0.56
2:H:139:VAL:HG23	2:H:186:VAL:HG23	1.86	0.55
1:L:96:ARG:NH1	2:H:50:MET:SD	2.80	0.54
2:H:35:ASN:HD22	2:H:35:ASN:N	2.06	0.54
1:L:147:LYS:HG2	1:L:195:GLU:HB3	1.88	0.54
1:L:124:GLN:HG3	2:H:125:PHE:CE1	2.47	0.50
1:L:150:ILE:HD11	1:L:179:LEU:HD21	1.93	0.50
3:Y:19:ASN:OD1	3:Y:22:GLY:HA2	2.13	0.49
1:L:150:ILE:HD12	1:L:155:ARG:HD2	1.95	0.48
3:Y:33:LYS:HB2	3:Y:38:PHE:CE2	2.49	0.48
1:L:85:SER:HA	1:L:102:THR:O	2.13	0.48
1:L:149:LYS:HG2	1:L:154:GLU:HA	1.96	0.48
1:L:51:THR:HG23	1:L:71:TYR:HD2	1.79	0.47
2:H:155:VAL:HG11	2:H:182:SER:OG	2.14	0.47
2:H:18:LEU:O	2:H:81:LYS:HA	2.14	0.47
2:H:198:CYS:O	2:H:210:ASP:HA	2.14	0.47
2:H:138:MET:HA	2:H:187:PRO:HA	1.96	0.47
2:H:180:LEU:HD23	2:H:181:SER:N	2.30	0.47
3:Y:13:LYS:HD3	3:Y:129:LEU:HD22	1.98	0.46
3:Y:62:TRP:HB2	3:Y:63:TRP:CD1	2.49	0.46
3:Y:94:CYS:O	3:Y:98:ILE:HG13	2.16	0.46
3:Y:71:GLY:O	3:Y:73:ARG:HD2	2.16	0.46
3:Y:33:LYS:HB2	3:Y:38:PHE:CZ	2.51	0.46
2:H:97:ARG:O	2:H:103:LEU:HA	2.16	0.45
1:L:125:LEU:O	1:L:183:LYS:HD3	2.15	0.45
3:Y:69:THR:HA	3:Y:70:PRO:HD3	1.76	0.45
2:H:67:LEU:CD2	2:H:80:LEU:HD11	2.47	0.45
2:H:140:THR:HA	2:H:184:VAL:O	2.18	0.44
2:H:126:PRO:HD3	2:H:211:LYS:HD2	1.99	0.44
3:Y:60:SER:HA	3:Y:64:CYS:SG	2.57	0.44
2:H:32:TYR:HE2	2:H:99:ARG:HG3	1.83	0.44
1:L:22:THR:HG23	1:L:70:GLN:NE2	2.32	0.44
2:H:149:PHE:HB2	2:H:177:LEU:HD23	2.00	0.44
2:H:67:LEU:HD22	2:H:80:LEU:HD11	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:85:LEU:HD23	2:H:89:ASP:OD1	2.18	0.43
3:Y:106:ASN:HD22	3:Y:106:ASN:H	1.64	0.43
3:Y:78:ILE:HA	3:Y:78:ILE:HD12	1.87	0.43
3:Y:78:ILE:HA	3:Y:79:PRO:HD2	1.79	0.42
1:L:58:VAL:HA	1:L:59:PRO:HD3	1.79	0.42
3:Y:5:ARG:NH1	3:Y:127:CYS:SG	2.92	0.42
1:L:33:LEU:HD22	1:L:71:TYR:CB	2.51	0.41
2:H:4:LEU:HG	2:H:24:VAL:HG12	2.01	0.41
1:L:52:THR:HG22	1:L:64:GLY:O	2.20	0.41
3:Y:58:ILE:HB	3:Y:83:LEU:HD13	2.02	0.41
1:L:49:TYR:CG	2:H:102:ARG:HD2	2.56	0.41
2:H:153:VAL:HG23	2:H:202:HIS:HD2	1.86	0.40
1:L:117:ILE:HG22	1:L:207:LYS:HG3	2.03	0.40
1:L:128:GLY:HA2	1:L:183:LYS:HB2	2.02	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	L	212/214 (99%)	199 (94%)	11 (5%)	2 (1%)	20	36
2	H	216/218 (99%)	201 (93%)	13 (6%)	2 (1%)	20	36
3	Y	127/129 (98%)	115 (91%)	12 (9%)	0	100	100
All	All	555/561 (99%)	515 (93%)	36 (6%)	4 (1%)	25	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	170	ASP
1	L	199	LYS
2	H	133	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	137	SER

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	L	189/189 (100%)	168 (89%)	21 (11%)	7	13
2	H	190/190 (100%)	169 (89%)	21 (11%)	7	13
3	Y	105/105 (100%)	103 (98%)	2 (2%)	62	85
All	All	484/484 (100%)	440 (91%)	44 (9%)	11	21

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	43	SER
1	L	45	GLN
1	L	70	GLN
1	L	95	PRO
1	L	105	GLU
1	L	110	ASP
1	L	125	LEU
1	L	147	LYS
1	L	154	GLU
1	L	160	LEU
1	L	170	ASP
1	L	172	THR
1	L	177	SER
1	L	190	ASN
1	L	193	THR
1	L	197	THR
1	L	202	THR
1	L	207	LYS
1	L	208	SER
1	L	209	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	7	SER
2	H	9	PRO
2	H	12	VAL
2	H	16	GLN
2	H	35	ASN
2	H	43	LYS
2	H	46	GLU
2	H	65	SER
2	H	68	SER
2	H	75	LYS
2	H	102	ARG
2	H	134	GLN
2	H	135	THR
2	H	152	PRO
2	H	153	VAL
2	H	175	SER
2	H	190	PRO
2	H	191	ARG
2	H	193	SER
2	H	195	THR
2	H	217	ASP
3	Y	91	SER
3	Y	99	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	30	HIS
1	L	70	GLN
1	L	76	ASN
1	L	89	GLN
1	L	90	HIS
1	L	189	HIS
3	Y	46	ASN
3	Y	106	ASN

5.3.3 RNA ⓘ

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.