Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2024 – 01:11 PM EDT

PDB ID	:	2IFF
Title	:	STRUCTURE OF AN ANTIBODY-LYSOZYME COMPLEX: EFFECT OF A CONSERVATIVE MUTATION
Authors	:	Chacko, S.; Davies, D.R.
Deposited on	:	1994-02-03
Resolution	:	2.65 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:

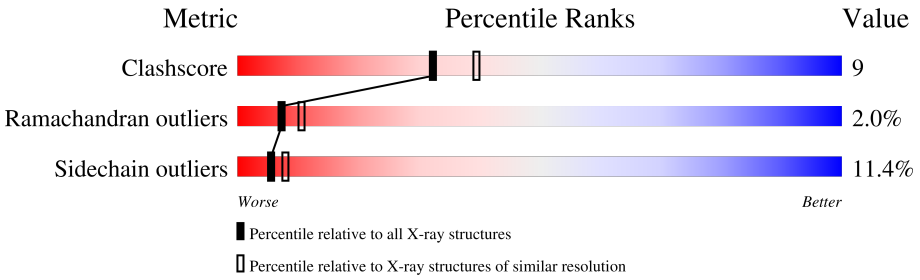
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.65 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	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)

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	L	212	67% 27% 5%
2	H	215	68% 28% .
3	Y	129	72% 23% . .

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4325 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 HYHEL-5 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	212	Total	C	N	O	S	0	0	0
			1635	1014	273	338	10			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	18	LYS	ARG	conflict	GB 1042224
L	26	SER	ASN	conflict	GB 1042224
L	30	ASN	SER	conflict	GB 1042224
L	33	TYR	HIS	conflict	GB 1042224
L	59	VAL	ALA	conflict	GB 1042224
L	79	THR	ALA	conflict	GB 1042224
L	91	GLY	SER	conflict	GB 1042224
L	92	ARG	SER	conflict	GB 1042224
L	93	ASN	HIS	conflict	GB 1042224
L	?	-	TYR	deletion	GB 1042224
L	111	PRO	GLN	conflict	GB 1042224

- Molecule 2 is a protein called IGG1 HYHEL-5 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total	C	N	O	S	0	0	0
			1607	1015	263	322	7			

- 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	1	0
			1003	616	192	185	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	68	LYS	ARG	conflict	UNP P00698

- Molecule 4 is water.

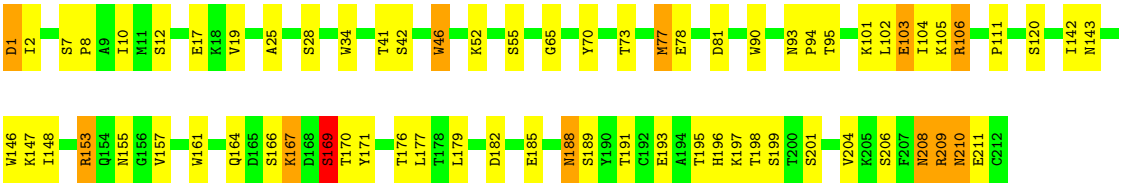
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	30	Total O 30 30	0	0
4	H	30	Total O 30 30	0	0
4	Y	20	Total O 20 20	0	0

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.

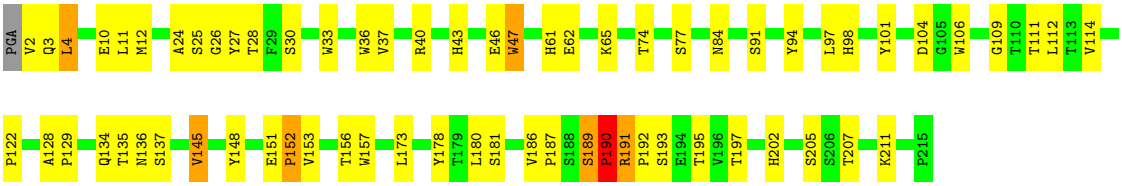
- Molecule 1: IGG1 HYHEL-5 FAB (LIGHT CHAIN)

Chain L:



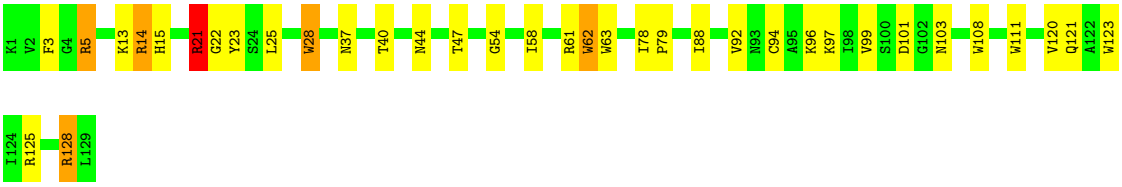
- Molecule 2: IGG1 HYHEL-5 FAB (HEAVY CHAIN)

Chain H:



- Molecule 3: HEN EGG WHITE LYSOZYME

Chain Y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.80Å 74.80Å 79.00Å 90.00° 101.80° 90.00°	Depositor
Resolution (Å)	10.00 – 2.65 43.59 – 2.58	Depositor EDS
% Data completeness (in resolution range)	69.2 (10.00-2.65) 65.0 (43.59-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.66 (at 2.58Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	(Not available) , (Not available) 0.160 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	25.4	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 107.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4325	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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	L	0.73	0/1673	1.45	23/2270 (1.0%)
2	H	0.75	0/1652	1.44	17/2257 (0.8%)
3	Y	0.74	0/1028	1.65	32/1387 (2.3%)
All	All	0.74	0/4353	1.49	72/5914 (1.2%)

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	L	0	1
2	H	0	1
All	All	0	2

There are no bond length outliers.

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	108	TRP	CD1-CG-CD2	9.15	113.62	106.30
2	H	190	PRO	O-C-N	-9.13	108.09	122.70
3	Y	62	TRP	CD1-CG-CD2	8.96	113.47	106.30
1	L	146	TRP	CD1-CG-CD2	8.95	113.46	106.30
3	Y	28	TRP	CD1-CG-CD2	8.87	113.40	106.30
1	L	161	TRP	CD1-CG-CD2	8.83	113.37	106.30
1	L	46	TRP	CD1-CG-CD2	8.77	113.32	106.30
2	H	33	TRP	CD1-CG-CD2	8.77	113.31	106.30
2	H	157	TRP	CD1-CG-CD2	8.64	113.21	106.30
1	L	90	TRP	CD1-CG-CD2	8.63	113.21	106.30
3	Y	123	TRP	CD1-CG-CD2	8.62	113.20	106.30
3	Y	63	TRP	CD1-CG-CD2	8.12	112.79	106.30
1	L	46	TRP	CE2-CD2-CG	-8.04	100.87	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	47	TRP	CD1-CG-CD2	7.97	112.67	106.30
1	L	161	TRP	CE2-CD2-CG	-7.91	100.97	107.30
3	Y	62	TRP	CE2-CD2-CG	-7.88	100.99	107.30
2	H	190	PRO	CA-C-N	7.87	134.52	117.20
3	Y	108	TRP	CE2-CD2-CG	-7.85	101.02	107.30
3	Y	28	TRP	CE2-CD2-CG	-7.75	101.10	107.30
1	L	146	TRP	CE2-CD2-CG	-7.67	101.17	107.30
3	Y	123	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	L	34	TRP	CD1-CG-CD2	7.62	112.40	106.30
3	Y	111	TRP	CD1-CG-CD2	7.62	112.40	106.30
2	H	33	TRP	CE2-CD2-CG	-7.62	101.21	107.30
3	Y	63	TRP	CE2-CD2-CG	-7.59	101.23	107.30
2	H	36	TRP	CD1-CG-CD2	7.57	112.36	106.30
2	H	106	TRP	CD1-CG-CD2	7.55	112.34	106.30
2	H	36	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	L	90	TRP	CE2-CD2-CG	-7.37	101.41	107.30
3	Y	125	ARG	NE-CZ-NH1	7.36	123.98	120.30
3	Y	111	TRP	CE2-CD2-CG	-7.31	101.45	107.30
2	H	47	TRP	CE2-CD2-CG	-7.28	101.47	107.30
2	H	157	TRP	CE2-CD2-CG	-7.28	101.48	107.30
1	L	34	TRP	CE2-CD2-CG	-7.00	101.70	107.30
3	Y	125	ARG	NE-CZ-NH2	-6.85	116.88	120.30
2	H	106	TRP	CE2-CD2-CG	-6.78	101.88	107.30
1	L	209	ARG	NE-CZ-NH2	6.77	123.68	120.30
1	L	46	TRP	CG-CD2-CE3	5.97	139.28	133.90
3	Y	5	ARG	NE-CZ-NH1	5.91	123.25	120.30
3	Y	21	ARG	NE-CZ-NH1	5.90	123.25	120.30
3	Y	108	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	L	161	TRP	CB-CG-CD1	-5.77	119.50	127.00
3	Y	108	TRP	CB-CG-CD1	-5.69	119.60	127.00
3	Y	108	TRP	CG-CD2-CE3	5.64	138.97	133.90
3	Y	111	TRP	CG-CD2-CE3	5.58	138.92	133.90
2	H	101	TYR	CB-CG-CD2	-5.54	117.67	121.00
2	H	36	TRP	CG-CD2-CE3	5.49	138.84	133.90
2	H	37	VAL	CG1-CB-CG2	-5.48	102.14	110.90
1	L	169	SER	O-C-N	-5.44	113.99	122.70
1	L	146	TRP	CG-CD1-NE1	-5.44	104.66	110.10
3	Y	111	TRP	CB-CG-CD1	-5.42	119.96	127.00
1	L	171	TYR	CB-CG-CD1	-5.41	117.76	121.00
3	Y	14	ARG	NE-CZ-NH2	-5.38	117.61	120.30
3	Y	23	TYR	CB-CG-CD1	-5.36	117.78	121.00
3	Y	5	ARG	NE-CZ-NH2	-5.36	117.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	28	TRP	CG-CD1-NE1	-5.36	104.74	110.10
1	L	199	SER	CA-C-N	-5.34	105.46	117.20
3	Y	62	TRP	CB-CG-CD1	-5.32	120.08	127.00
3	Y	62	TRP	CG-CD1-NE1	-5.32	104.78	110.10
3	Y	14	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	H	33	TRP	CG-CD1-NE1	-5.29	104.81	110.10
1	L	46	TRP	CG-CD1-NE1	-5.29	104.81	110.10
3	Y	123	TRP	CG-CD1-NE1	-5.29	104.81	110.10
2	H	157	TRP	CG-CD1-NE1	-5.28	104.83	110.10
1	L	161	TRP	CG-CD1-NE1	-5.18	104.92	110.10
3	Y	3	PHE	N-CA-C	5.12	124.83	111.00
1	L	46	TRP	CB-CG-CD1	-5.11	120.35	127.00
1	L	161	TRP	CG-CD2-CE3	5.11	138.49	133.90
1	L	153	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	L	90	TRP	CG-CD1-NE1	-5.03	105.07	110.10
3	Y	28	TRP	CB-CG-CD1	-5.03	120.46	127.00
3	Y	128	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	4	LEU	Mainchain
1	L	169	SER	Mainchain

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	L	1635	0	1557	29	0
2	H	1607	0	1547	36	0
3	Y	1003	0	968	10	0
4	H	30	0	0	2	0
4	L	30	0	0	0	0
4	Y	20	0	0	0	0
All	All	4325	0	4072	73	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 9.

All (73) 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:26:GLY:HA3	4:H:793:HOH:O	1.49	1.10
2:H:187:PRO:O	2:H:190:PRO:HD2	1.79	0.81
1:L:143:ASN:HB3	1:L:195:THR:HB	1.62	0.81
2:H:122:PRO:HB3	2:H:148:TYR:HB3	1.69	0.73
1:L:142:ILE:HD12	1:L:196:HIS:HB2	1.78	0.66
1:L:1:ASP:HB2	1:L:2:ILE:HD12	1.79	0.65
2:H:10:GLU:HB2	2:H:112:LEU:HD12	1.78	0.64
2:H:191:ARG:HH11	2:H:191:ARG:HB3	1.63	0.64
2:H:186:VAL:HB	2:H:190:PRO:HG2	1.83	0.61
2:H:189:SER:H	2:H:190:PRO:HD2	1.66	0.60
1:L:10:ILE:HG23	1:L:101:LYS:HB3	1.84	0.58
2:H:2:VAL:N	2:H:25:SER:HG	2.02	0.58
2:H:151:GLU:HG2	2:H:152:PRO:HA	1.84	0.58
2:H:2:VAL:HG12	2:H:3:GLN:H	1.68	0.57
3:Y:120:VAL:HG23	3:Y:121:GLN:HE21	1.71	0.56
1:L:167:LYS:HD2	1:L:167:LYS:H	1.71	0.54
1:L:17:GLU:O	1:L:77:MET:HB2	2.08	0.54
1:L:52:LYS:N	1:L:52:LYS:HD2	2.24	0.53
3:Y:13:LYS:HB2	3:Y:25:LEU:HD11	1.91	0.53
3:Y:92:VAL:O	3:Y:96:LYS:HG2	2.09	0.52
1:L:94:PRO:HD2	2:H:47:TRP:CE3	2.44	0.52
1:L:147:LYS:HB2	1:L:191:THR:HB	1.92	0.52
2:H:94:TYR:O	2:H:109:GLY:HA2	2.11	0.51
1:L:93:ASN:HB2	2:H:61:HIS:CD2	2.46	0.51
3:Y:58:ILE:HD13	3:Y:94:CYS:SG	2.51	0.50
1:L:2:ILE:HG21	1:L:25:ALA:HB1	1.94	0.50
1:L:12:SER:HA	1:L:103:GLU:O	2.11	0.50
1:L:164:GLN:CD	1:L:169:SER:HB3	2.32	0.50
1:L:164:GLN:NE2	1:L:169:SER:HB3	2.27	0.49
3:Y:40:THR:O	3:Y:54:GLY:HA2	2.13	0.49
2:H:2:VAL:HA	2:H:25:SER:O	2.13	0.49
1:L:189:SER:HA	1:L:208:ASN:HA	1.94	0.48
2:H:4:LEU:HD21	2:H:98:HIS:CD2	2.49	0.48
1:L:182:ASP:HA	1:L:185:GLU:HG2	1.95	0.47
3:Y:15:HIS:HB3	3:Y:92:VAL:HG11	1.96	0.47
2:H:191:ARG:HB3	2:H:191:ARG:NH1	2.29	0.47
2:H:62:GLU:O	2:H:65:LYS:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:65:GLY:HA3	1:L:70:TYR:HA	1.96	0.47
1:L:81:ASP:O	1:L:102:LEU:HD23	2.15	0.47
2:H:191:ARG:HD2	2:H:192:PRO:HA	1.97	0.46
3:Y:28:TRP:HH2	3:Y:99:VAL:HG21	1.80	0.46
2:H:27:TYR:OH	2:H:98:HIS:HE1	1.99	0.45
2:H:205:SER:HB2	2:H:207:THR:OG1	2.16	0.45
2:H:24:ALA:O	2:H:77:SER:HB3	2.18	0.44
1:L:148:ILE:HD11	1:L:177:LEU:HD21	2.00	0.44
2:H:148:TYR:HE2	2:H:151:GLU:HG3	1.82	0.44
1:L:12:SER:HB3	1:L:105:LYS:HB3	1.99	0.43
2:H:40:ARG:HB3	2:H:43:HIS:HB3	2.00	0.43
2:H:12:MET:O	2:H:114:VAL:HA	2.18	0.43
3:Y:21:ARG:HD3	3:Y:99:VAL:HG12	2.00	0.43
2:H:197:THR:HA	2:H:211:LYS:O	2.19	0.43
3:Y:58:ILE:HG21	3:Y:94:CYS:SG	2.58	0.43
2:H:26:GLY:CA	4:H:793:HOH:O	2.31	0.43
2:H:173:LEU:HD13	2:H:178:TYR:CE1	2.54	0.43
2:H:145:VAL:HG22	2:H:180:LEU:HB3	2.00	0.42
1:L:193:GLU:HG3	1:L:204:VAL:HG12	2.01	0.42
1:L:93:ASN:HA	1:L:94:PRO:HD3	1.76	0.42
2:H:202:HIS:HB3	2:H:207:THR:HB	2.01	0.42
1:L:19:VAL:O	1:L:73:THR:HA	2.20	0.42
2:H:122:PRO:HD2	2:H:207:THR:HG21	2.02	0.42
2:H:91:SER:HA	2:H:112:LEU:O	2.20	0.41
2:H:27:TYR:OH	2:H:98:HIS:CE1	2.73	0.41
1:L:106:ARG:HG2	1:L:169:SER:HB2	2.02	0.41
1:L:188:ASN:HA	1:L:210:ASN:OD1	2.19	0.41
1:L:188:ASN:O	1:L:208:ASN:HA	2.21	0.41
2:H:129:PRO:HD2	2:H:191:ARG:NH2	2.36	0.41
2:H:187:PRO:HG2	2:H:190:PRO:CD	2.50	0.41
2:H:189:SER:H	2:H:190:PRO:CD	2.33	0.41
1:L:111:PRO:HD3	1:L:196:HIS:CD2	2.56	0.40
1:L:157:VAL:HA	1:L:176:THR:O	2.20	0.40
2:H:128:ALA:HB1	2:H:191:ARG:HH21	1.84	0.40
1:L:7:SER:HA	1:L:8:PRO:HA	1.89	0.40
3:Y:78:ILE:HD12	3:Y:79:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

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	L	210/212 (99%)	187 (89%)	19 (9%)	4 (2%)	8 11
2	H	212/215 (99%)	190 (90%)	18 (8%)	4 (2%)	8 11
3	Y	128/129 (99%)	116 (91%)	9 (7%)	3 (2%)	6 8
All	All	550/556 (99%)	493 (90%)	46 (8%)	11 (2%)	7 10

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	55	SER
1	L	197	LYS
2	H	189	SER
2	H	136	ASN
3	Y	22	GLY
2	H	134	GLN
2	H	190	PRO
1	L	188	ASN
1	L	209	ARG
3	Y	5	ARG
3	Y	88	ILE

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	187/187 (100%)	163 (87%)	24 (13%)	4 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	182/182 (100%)	163 (90%)	19 (10%)	7 10
3	Y	106/105 (101%)	95 (90%)	11 (10%)	7 10
All	All	475/474 (100%)	421 (89%)	54 (11%)	5 8

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

Mol	Chain	Res	Type
1	L	1	ASP
1	L	28	SER
1	L	41	THR
1	L	42	SER
1	L	46	TRP
1	L	77	MET
1	L	78	GLU
1	L	95	THR
1	L	103	GLU
1	L	104	ILE
1	L	106	ARG
1	L	120	SER
1	L	153	ARG
1	L	155	ASN
1	L	166	SER
1	L	167	LYS
1	L	170	THR
1	L	179	LEU
1	L	198	THR
1	L	201	SER
1	L	206	SER
1	L	208	ASN
1	L	210	ASN
1	L	211	GLU
2	H	11	LEU
2	H	28	THR
2	H	30	SER
2	H	46	GLU
2	H	74	THR
2	H	84	ASN
2	H	97	LEU
2	H	104	ASP
2	H	111	THR
2	H	135	THR

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Mol	Chain	Res	Type
2	H	137	SER
2	H	145	VAL
2	H	152	PRO
2	H	153	VAL
2	H	156	THR
2	H	181	SER
2	H	191	ARG
2	H	193	SER
2	H	195	THR
3	Y	14	ARG
3	Y	21	ARG
3	Y	37	ASN
3	Y	44	ASN
3	Y	47	THR
3	Y	61	ARG
3	Y	62	TRP
3	Y	97	LYS
3	Y	101	ASP
3	Y	103	ASN
3	Y	128	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	155	ASN
2	H	98	HIS
3	Y	27	ASN
3	Y	121	GLN

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 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.