



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:33 PM UTC

PDB ID : 1BQL / pdb_00001bql
Title : STRUCTURE OF AN ANTI-HEL FAB FRAGMENT COMPLEXED WITH
BOBWHITE QUAIL LYSOZYME
Authors : Chacko, S.; Davies, D.R.
Deposited on : 1995-02-03
Resolution : 2.60 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

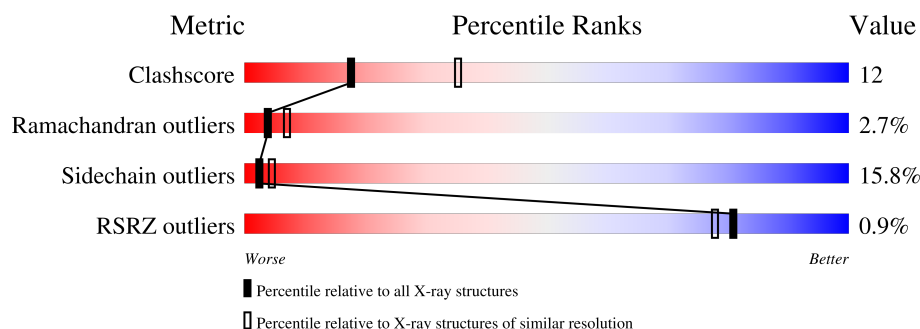
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	L	212	44% 41% 14% .
2	H	215	51% 39% 9%
3	Y	129	53% 36% 9% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4326 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 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 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 BOBWHITE QUAIL LYSOZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	129	Total	C	N	O	S	0	0	0
			998	612	191	185	10			

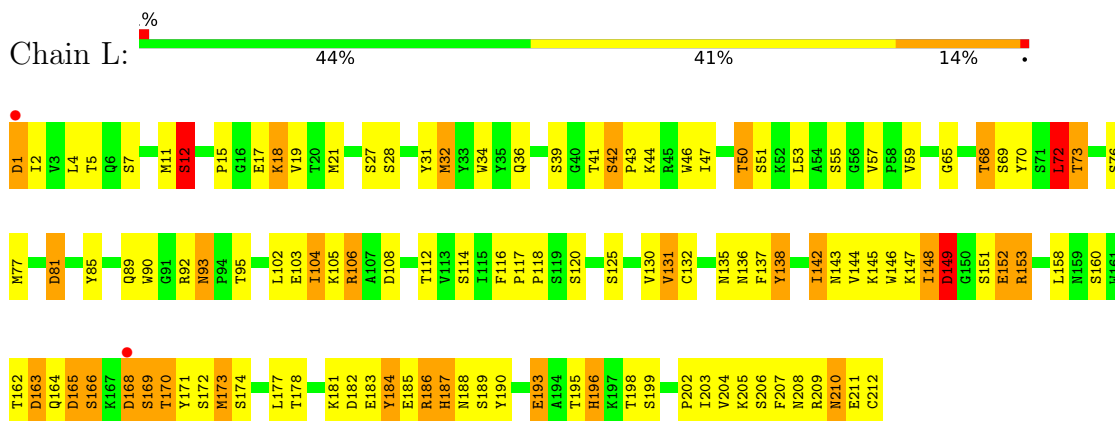
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	28	Total 28	O 28	0	0
4	H	38	Total 38	O 38	0	0
4	Y	20	Total 20	O 20	0	0

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 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.

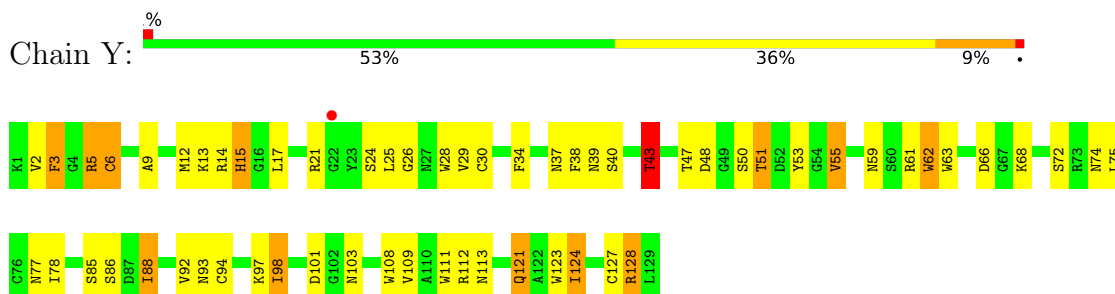
• Molecule 1: HYHEL-5 FAB (LIGHT CHAIN)



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



• Molecule 3: BOBWHITE QUAIL LYSOZYME



4 Data and refinement statistics

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)	8.00 – 2.60 8.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	55.0 (8.00-2.60) 81.1 (8.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.58Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.191 , 0.291 0.198 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 74.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4326	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1.07	3/1673 (0.2%)	2.09	62/2270 (2.7%)
2	H	1.16	9/1652 (0.5%)	2.03	52/2257 (2.3%)
3	Y	1.03	2/1018 (0.2%)	2.15	51/1375 (3.7%)
All	All	1.10	14/4343 (0.3%)	2.08	165/5902 (2.8%)

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	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	142	ILE	CA-CB	8.67	1.66	1.54
1	L	196	HIS	CD2-NE2	-7.98	1.29	1.37
2	H	98	HIS	CD2-NE2	-7.17	1.29	1.37
1	L	187	HIS	CD2-NE2	-7.11	1.30	1.37
2	H	202	HIS	CD2-NE2	-6.92	1.30	1.37
2	H	167	HIS	CD2-NE2	-6.79	1.30	1.37
2	H	145	VAL	CA-CB	6.37	1.61	1.54
2	H	61	HIS	CD2-NE2	-6.33	1.30	1.37
3	Y	15	HIS	CD2-NE2	-6.19	1.31	1.37
2	H	202	HIS	CG-ND1	-5.86	1.31	1.38
2	H	43	HIS	CD2-NE2	-5.62	1.31	1.37
2	H	186	VAL	CA-CB	5.51	1.61	1.55
3	Y	15	HIS	CG-ND1	-5.41	1.32	1.38
2	H	167	HIS	CG-ND1	-5.29	1.32	1.38

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	3	PHE	N-CA-C	11.31	123.18	111.07
1	L	169	SER	N-CA-CB	-10.34	95.41	111.23
2	H	135	THR	N-CA-C	-10.06	99.12	111.40
2	H	61	HIS	CB-CG-CD2	-9.97	118.23	131.20
1	L	210	ASN	OD1-CG-ND2	-9.83	112.77	122.60
1	L	196	HIS	CB-CG-CD2	-9.47	118.88	131.20
1	L	1	ASP	CA-CB-CG	8.76	121.36	112.60
2	H	134	GLN	CA-C-O	8.76	130.26	120.80
1	L	169	SER	N-CA-C	8.43	122.40	108.49
1	L	196	HIS	CB-CG-ND1	8.38	135.27	122.70
2	H	158	ASN	CA-CB-CG	-8.30	104.30	112.60
3	Y	6	CYS	CA-C-O	-8.12	111.86	120.63
2	H	90	ASP	CA-CB-CG	8.03	120.63	112.60
2	H	36	TRP	CG-CD2-CE3	7.95	141.85	133.90
1	L	138	TYR	O-C-N	-7.82	115.08	121.80
2	H	3	GLN	OE1-CD-NE2	-7.77	114.83	122.60
3	Y	2	VAL	N-CA-C	-7.70	96.75	107.99
3	Y	113	ASN	OD1-CG-ND2	-7.64	114.96	122.60
3	Y	98	ILE	N-CA-C	-7.51	104.46	111.45
2	H	98	HIS	CA-CB-CG	-7.42	106.38	113.80
3	Y	55	VAL	CB-CA-C	-7.38	102.18	112.14
1	L	136	ASN	N-CA-C	7.35	126.46	110.80
3	Y	66	ASP	CA-CB-CG	7.32	119.92	112.60
2	H	61	HIS	CB-CG-ND1	7.28	133.62	122.70
2	H	31	ASP	N-CA-C	7.25	122.12	113.28
1	L	165	ASP	CA-CB-CG	7.13	119.73	112.60
3	Y	78	ILE	CB-CA-C	7.12	116.31	109.33
3	Y	63	TRP	N-CA-C	7.06	121.94	113.12
1	L	199	SER	CA-C-O	7.05	129.72	120.21
2	H	36	TRP	CB-CG-CD1	-7.01	116.38	126.90
1	L	89	GLN	N-CA-C	-6.95	97.92	108.96
1	L	148	ILE	N-CA-C	-6.94	99.73	108.89
1	L	93	ASN	CA-C-N	6.89	126.93	119.90
1	L	93	ASN	C-N-CA	6.89	126.93	119.90
1	L	203	ILE	N-CA-C	-6.87	99.83	108.89
2	H	167	HIS	CB-CG-CD2	-6.82	122.33	131.20
1	L	174	SER	CA-CB-OG	6.79	124.67	111.10
1	L	93	ASN	CA-CB-CG	6.73	119.33	112.60
1	L	89	GLN	CB-CG-CD	6.62	123.86	112.60
1	L	187	HIS	CB-CG-CD2	-6.61	122.61	131.20
1	L	168	ASP	CA-C-N	-6.59	114.20	123.03
1	L	168	ASP	C-N-CA	-6.59	114.20	123.03
2	H	98	HIS	CB-CG-CD2	-6.59	122.64	131.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	136	ASN	OD1-CG-ND2	-6.51	116.09	122.60
3	Y	21	ARG	N-CA-C	-6.48	97.13	108.08
1	L	209	ARG	N-CA-C	6.41	120.03	107.98
2	H	117	ALA	N-CA-CB	-6.40	101.61	110.38
1	L	173	MET	CG-SD-CE	-6.39	86.84	100.90
3	Y	128	ARG	N-CA-C	-6.39	101.03	110.48
2	H	149	PHE	CA-CB-CG	-6.37	107.43	113.80
1	L	17	GLU	N-CA-C	6.33	119.88	110.52
3	Y	123	TRP	CA-CB-CG	-6.28	101.66	113.60
2	H	197	THR	CA-C-O	-6.24	113.96	120.70
2	H	186	VAL	O-C-N	-6.23	116.03	121.57
3	Y	93	ASN	OD1-CG-ND2	-6.23	116.37	122.60
1	L	12	SER	CA-CB-OG	6.16	123.43	111.10
3	Y	28	TRP	CG-CD2-CE3	6.15	140.05	133.90
1	L	125	SER	N-CA-C	-6.12	104.89	112.90
3	Y	111	TRP	CG-CD2-CE3	6.11	140.01	133.90
1	L	108	ASP	CA-CB-CG	6.10	118.70	112.60
1	L	89	GLN	OE1-CD-NE2	-6.10	116.50	122.60
1	L	142	ILE	N-CA-CB	-6.10	101.17	111.23
2	H	104	ASP	CA-CB-CG	6.02	118.62	112.60
1	L	186	ARG	N-CA-C	-5.98	105.56	112.92
3	Y	78	ILE	N-CA-CB	-5.97	105.25	111.64
1	L	174	SER	N-CA-C	-5.94	99.32	109.24
2	H	45	LEU	N-CA-C	5.93	119.57	110.20
3	Y	74	ASN	OD1-CG-ND2	-5.92	116.68	122.60
3	Y	112	ARG	N-CA-C	-5.90	104.77	111.14
2	H	174	GLN	N-CA-C	-5.89	98.24	110.80
3	Y	111	TRP	CB-CG-CD1	-5.89	118.06	126.90
3	Y	62	TRP	CE2-CD2-CG	-5.88	100.14	107.20
1	L	72	LEU	N-CA-C	-5.84	99.38	108.90
3	Y	103	ASN	CA-C-O	5.84	125.73	118.43
1	L	208	ASN	OD1-CG-ND2	-5.82	116.78	122.60
3	Y	123	TRP	N-CA-C	5.82	119.85	112.87
3	Y	75	LEU	N-CA-C	5.81	119.47	112.38
1	L	165	ASP	CA-C-N	5.79	132.59	121.54
1	L	165	ASP	C-N-CA	5.79	132.59	121.54
2	H	194	GLU	N-CA-C	-5.74	100.53	109.72
2	H	23	LYS	O-C-N	5.74	129.89	122.43
1	L	193	GLU	CA-CB-CG	5.72	125.54	114.10
2	H	167	HIS	CB-CG-ND1	5.70	131.26	122.70
2	H	128	ALA	CA-C-N	5.67	125.03	118.85
2	H	128	ALA	C-N-CA	5.67	125.03	118.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	68	THR	N-CA-CB	-5.63	100.94	110.51
3	Y	50	SER	CA-CB-OG	5.63	122.36	111.10
3	Y	63	TRP	CG-CD2-CE3	5.63	139.53	133.90
1	L	76	SER	O-C-N	-5.61	116.68	123.13
3	Y	111	TRP	CE2-CD2-CG	-5.61	100.47	107.20
3	Y	21	ARG	CB-CG-CD	5.60	124.19	111.30
3	Y	55	VAL	N-CA-CB	5.59	118.14	110.54
1	L	81	ASP	CA-CB-CG	5.57	118.17	112.60
2	H	33	TRP	CE2-CD2-CG	-5.57	100.52	107.20
3	Y	34	PHE	CA-CB-CG	-5.57	108.23	113.80
2	H	129	PRO	N-CA-C	5.56	120.85	113.40
1	L	178	THR	CA-C-O	5.56	126.43	120.32
1	L	142	ILE	CB-CA-C	5.53	120.36	111.29
2	H	157	TRP	CE2-CD2-CG	-5.53	100.57	107.20
3	Y	51	THR	N-CA-CB	-5.51	102.36	110.85
3	Y	88	ILE	N-CA-C	5.50	120.79	109.34
3	Y	108	TRP	CG-CD2-CE3	5.49	139.39	133.90
1	L	184	TYR	CA-C-O	-5.46	115.27	121.00
2	H	20	ILE	CA-C-O	-5.45	114.74	120.57
1	L	46	TRP	CA-C-N	-5.42	116.46	123.19
1	L	46	TRP	C-N-CA	-5.42	116.46	123.19
3	Y	108	TRP	CE2-CD2-CG	-5.42	100.70	107.20
3	Y	112	ARG	CA-CB-CG	5.42	124.93	114.10
2	H	155	VAL	N-CA-C	-5.41	102.09	109.55
2	H	39	GLN	CA-C-O	5.40	126.08	120.30
3	Y	63	TRP	CE2-CD2-CG	-5.40	100.72	107.20
3	Y	48	ASP	CA-CB-CG	5.38	117.98	112.60
2	H	69	THR	O-C-N	-5.38	116.82	123.33
1	L	46	TRP	CG-CD2-CE3	5.36	139.26	133.90
2	H	204	ALA	N-CA-C	5.35	119.30	112.87
3	Y	53	TYR	N-CA-C	5.35	117.63	108.90
2	H	6	GLN	OE1-CD-NE2	-5.33	117.27	122.60
1	L	181	LYS	N-CA-C	5.32	117.08	111.28
1	L	187	HIS	CB-CG-ND1	5.32	130.68	122.70
2	H	3	GLN	CA-CB-CG	5.31	124.73	114.10
1	L	153	ARG	NE-CZ-NH2	5.29	123.96	119.20
3	Y	63	TRP	CG-CD1-NE1	-5.29	103.33	110.20
1	L	92	ARG	CA-C-N	-5.28	115.56	122.74
1	L	92	ARG	C-N-CA	-5.28	115.56	122.74
3	Y	121	GLN	OE1-CD-NE2	-5.27	117.33	122.60
3	Y	128	ARG	CA-C-N	5.26	131.17	121.70
3	Y	128	ARG	C-N-CA	5.26	131.17	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	40	ARG	N-CA-C	-5.25	99.08	109.10
2	H	120	THR	CA-C-N	5.23	123.42	119.66
2	H	120	THR	C-N-CA	5.23	123.42	119.66
1	L	211	GLU	CB-CG-CD	5.22	121.47	112.60
2	H	69	THR	CA-CB-OG1	-5.21	101.78	109.60
1	L	149	ASP	CA-C-N	-5.21	105.32	120.36
1	L	149	ASP	C-N-CA	-5.21	105.32	120.36
2	H	118	LYS	CA-CB-CG	5.19	124.48	114.10
1	L	18	LYS	N-CA-C	5.15	118.01	109.46
1	L	202	PRO	N-CA-CB	5.15	107.78	103.25
2	H	36	TRP	CE2-CD2-CG	-5.14	101.03	107.20
2	H	212	LYS	CG-CD-CE	-5.14	99.49	111.30
3	Y	109	VAL	CA-C-O	-5.13	116.08	121.41
2	H	208	LYS	N-CA-C	-5.12	101.06	109.40
3	Y	63	TRP	CD1-CG-CD2	5.11	114.47	106.30
2	H	153	VAL	O-C-N	-5.09	117.39	123.04
1	L	34	TRP	CG-CD2-CE3	5.09	138.99	133.90
2	H	29	PHE	CA-CB-CG	5.09	118.89	113.80
3	Y	113	ASN	N-CA-C	5.08	118.63	112.23
1	L	160	SER	N-CA-C	-5.07	100.80	108.46
1	L	142	ILE	O-C-N	-5.07	116.23	122.57
3	Y	6	CYS	CB-CA-C	-5.07	102.06	110.68
2	H	206	SER	N-CA-C	5.06	121.59	110.80
3	Y	43	THR	CA-CB-OG1	5.06	117.20	109.60
3	Y	40	SER	N-CA-C	5.06	117.45	111.33
3	Y	28	TRP	CE2-CD2-CG	-5.06	101.13	107.20
3	Y	123	TRP	CG-CD2-CE3	5.05	138.95	133.90
2	H	40	ARG	CA-C-N	5.05	125.05	119.90
2	H	40	ARG	C-N-CA	5.05	125.05	119.90
2	H	88	SER	CA-C-O	5.04	125.76	120.42
2	H	121	PRO	O-C-N	-5.03	118.78	121.15
3	Y	39	ASN	OD1-CG-ND2	-5.03	117.57	122.60
1	L	207	PHE	CA-CB-CG	5.03	118.83	113.80
2	H	69	THR	CA-CB-CG2	5.01	119.02	110.50
1	L	163	ASP	CA-CB-CG	5.01	117.61	112.60
1	L	90	TRP	CE2-CD2-CG	-5.01	101.19	107.20
3	Y	28	TRP	CB-CG-CD1	-5.01	119.39	126.90
2	H	118	LYS	CB-CG-CD	-5.00	99.80	111.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	104	ILE	Mainchain
1	L	171	TYR	Sidechain

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	1635	0	1557	55	0
2	H	1607	0	1547	39	0
3	Y	998	0	957	18	0
4	H	38	0	0	2	0
4	L	28	0	0	6	0
4	Y	20	0	0	2	0
All	All	4326	0	4061	103	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 12.

All (103) 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:L:1:ASP:HB2	1:L:2:ILE:HD12	1.66	0.77
2:H:191:ARG:HD2	2:H:192:PRO:HA	1.68	0.76
1:L:2:ILE:HG12	1:L:27:SER:HB2	1.68	0.75
3:Y:59:ASN:OD1	3:Y:61:ARG:HB3	1.89	0.72
1:L:77:MET:HE1	1:L:104:ILE:HG22	1.73	0.71
1:L:4:LEU:HG	4:L:235:HOH:O	1.92	0.69
1:L:182:ASP:HA	1:L:185:GLU:HG2	1.76	0.68
1:L:144:VAL:HG21	1:L:173:MET:HE1	1.77	0.67
1:L:12:SER:HB3	1:L:103:GLU:HG3	1.78	0.66
2:H:10:GLU:HB2	2:H:112:LEU:HD13	1.81	0.61
2:H:2:VAL:N	2:H:25:SER:HG	1.99	0.60
3:Y:15:HIS:HA	4:Y:144:HOH:O	2.02	0.60
1:L:148:ILE:HD11	1:L:177:LEU:HD21	1.84	0.59
2:H:91:SER:HA	2:H:112:LEU:O	2.03	0.59
1:L:147:LYS:HG3	1:L:151:SER:HA	1.84	0.59
1:L:81:ASP:O	1:L:102:LEU:HD23	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:15:PRO:HA	1:L:77:MET:O	2.03	0.58
1:L:187:HIS:H	1:L:210:ASN:HD21	1.51	0.58
2:H:108:GLN:HB3	4:H:235:HOH:O	2.04	0.58
1:L:142:ILE:HG13	4:L:226:HOH:O	2.02	0.57
2:H:191:ARG:HH11	2:H:191:ARG:HB3	1.68	0.57
2:H:57:SER:HB3	3:Y:43:THR:OG1	2.04	0.57
1:L:53:LEU:HB3	1:L:57:VAL:HB	1.85	0.57
3:Y:9:ALA:HB2	3:Y:29:VAL:HG21	1.86	0.57
1:L:142:ILE:HD13	1:L:196:HIS:CD2	2.40	0.56
2:H:166:VAL:HA	2:H:183:SER:O	2.06	0.56
1:L:138:TYR:O	1:L:196:HIS:HE1	1.89	0.56
1:L:144:VAL:HG21	1:L:173:MET:CE	2.37	0.55
2:H:122:PRO:HB3	2:H:148:TYR:HB3	1.88	0.55
2:H:110:THR:HG21	4:H:245:HOH:O	2.07	0.53
3:Y:13:LYS:HB2	3:Y:25:LEU:HD11	1.90	0.53
1:L:158:LEU:HD11	2:H:174:GLN:HB3	1.89	0.53
1:L:11:MET:HE3	1:L:102:LEU:HD13	1.91	0.52
1:L:131:VAL:HG11	2:H:127:LEU:HD13	1.90	0.52
1:L:166:SER:C	1:L:168:ASP:H	2.16	0.51
1:L:135:ASN:OD1	2:H:167:HIS:HD2	1.94	0.50
2:H:33:TRP:CD1	3:Y:68:LYS:HZ3	2.29	0.50
3:Y:15:HIS:HB3	3:Y:92:VAL:HG11	1.93	0.50
3:Y:94:CYS:O	3:Y:98:ILE:HG13	2.11	0.50
1:L:47:ILE:HD12	1:L:72:LEU:HD12	1.94	0.50
1:L:31:TYR:HA	1:L:50:THR:HG23	1.94	0.49
1:L:44:LYS:HA	4:L:229:HOH:O	2.11	0.49
2:H:171:ALA:HB1	2:H:178:TYR:HB3	1.94	0.49
1:L:184:TYR:O	1:L:210:ASN:ND2	2.44	0.49
2:H:51:ILE:O	2:H:53:PRO:HD3	2.12	0.49
1:L:65:GLY:HA3	1:L:70:TYR:HA	1.94	0.49
3:Y:17:LEU:HD11	3:Y:92:VAL:HG22	1.95	0.49
2:H:140:THR:HA	2:H:184:VAL:O	2.14	0.48
1:L:146:TRP:HE3	4:L:231:HOH:O	1.96	0.48
3:Y:26:GLY:O	3:Y:30:CYS:HB2	2.14	0.48
2:H:158:ASN:ND2	2:H:196:VAL:HA	2.28	0.48
2:H:173:LEU:HD13	2:H:178:TYR:CE1	2.49	0.48
3:Y:124:ILE:O	3:Y:127:CYS:HB2	2.15	0.47
2:H:154:THR:OG1	2:H:201:ALA:HB3	2.15	0.47
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.97	0.47
2:H:81:MET:HE1	2:H:94:TYR:CD2	2.50	0.46
2:H:158:ASN:HB2	2:H:162:LEU:HB2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:128:ARG:HB2	4:Y:149:HOH:O	2.15	0.46
1:L:118:PRO:HD2	1:L:184:TYR:OH	2.16	0.45
1:L:193:GLU:HB3	1:L:204:VAL:HG12	1.98	0.45
2:H:191:ARG:NH1	2:H:192:PRO:HG3	2.32	0.45
3:Y:3:PHE:HB2	3:Y:38:PHE:HB3	1.98	0.45
1:L:93:ASN:HB2	2:H:61:HIS:CD2	2.52	0.45
1:L:164:GLN:HA	1:L:170:THR:O	2.17	0.44
2:H:115:SER:HG	2:H:149:PHE:HZ	1.64	0.44
1:L:11:MET:HE2	1:L:11:MET:HB3	1.87	0.44
1:L:18:LYS:HE2	1:L:18:LYS:HB3	1.58	0.44
1:L:31:TYR:HA	1:L:50:THR:CG2	2.47	0.44
1:L:148:ILE:HG12	1:L:190:TYR:CE2	2.53	0.44
1:L:187:HIS:N	1:L:210:ASN:HD21	2.14	0.44
1:L:32:MET:H	1:L:50:THR:HG22	1.81	0.44
1:L:12:SER:HB2	1:L:105:LYS:HG3	1.99	0.44
1:L:182:ASP:O	1:L:186:ARG:HB2	2.18	0.44
3:Y:43:THR:HG22	3:Y:51:THR:HG22	1.98	0.44
2:H:191:ARG:HB3	2:H:191:ARG:NH1	2.31	0.44
1:L:19:VAL:O	1:L:73:THR:HA	2.18	0.43
2:H:162:LEU:O	2:H:166:VAL:HG21	2.17	0.43
1:L:137:PHE:CE1	1:L:172:SER:HA	2.53	0.43
1:L:183:GLU:O	1:L:187:HIS:HD2	2.01	0.43
2:H:27:TYR:OH	2:H:98:HIS:CE1	2.72	0.43
3:Y:62:TRP:H	3:Y:62:TRP:CD1	2.36	0.43
3:Y:12:MET:HB3	3:Y:17:LEU:HD12	2.00	0.42
1:L:21:MET:SD	1:L:85:TYR:HB2	2.59	0.42
1:L:114:SER:O	1:L:132:CYS:HA	2.20	0.42
2:H:38:LYS:HD2	2:H:94:TYR:OH	2.20	0.42
3:Y:6:CYS:HB3	3:Y:128:ARG:NH1	2.35	0.42
1:L:44:LYS:HD2	4:L:229:HOH:O	2.19	0.42
1:L:12:SER:HB3	4:L:218:HOH:O	2.19	0.42
1:L:106:ARG:HH11	1:L:106:ARG:HD3	1.65	0.41
1:L:43:PRO:HD2	2:H:106:TRP:CE3	2.55	0.41
3:Y:121:GLN:O	3:Y:124:ILE:HD12	2.20	0.41
2:H:33:TRP:CE3	2:H:50:GLU:HG3	2.55	0.41
2:H:202:HIS:ND1	2:H:205:SER:OG	2.50	0.41
1:L:65:GLY:HA3	1:L:69:SER:O	2.20	0.41
1:L:158:LEU:HD22	2:H:172:VAL:HG11	2.02	0.41
1:L:168:ASP:CG	1:L:169:SER:N	2.78	0.41
1:L:42:SER:HB3	2:H:95:TYR:CE1	2.56	0.41
2:H:51:ILE:HA	2:H:57:SER:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:116:PHE:HA	1:L:117:PRO:HD2	1.90	0.40
2:H:62:GLU:O	2:H:65:LYS:HE2	2.21	0.40
2:H:28:THR:O	2:H:31:ASP:HB2	2.21	0.40
1:L:118:PRO:HG2	1:L:184:TYR:CZ	2.56	0.40
2:H:143:CYS:O	2:H:181:SER:HA	2.22	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	210/212 (99%)	181 (86%)	21 (10%)	8 (4%)	2	3
2	H	212/215 (99%)	186 (88%)	21 (10%)	5 (2%)	4	9
3	Y	127/129 (98%)	113 (89%)	12 (9%)	2 (2%)	7	16
All	All	549/556 (99%)	480 (87%)	54 (10%)	15 (3%)	4	7

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	175	SER
2	H	189	SER
2	H	206	SER
3	Y	5	ARG
3	Y	88	ILE
1	L	50	THR
1	L	165	ASP
1	L	166	SER
2	H	132	ALA
1	L	149	ASP
1	L	152	GLU
1	L	153	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	188	ASN
2	H	190	PRO
1	L	55	SER

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	L	187/187 (100%)	154 (82%)	33 (18%)	2	3
2	H	182/182 (100%)	154 (85%)	28 (15%)	2	5
3	Y	105/105 (100%)	91 (87%)	14 (13%)	4	8
All	All	474/474 (100%)	399 (84%)	75 (16%)	2	4

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	THR
1	L	7	SER
1	L	12	SER
1	L	28	SER
1	L	32	MET
1	L	36	GLN
1	L	39	SER
1	L	41	THR
1	L	42	SER
1	L	51	SER
1	L	59	VAL
1	L	68	THR
1	L	72	LEU
1	L	73	THR
1	L	95	THR
1	L	106	ARG
1	L	112	THR
1	L	120	SER
1	L	130	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	131	VAL
1	L	143	ASN
1	L	145	LYS
1	L	149	ASP
1	L	152	GLU
1	L	162	THR
1	L	163	ASP
1	L	170	THR
1	L	189	SER
1	L	195	THR
1	L	198	THR
1	L	205	LYS
1	L	206	SER
1	L	212	CYS
2	H	28	THR
2	H	30	SER
2	H	53	PRO
2	H	71	THR
2	H	74	THR
2	H	83	LEU
2	H	97	LEU
2	H	103	PHE
2	H	131	SER
2	H	135	THR
2	H	141	LEU
2	H	145	VAL
2	H	151	GLU
2	H	152	PRO
2	H	153	VAL
2	H	154	THR
2	H	155	VAL
2	H	156	THR
2	H	162	LEU
2	H	164	SER
2	H	174	GLN
2	H	180	LEU
2	H	184	VAL
2	H	188	SER
2	H	191	ARG
2	H	198	CYS
2	H	208	LYS
2	H	214	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Y	5	ARG
3	Y	14	ARG
3	Y	24	SER
3	Y	37	ASN
3	Y	43	THR
3	Y	47	THR
3	Y	55	VAL
3	Y	72	SER
3	Y	77	ASN
3	Y	85	SER
3	Y	86	SER
3	Y	97	LYS
3	Y	101	ASP
3	Y	124	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	30	ASN
1	L	37	GLN
1	L	88	GLN
1	L	187	HIS
1	L	208	ASN
2	H	39	GLN
2	H	82	GLN
2	H	84	ASN
2	H	134	GLN
3	Y	27	ASN
3	Y	37	ASN
3	Y	39	ASN
3	Y	103	ASN
3	Y	106	ASN
3	Y	121	GLN

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 oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	L	212/212 (100%)	-0.46	2 (0%) 81 78	5, 21, 48, 71	0
2	H	214/215 (99%)	-0.54	2 (0%) 81 78	2, 18, 45, 71	0
3	Y	129/129 (100%)	-0.48	1 (0%) 82 80	5, 20, 40, 56	1 (0%)
All	All	555/556 (99%)	-0.50	5 (0%) 81 78	2, 20, 45, 71	1 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	168	ASP	2.5
2	H	135	THR	2.3
3	Y	22	GLY	2.2
1	L	1	ASP	2.2
2	H	175	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.