



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:38 PM UTC

PDB ID : 3HFM / pdb_00003hfm
Title : STRUCTURE OF AN ANTIBODY-ANTIGEN COMPLEX. CRYSTAL
STRUCTURE OF THE HY/HEL-10 FAB-LYSOZYME COMPLEX
Authors : Padlan, E.A.; Davies, D.R.
Deposited on : 1988-08-11
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

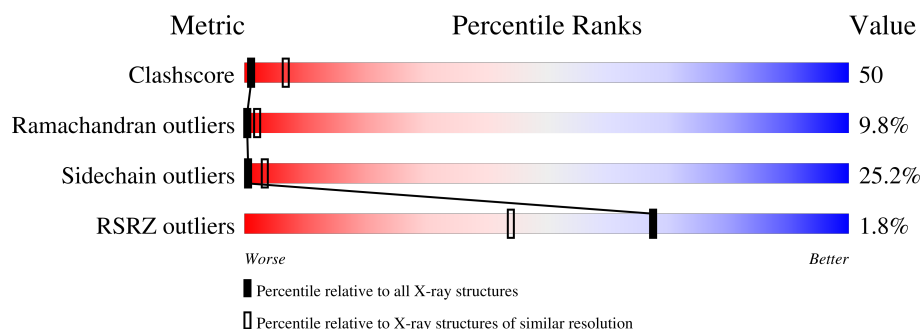
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	214	21% 49% 24% 6%
2	H	215	4% 23% 44% 25% 8%
3	Y	129	17% 47% 30% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4297 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-10 IGG1 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1655	1026	281	341	7			

- Molecule 2 is a protein called HYHEL-10 IGG1 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	0	0
			1640	1032	266	335	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	0	0
			1001	613	193	185	10			

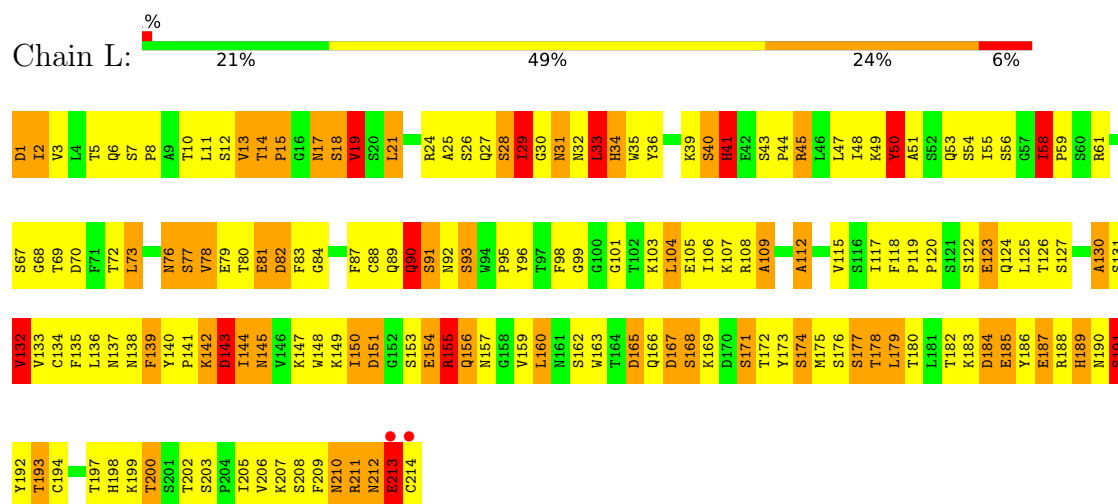
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Y	1	Total	O	0
			1	1	

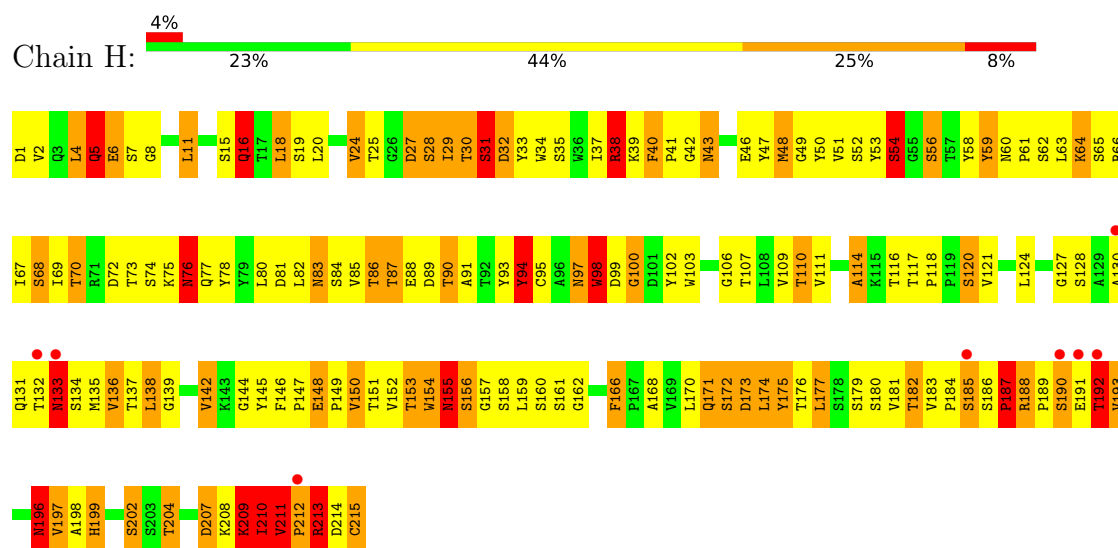
3 Residue-property plots

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.

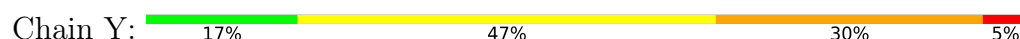
• Molecule 1: HYHEL-10 IGG1 FAB (LIGHT CHAIN)

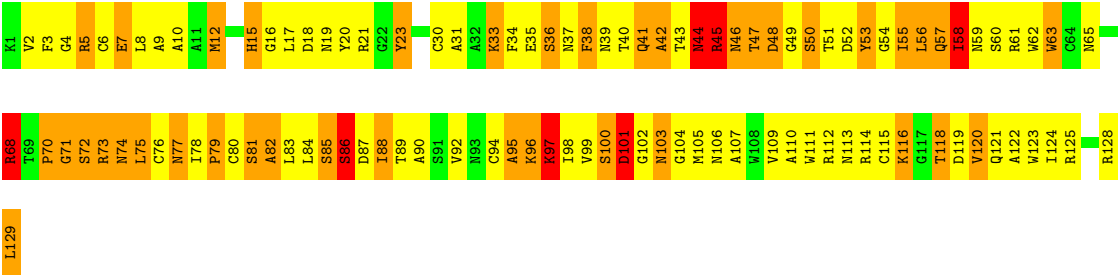


• Molecule 2: HYHEL-10 IGG1 FAB (HEAVY CHAIN)



• Molecule 3: HEN EGG WHITE LYSOZYME





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.47Å 118.73Å 137.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 10.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-3.00) 63.9 (10.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.246 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 38.6	EDS
L-test for twinning ¹	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	4297	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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

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	1.02	0/1693	2.21	69/2297 (3.0%)
2	H	1.05	2/1684 (0.1%)	2.24	80/2310 (3.5%)
3	Y	1.00	0/1021	2.04	45/1379 (3.3%)
All	All	1.03	2/4398 (0.0%)	2.18	194/5986 (3.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	49	GLY	N-CA	5.17	1.50	1.45
2	H	211	VAL	N-CA	5.08	1.50	1.46

All (194) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	45	ARG	CD-NE-CZ	19.57	151.81	124.40
1	L	145	ASN	CA-CB-CG	18.90	131.50	112.60
1	L	212	ASN	CA-CB-CG	18.54	131.14	112.60
2	H	133	ASN	CA-CB-CG	15.42	128.02	112.60
2	H	208	LYS	CA-C-N	13.22	139.45	120.95
2	H	208	LYS	C-N-CA	13.22	139.45	120.95
2	H	211	VAL	N-CA-C	-13.10	94.58	107.55
2	H	40	PHE	CA-CB-CG	11.54	125.34	113.80
2	H	175	TYR	N-CA-C	11.44	127.21	110.28
3	Y	101	ASP	CA-CB-CG	11.16	123.76	112.60
2	H	162	GLY	N-CA-C	11.06	139.39	113.18
2	H	174	LEU	CA-C-N	10.97	136.45	120.87
2	H	174	LEU	C-N-CA	10.97	136.45	120.87
2	H	196	ASN	CA-CB-CG	-10.22	102.38	112.60
1	L	143	ASP	CA-CB-CG	-9.93	102.67	112.60
1	L	138	ASN	N-CA-C	9.92	123.42	111.02
2	H	97	ASN	CA-CB-CG	9.75	122.35	112.60
2	H	211	VAL	O-C-N	9.52	127.36	121.37
2	H	211	VAL	CB-CA-C	9.41	122.15	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	83	ASN	CA-CB-CG	9.38	121.98	112.60
1	L	189	HIS	CA-CB-CG	-9.24	104.56	113.80
2	H	106	GLY	N-CA-C	-9.04	102.17	112.29
3	Y	103	ASN	N-CA-C	-8.87	102.47	113.38
3	Y	38	PHE	CA-CB-CG	8.66	122.46	113.80
1	L	188	ARG	CA-C-O	8.51	129.45	119.32
1	L	13	VAL	CA-C-O	8.50	130.19	120.67
2	H	16	GLN	N-CA-CB	8.33	119.21	108.96
1	L	153	SER	N-CA-C	8.18	122.32	109.81
2	H	94	TYR	CA-CB-CG	8.15	128.57	113.90
1	L	132	VAL	N-CA-C	-8.10	96.55	108.87
1	L	213	GLU	N-CA-C	8.05	127.94	110.80
2	H	202	SER	N-CA-C	-8.00	102.42	112.90
2	H	5	GLN	CB-CG-CD	7.99	126.18	112.60
1	L	188	ARG	N-CA-C	-7.90	102.72	113.30
2	H	107	THR	CB-CA-C	7.89	121.77	110.24
3	Y	46	ASN	CB-CA-C	7.86	123.08	110.19
3	Y	65	ASN	CA-CB-CG	-7.82	104.78	112.60
1	L	153	SER	CA-C-N	7.76	136.36	121.54
1	L	153	SER	C-N-CA	7.76	136.36	121.54
1	L	19	VAL	N-CA-CB	-7.72	103.80	112.45
1	L	76	ASN	CA-CB-CG	7.72	120.32	112.60
2	H	16	GLN	N-CA-C	-7.64	98.52	109.29
2	H	160	SER	N-CA-C	-7.62	102.97	112.72
1	L	132	VAL	CB-CA-C	7.61	121.64	111.21
1	L	109	ALA	CA-C-O	-7.61	112.35	121.56
1	L	155	ARG	CD-NE-CZ	7.54	134.96	124.40
1	L	50	TYR	CA-CB-CG	-7.42	100.54	113.90
1	L	112	ALA	N-CA-C	7.42	120.04	110.39
3	Y	101	ASP	N-CA-C	7.21	119.42	109.54
2	H	148	GLU	N-CA-C	-7.18	101.87	110.13
2	H	89	ASP	CA-CB-CG	7.09	119.69	112.60
2	H	128	SER	N-CA-C	-7.04	104.57	113.72
1	L	24	ARG	CD-NE-CZ	6.92	134.09	124.40
1	L	41	HIS	CA-CB-CG	-6.91	106.89	113.80
1	L	90	GLN	N-CA-C	-6.85	100.65	110.59
2	H	154	TRP	CB-CA-C	6.85	121.00	109.84
1	L	150	ILE	N-CA-C	-6.85	97.23	107.37
3	Y	23	TYR	N-CA-C	6.85	119.89	108.73
3	Y	100	SER	CA-C-O	-6.80	111.22	119.59
2	H	148	GLU	N-CA-CB	6.79	117.16	109.49
1	L	1	ASP	CA-CB-CG	6.77	119.37	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	90	ALA	CA-C-N	6.74	129.21	120.44
3	Y	90	ALA	C-N-CA	6.74	129.21	120.44
3	Y	118	THR	CA-C-O	-6.74	113.41	121.56
2	H	81	ASP	CA-CB-CG	-6.73	105.87	112.60
3	Y	20	TYR	N-CA-CB	6.68	121.79	110.49
3	Y	21	ARG	CD-NE-CZ	-6.68	115.05	124.40
3	Y	119	ASP	CA-C-O	-6.64	113.38	121.02
3	Y	119	ASP	N-CA-C	-6.63	98.01	108.63
1	L	205	ILE	N-CA-C	-6.60	97.43	107.73
1	L	213	GLU	CA-C-O	6.56	129.88	120.51
3	Y	63	TRP	N-CA-C	6.54	121.67	113.43
1	L	206	VAL	N-CA-C	6.48	116.96	107.37
2	H	38	ARG	CA-CB-CG	6.46	127.03	114.10
3	Y	46	ASN	N-CA-C	-6.44	98.02	108.52
1	L	70	ASP	CA-CB-CG	6.39	118.99	112.60
3	Y	15	HIS	CA-CB-CG	-6.39	107.41	113.80
1	L	138	ASN	CA-CB-CG	-6.38	106.22	112.60
2	H	208	LYS	CA-C-O	6.36	128.80	120.21
3	Y	45	ARG	CD-NE-CZ	6.34	133.28	124.40
2	H	40	PHE	CA-C-N	6.31	126.51	119.32
2	H	40	PHE	C-N-CA	6.31	126.51	119.32
2	H	207	ASP	CB-CA-C	6.28	120.50	110.19
1	L	184	ASP	CA-CB-CG	6.26	118.86	112.60
2	H	5	GLN	N-CA-C	6.25	120.74	107.67
2	H	27	ASP	CA-C-N	6.23	132.31	120.97
2	H	27	ASP	C-N-CA	6.23	132.31	120.97
2	H	74	SER	N-CA-C	-6.22	104.42	111.14
1	L	79	GLU	CB-CG-CD	6.21	123.16	112.60
2	H	106	GLY	CA-C-O	-6.21	117.95	122.23
1	L	212	ASN	N-CA-C	-6.16	104.94	112.88
3	Y	65	ASN	N-CA-C	6.06	118.57	108.20
1	L	83	PHE	N-CA-C	-6.06	100.63	110.20
3	Y	79	PRO	N-CA-C	-6.06	100.27	110.21
1	L	165	ASP	N-CA-C	-6.04	101.58	110.52
3	Y	119	ASP	N-CA-CB	6.03	119.40	109.88
1	L	150	ILE	CB-CA-C	6.00	119.53	111.19
3	Y	46	ASN	CA-CB-CG	-5.99	106.61	112.60
3	Y	95	ALA	N-CA-C	-5.99	104.44	110.97
2	H	128	SER	CB-CA-C	5.99	119.61	109.55
2	H	65	SER	N-CA-C	-5.98	103.51	112.54
2	H	120	SER	N-CA-C	-5.97	97.39	108.02
1	L	205	ILE	CA-C-O	-5.95	113.49	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	44	ASN	CA-CB-CG	5.94	118.54	112.60
2	H	209	LYS	N-CA-C	5.92	118.83	109.96
2	H	214	ASP	CA-CB-CG	-5.91	106.69	112.60
2	H	56	SER	N-CA-C	-5.90	100.38	109.76
2	H	90	THR	N-CA-CB	5.90	119.38	109.94
3	Y	74	ASN	CA-CB-CG	5.89	118.49	112.60
2	H	70	THR	CA-C-O	-5.88	114.63	121.10
1	L	139	PHE	CA-CB-CG	5.88	119.67	113.80
3	Y	79	PRO	CB-CA-C	5.86	116.73	111.40
2	H	1	ASP	CA-CB-CG	-5.85	106.75	112.60
3	Y	2	VAL	CB-CA-C	5.85	117.59	111.09
2	H	187	PRO	CA-N-CD	-5.82	103.35	111.50
2	H	81	ASP	N-CA-CB	-5.82	102.16	111.58
2	H	73	THR	N-CA-C	5.80	117.68	111.36
2	H	187	PRO	N-CA-C	5.80	127.17	112.10
2	H	48	MET	CB-CA-C	5.77	121.90	110.42
1	L	92	ASN	O-C-N	5.76	128.31	122.09
1	L	36	TYR	CA-CB-CG	5.75	124.26	113.90
2	H	16	GLN	CA-C-O	-5.75	114.39	119.91
3	Y	34	PHE	CA-CB-CG	-5.74	108.06	113.80
1	L	33	LEU	CB-CA-C	5.73	119.31	110.14
2	H	128	SER	CA-C-O	5.70	125.32	119.05
1	L	138	ASN	N-CA-CB	-5.69	101.44	111.40
3	Y	71	GLY	CA-C-O	5.69	126.25	120.45
2	H	81	ASP	N-CA-C	5.65	119.60	107.67
2	H	127	GLY	N-CA-C	-5.65	101.85	112.64
1	L	83	PHE	N-CA-CB	5.63	118.56	110.06
2	H	175	TYR	N-CA-CB	-5.62	101.71	109.97
2	H	24	VAL	N-CA-C	-5.61	100.31	108.17
2	H	65	SER	CA-C-O	5.61	125.34	119.51
1	L	84	GLY	N-CA-C	-5.60	102.62	110.63
3	Y	41	GLN	N-CA-C	5.59	119.83	112.89
3	Y	74	ASN	N-CA-CB	-5.58	102.17	110.60
1	L	210	ASN	CA-C-O	-5.58	114.25	120.66
1	L	58	ILE	O-C-N	5.57	127.44	121.10
2	H	11	LEU	N-CA-C	5.54	117.53	108.55
3	Y	71	GLY	N-CA-C	-5.53	105.91	113.27
1	L	155	ARG	NE-CZ-NH1	5.50	127.00	121.50
2	H	171	GLN	CA-CB-CG	5.50	125.10	114.10
2	H	114	ALA	N-CA-C	-5.48	102.79	110.35
1	L	87	PHE	CA-CB-CG	5.47	119.27	113.80
1	L	188	ARG	CA-CB-CG	5.45	125.00	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	58	ILE	CB-CA-C	5.45	119.08	111.34
2	H	32	ASP	CB-CA-C	5.44	118.20	109.61
1	L	179	LEU	O-C-N	5.43	129.76	123.30
2	H	190	SER	N-CA-C	5.41	122.33	110.80
1	L	167	ASP	N-CA-C	5.39	118.42	109.46
3	Y	53	TYR	N-CA-C	5.39	116.83	107.93
2	H	28	SER	CA-C-O	-5.37	115.64	121.87
1	L	5	THR	N-CA-C	5.31	118.14	107.41
2	H	204	THR	CA-CB-OG1	-5.30	101.65	109.60
1	L	91	SER	N-CA-C	-5.29	104.48	112.99
2	H	59	TYR	CA-CB-CG	5.28	123.40	113.90
3	Y	118	THR	N-CA-C	-5.27	101.98	110.14
3	Y	75	LEU	CB-CA-C	5.26	119.52	110.79
2	H	174	LEU	CA-C-O	5.25	128.02	120.51
2	H	58	TYR	CA-C-O	-5.25	114.97	121.06
2	H	199	HIS	O-C-N	5.25	126.15	120.85
1	L	179	LEU	N-CA-C	-5.24	100.35	108.90
3	Y	107	ALA	N-CA-C	-5.24	105.74	111.82
3	Y	81	SER	N-CA-C	-5.24	102.78	111.37
1	L	13	VAL	CA-C-N	5.24	134.58	121.80
1	L	13	VAL	C-N-CA	5.24	134.58	121.80
1	L	68	GLY	N-CA-C	-5.23	100.78	113.18
2	H	24	VAL	CB-CA-C	5.23	118.62	110.83
3	Y	68	ARG	CA-C-O	5.22	124.24	118.65
1	L	185	GLU	N-CA-C	-5.21	105.80	113.61
2	H	213	ARG	CA-CB-CG	5.20	124.50	114.10
1	L	90	GLN	N-CA-CB	5.20	118.32	110.42
1	L	212	ASN	CB-CA-C	5.19	119.48	110.72
2	H	133	ASN	N-CA-C	-5.17	99.78	110.80
2	H	136	VAL	N-CA-C	5.16	115.66	108.84
2	H	118	PRO	CB-CA-C	5.16	117.21	110.92
2	H	118	PRO	N-CA-C	-5.16	104.41	110.70
1	L	137	ASN	N-CA-C	5.15	118.10	110.48
1	L	82	ASP	O-C-N	5.13	128.57	122.26
3	Y	97	LYS	N-CA-C	5.13	117.66	111.40
3	Y	58	ILE	N-CA-C	-5.12	102.25	109.21
1	L	191	SER	N-CA-C	5.12	117.05	107.99
3	Y	73	ARG	CD-NE-CZ	-5.11	117.25	124.40
3	Y	114	ARG	N-CA-C	5.10	119.77	113.50
1	L	50	TYR	CA-C-O	-5.09	113.23	120.51
1	L	99	GLY	CA-C-N	5.09	126.54	120.13
1	L	99	GLY	C-N-CA	5.09	126.54	120.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	86	SER	N-CA-C	-5.09	105.82	112.23
2	H	76	ASN	CA-C-O	-5.05	113.28	120.51
2	H	114	ALA	CA-C-O	-5.05	116.17	121.88
2	H	100	GLY	N-CA-C	-5.01	101.30	113.18
1	L	84	GLY	O-C-N	5.01	128.92	123.96
1	L	31	ASN	N-CA-CB	-5.00	102.03	110.49
2	H	130	ALA	N-CA-C	5.00	117.59	109.79

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	1655	0	1572	146	0
2	H	1640	0	1582	179	0
3	Y	1001	0	959	107	0
4	Y	1	0	0	0	0
All	All	4297	0	4113	417	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 50.

All (417) 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:214:CYS:HA	2:H:215:CYS:CB	1.80	1.11
1:L:214:CYS:CA	2:H:215:CYS:HB3	1.79	1.10
2:H:53:TYR:O	2:H:54:SER:HB3	1.35	1.08
2:H:183:VAL:HB	2:H:184:PRO:HD2	1.27	1.08
1:L:156:GLN:HG3	1:L:157:ASN:H	1.17	1.07
1:L:30:GLY:O	1:L:31:ASN:HB3	1.54	1.05
2:H:188:ARG:CB	2:H:189:PRO:HD3	1.88	1.03
1:L:150:ILE:HD11	1:L:155:ARG:HH11	1.24	1.03
1:L:112:ALA:HB2	1:L:200:THR:HG21	1.40	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:188:ARG:HB3	2:H:189:PRO:CD	1.90	1.01
2:H:155:ASN:HD21	2:H:193:VAL:HA	1.25	1.01
2:H:146:PHE:HD2	2:H:147:PRO:HA	1.25	1.00
2:H:64:LYS:H	2:H:64:LYS:HD2	1.22	1.00
2:H:2:VAL:HG22	2:H:27:ASP:HB2	1.41	0.99
2:H:188:ARG:HB3	2:H:189:PRO:HD3	1.01	0.99
1:L:151:ASP:N	1:L:191:SER:O	1.95	0.98
2:H:48:MET:HE2	2:H:63:LEU:HD11	1.49	0.94
3:Y:45:ARG:HH11	3:Y:45:ARG:HB2	1.28	0.94
3:Y:121:GLN:HB3	3:Y:125:ARG:HE	1.30	0.93
2:H:98:TRP:HA	2:H:98:TRP:CE3	2.03	0.92
2:H:186:SER:HA	2:H:188:ARG:N	1.84	0.91
2:H:132:THR:O	2:H:133:ASN:HB2	1.68	0.90
3:Y:53:TYR:CD1	3:Y:84:LEU:HD11	2.07	0.90
2:H:98:TRP:HA	2:H:98:TRP:HE3	1.36	0.89
3:Y:53:TYR:HD1	3:Y:84:LEU:HD11	1.37	0.89
1:L:156:GLN:CG	1:L:157:ASN:H	1.80	0.89
1:L:213:GLU:HG2	1:L:214:CYS:H	1.37	0.88
3:Y:111:TRP:HA	3:Y:115:CYS:HB2	1.54	0.88
1:L:149:LYS:HB2	1:L:193:THR:HG22	1.55	0.88
1:L:156:GLN:HG3	1:L:157:ASN:N	1.84	0.88
1:L:186:TYR:O	1:L:192:TYR:OH	1.91	0.88
2:H:121:VAL:HG21	2:H:197:VAL:HG11	1.55	0.87
3:Y:62:TRP:O	3:Y:75:LEU:HG	1.74	0.87
2:H:18:LEU:CD2	2:H:82:LEU:HB3	2.04	0.86
1:L:49:LYS:HG3	1:L:55:ILE:HD11	1.56	0.86
2:H:146:PHE:HD2	2:H:147:PRO:CA	1.89	0.86
3:Y:5:ARG:NH1	3:Y:123:TRP:O	2.09	0.85
1:L:143:ASP:O	1:L:144:ILE:HB	1.75	0.84
3:Y:59:ASN:ND2	3:Y:60:SER:H	1.75	0.84
1:L:213:GLU:CG	1:L:214:CYS:H	1.89	0.84
2:H:18:LEU:HD21	2:H:82:LEU:HB3	1.59	0.83
1:L:155:ARG:HE	1:L:155:ARG:HA	1.42	0.83
3:Y:12:MET:HG2	3:Y:17:LEU:HD12	1.59	0.83
1:L:47:LEU:HD22	1:L:58:ILE:HD12	1.59	0.82
1:L:132:VAL:HG22	1:L:179:LEU:HB3	1.60	0.82
3:Y:115:CYS:O	3:Y:118:THR:HG23	1.80	0.82
2:H:30:THR:HB	3:Y:73:ARG:NH1	1.96	0.81
2:H:183:VAL:HB	2:H:184:PRO:CD	2.10	0.80
2:H:147:PRO:O	2:H:199:HIS:NE2	2.13	0.80
2:H:48:MET:CE	2:H:63:LEU:HD11	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:146:PHE:CD2	2:H:147:PRO:HA	2.13	0.80
2:H:136:VAL:HG13	2:H:183:VAL:HG23	1.63	0.80
2:H:90:THR:HG22	2:H:111:VAL:H	1.45	0.80
3:Y:55:ILE:HG22	3:Y:56:LEU:HD13	1.64	0.79
2:H:199:HIS:ND1	2:H:202:SER:HB2	1.98	0.79
2:H:172:SER:O	2:H:173:ASP:HB2	1.84	0.78
2:H:6:GLU:OE1	2:H:94:TYR:HA	1.83	0.78
2:H:64:LYS:HB2	2:H:66:ARG:CG	2.13	0.78
2:H:156:SER:O	2:H:158:SER:N	2.16	0.77
2:H:148:GLU:HB3	2:H:149:PRO:HA	1.65	0.77
3:Y:74:ASN:OD1	3:Y:77:ASN:HA	1.85	0.77
2:H:53:TYR:O	2:H:54:SER:CB	2.25	0.76
2:H:64:LYS:HD3	2:H:66:ARG:HE	1.49	0.76
2:H:29:ILE:O	2:H:31:SER:N	2.18	0.75
1:L:155:ARG:O	1:L:156:GLN:HB3	1.86	0.74
3:Y:46:ASN:ND2	3:Y:52:ASP:OD1	2.19	0.74
2:H:64:LYS:HB2	2:H:66:ARG:HG3	1.68	0.74
2:H:16:GLN:HA	2:H:16:GLN:HE21	1.52	0.74
2:H:188:ARG:HG2	2:H:212:PRO:HB2	1.67	0.74
2:H:183:VAL:CB	2:H:184:PRO:HD2	2.13	0.74
1:L:33:LEU:HD21	1:L:88:CYS:HB2	1.69	0.74
1:L:17:ASN:O	1:L:78:VAL:HG13	1.90	0.72
1:L:190:ASN:HA	1:L:211:ARG:HG3	1.70	0.71
2:H:90:THR:CG2	2:H:111:VAL:H	2.03	0.71
2:H:148:GLU:HB3	2:H:149:PRO:CA	2.19	0.71
1:L:90:GLN:NE2	1:L:93:SER:H	1.88	0.71
2:H:86:THR:OG1	2:H:87:THR:N	2.24	0.71
1:L:26:SER:O	1:L:27:GLN:HG2	1.91	0.70
2:H:64:LYS:HD2	2:H:64:LYS:N	2.04	0.70
2:H:168:ALA:HB2	2:H:177:LEU:HB3	1.73	0.69
2:H:34:TRP:O	2:H:50:TYR:HB2	1.93	0.69
3:Y:45:ARG:HD3	3:Y:50:SER:O	1.92	0.69
1:L:132:VAL:HG23	1:L:148:TRP:CH2	2.28	0.69
1:L:112:ALA:HB2	1:L:200:THR:CG2	2.19	0.69
1:L:198:HIS:ND1	1:L:200:THR:OG1	2.22	0.69
2:H:134:SER:O	2:H:185:SER:HB2	1.91	0.69
2:H:186:SER:HA	2:H:188:ARG:H	1.57	0.69
1:L:95:PRO:HG3	2:H:61:PRO:HD2	1.75	0.68
2:H:142:VAL:HG23	2:H:177:LEU:O	1.94	0.68
3:Y:80:CYS:O	3:Y:81:SER:C	2.36	0.68
1:L:90:GLN:HE22	1:L:93:SER:H	1.39	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:120:PRO:HD3	1:L:132:VAL:HG12	1.75	0.68
2:H:40:PHE:HD1	2:H:91:ALA:HB2	1.59	0.67
3:Y:12:MET:O	3:Y:15:HIS:N	2.23	0.67
3:Y:85:SER:OG	3:Y:87:ASP:N	2.26	0.67
1:L:40:SER:O	1:L:41:HIS:HB2	1.93	0.67
1:L:18:SER:OG	1:L:76:ASN:HA	1.95	0.67
2:H:177:LEU:C	2:H:177:LEU:HD12	2.20	0.67
2:H:172:SER:O	2:H:173:ASP:CB	2.43	0.66
2:H:39:LYS:HE2	2:H:43:ASN:HA	1.76	0.66
2:H:40:PHE:HB3	2:H:41:PRO:HD2	1.76	0.66
1:L:190:ASN:O	1:L:210:ASN:HA	1.95	0.66
2:H:4:LEU:HG	2:H:24:VAL:HG12	1.77	0.66
1:L:150:ILE:CD1	1:L:155:ARG:HD2	2.26	0.66
1:L:142:LYS:O	1:L:163:TRP:HZ3	1.79	0.66
1:L:139:PHE:O	1:L:173:TYR:N	2.30	0.65
2:H:30:THR:HB	3:Y:73:ARG:CZ	2.26	0.65
2:H:48:MET:HE2	2:H:63:LEU:CD1	2.23	0.65
1:L:49:LYS:O	1:L:51:ALA:N	2.29	0.65
1:L:120:PRO:HB3	1:L:130:ALA:HA	1.79	0.65
3:Y:59:ASN:ND2	3:Y:60:SER:N	2.44	0.64
2:H:37:ILE:HG12	2:H:47:TYR:CD1	2.33	0.64
1:L:134:CYS:HB2	1:L:148:TRP:CZ2	2.33	0.63
1:L:124:GLN:NE2	1:L:130:ALA:H	1.96	0.63
1:L:28:SER:O	1:L:29:ILE:C	2.42	0.63
2:H:192:THR:HB	2:H:211:VAL:HG13	1.81	0.63
1:L:182:THR:HG23	1:L:185:GLU:OE1	1.99	0.63
3:Y:4:GLY:O	3:Y:7:GLU:N	2.31	0.62
2:H:98:TRP:CE3	2:H:98:TRP:CA	2.81	0.62
3:Y:88:ILE:HG13	3:Y:92:VAL:HG23	1.82	0.62
3:Y:111:TRP:O	3:Y:116:LYS:HB2	1.99	0.62
2:H:188:ARG:HG2	2:H:212:PRO:CB	2.30	0.62
3:Y:10:ALA:HA	3:Y:129:LEU:HD23	1.81	0.61
2:H:156:SER:C	2:H:158:SER:H	2.08	0.61
2:H:202:SER:HB3	2:H:204:THR:OG1	1.99	0.61
2:H:136:VAL:CG1	2:H:183:VAL:HG23	2.30	0.61
1:L:115:VAL:HG22	1:L:136:LEU:HD23	1.83	0.61
3:Y:94:CYS:O	3:Y:97:LYS:HB3	2.01	0.61
1:L:11:LEU:HD13	1:L:19:VAL:HG22	1.82	0.60
2:H:116:THR:HA	2:H:146:PHE:O	2.00	0.60
3:Y:4:GLY:O	3:Y:5:ARG:C	2.44	0.60
1:L:58:ILE:HG13	1:L:59:PRO:HD2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:33:LYS:NZ	3:Y:37:ASN:OD1	2.34	0.60
1:L:108:ARG:HG2	1:L:109:ALA:H	1.66	0.60
2:H:5:GLN:HE22	2:H:25:THR:CG2	2.14	0.60
2:H:5:GLN:NE2	2:H:25:THR:HG23	2.17	0.60
2:H:31:SER:O	2:H:32:ASP:C	2.42	0.60
1:L:122:SER:N	1:L:123:GLU:OE2	2.35	0.60
2:H:29:ILE:HG21	2:H:76:ASN:O	2.02	0.60
2:H:154:TRP:O	2:H:155:ASN:C	2.45	0.60
3:Y:23:TYR:CE1	3:Y:105:MET:HG3	2.36	0.60
3:Y:37:ASN:O	3:Y:38:PHE:HB2	2.01	0.60
1:L:208:SER:OG	1:L:209:PHE:N	2.35	0.59
2:H:2:VAL:CG2	2:H:27:ASP:HB2	2.25	0.59
2:H:53:TYR:C	2:H:53:TYR:CD2	2.81	0.59
3:Y:40:THR:O	3:Y:54:GLY:HA2	2.02	0.59
1:L:40:SER:O	1:L:41:HIS:CB	2.51	0.59
1:L:108:ARG:HB2	1:L:171:SER:HB2	1.85	0.59
2:H:39:LYS:O	2:H:91:ALA:HB1	2.03	0.58
1:L:11:LEU:HD13	1:L:19:VAL:CG2	2.33	0.58
3:Y:18:ASP:O	3:Y:19:ASN:HB2	2.03	0.58
3:Y:84:LEU:HD12	3:Y:84:LEU:N	2.18	0.58
2:H:16:GLN:HA	2:H:16:GLN:NE2	2.15	0.58
3:Y:85:SER:OG	3:Y:86:SER:N	2.33	0.58
1:L:125:LEU:O	1:L:183:LYS:HD2	2.03	0.58
2:H:52:SER:OG	3:Y:101:ASP:HB2	2.03	0.58
1:L:175:MET:HG3	1:L:176:SER:N	2.19	0.58
1:L:214:CYS:HA	2:H:215:CYS:HB3	0.84	0.58
2:H:135:MET:HE2	2:H:182:THR:OG1	2.03	0.57
3:Y:103:ASN:O	3:Y:104:GLY:C	2.47	0.57
1:L:150:ILE:CD1	1:L:155:ARG:HH11	2.09	0.57
1:L:30:GLY:O	3:Y:16:GLY:HA3	2.03	0.57
2:H:75:LYS:O	2:H:77:GLN:N	2.38	0.57
2:H:188:ARG:HE	2:H:212:PRO:CB	2.18	0.57
2:H:184:PRO:HG2	2:H:187:PRO:HB3	1.86	0.56
1:L:10:THR:HG22	1:L:103:LYS:HB3	1.87	0.56
2:H:38:ARG:HD3	2:H:93:TYR:CE2	2.41	0.56
2:H:59:TYR:HE1	2:H:69:ILE:HG13	1.71	0.56
3:Y:78:ILE:HG13	3:Y:79:PRO:HD2	1.86	0.56
3:Y:103:ASN:O	3:Y:106:ASN:N	2.33	0.56
1:L:124:GLN:NE2	1:L:130:ALA:N	2.54	0.55
1:L:176:SER:OG	1:L:177:SER:N	2.39	0.55
2:H:188:ARG:CG	2:H:212:PRO:HB2	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:38:ARG:NH2	2:H:46:GLU:OE2	2.36	0.55
3:Y:121:GLN:HB3	3:Y:125:ARG:NE	2.11	0.55
3:Y:111:TRP:O	3:Y:116:LYS:N	2.32	0.55
2:H:52:SER:CB	3:Y:101:ASP:HB2	2.37	0.55
1:L:80:THR:HG22	1:L:106:ILE:HG21	1.88	0.55
2:H:90:THR:HG22	2:H:110:THR:HA	1.87	0.55
2:H:52:SER:OG	2:H:56:SER:HB3	2.07	0.55
1:L:21:LEU:HD12	1:L:73:LEU:HD23	1.89	0.55
1:L:112:ALA:CB	1:L:200:THR:HG21	2.27	0.55
3:Y:58:ILE:HB	3:Y:83:LEU:HD13	1.87	0.55
3:Y:74:ASN:HD21	3:Y:78:ILE:N	2.04	0.55
3:Y:59:ASN:HD22	3:Y:60:SER:H	1.53	0.54
2:H:154:TRP:NE1	2:H:179:SER:OG	2.30	0.54
2:H:211:VAL:O	2:H:213:ARG:N	2.41	0.54
2:H:16:GLN:H	2:H:85:VAL:HG22	1.72	0.54
2:H:61:PRO:O	2:H:62:SER:C	2.50	0.54
3:Y:45:ARG:NH2	3:Y:68:ARG:HD2	2.22	0.54
3:Y:81:SER:O	3:Y:83:LEU:N	2.41	0.54
1:L:13:VAL:N	1:L:105:GLU:O	2.34	0.54
1:L:104:LEU:HD23	1:L:104:LEU:C	2.33	0.54
3:Y:95:ALA:O	3:Y:97:LYS:N	2.41	0.54
3:Y:47:THR:C	3:Y:49:GLY:H	2.15	0.54
2:H:72:ASP:CG	2:H:75:LYS:HB2	2.33	0.54
2:H:155:ASN:ND2	2:H:193:VAL:HA	2.07	0.54
2:H:72:ASP:OD2	2:H:75:LYS:HB2	2.08	0.53
3:Y:95:ALA:O	3:Y:96:LYS:C	2.51	0.53
1:L:33:LEU:CD2	1:L:88:CYS:HB2	2.37	0.53
2:H:145:TYR:CZ	2:H:175:TYR:HB3	2.43	0.53
3:Y:23:TYR:CD1	3:Y:105:MET:HG3	2.42	0.53
3:Y:101:ASP:CG	3:Y:101:ASP:O	2.49	0.53
1:L:34:HIS:N	1:L:34:HIS:CD2	2.77	0.53
1:L:150:ILE:HG22	1:L:192:TYR:CD1	2.43	0.53
3:Y:92:VAL:O	3:Y:95:ALA:N	2.41	0.53
1:L:2:ILE:HD12	1:L:29:ILE:HG21	1.91	0.53
1:L:167:ASP:C	1:L:169:LYS:H	2.17	0.53
1:L:31:ASN:HB3	3:Y:16:GLY:HA3	1.91	0.53
2:H:83:ASN:O	2:H:84:SER:C	2.52	0.53
2:H:64:LYS:HD3	2:H:66:ARG:NE	2.20	0.53
2:H:66:ARG:HB2	2:H:82:LEU:HD11	1.91	0.53
2:H:32:ASP:O	2:H:34:TRP:CD1	2.63	0.52
2:H:168:ALA:CB	2:H:177:LEU:HB3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:144:GLY:HA2	2:H:174:LEU:HD21	1.92	0.52
2:H:151:THR:HB	2:H:198:ALA:HB3	1.90	0.52
2:H:114:ALA:HB3	2:H:146:PHE:HE1	1.74	0.52
2:H:66:ARG:HB2	2:H:82:LEU:CD1	2.40	0.52
1:L:139:PHE:CZ	1:L:144:ILE:HG21	2.44	0.52
2:H:90:THR:HG22	2:H:111:VAL:N	2.18	0.52
1:L:61:ARG:NH1	1:L:82:ASP:OD2	2.33	0.52
1:L:150:ILE:HD13	1:L:155:ARG:HD2	1.91	0.52
2:H:7:SER:OG	2:H:8:GLY:N	2.42	0.52
1:L:6:GLN:OE1	1:L:101:GLY:N	2.40	0.52
1:L:213:GLU:CG	1:L:214:CYS:N	2.65	0.52
3:Y:61:ARG:HD3	3:Y:62:TRP:CE2	2.44	0.52
1:L:190:ASN:HD22	1:L:211:ARG:HG3	1.74	0.51
3:Y:36:SER:O	3:Y:39:ASN:HB3	2.10	0.51
3:Y:124:ILE:HG13	3:Y:124:ILE:O	2.10	0.51
1:L:11:LEU:O	1:L:105:GLU:N	2.27	0.51
1:L:91:SER:HA	1:L:96:TYR:CD1	2.45	0.51
2:H:124:LEU:HB2	2:H:139:GLY:C	2.36	0.51
3:Y:120:VAL:O	3:Y:121:GLN:C	2.54	0.51
1:L:48:ILE:CD1	1:L:54:SER:HA	2.41	0.51
2:H:29:ILE:HG23	2:H:76:ASN:OD1	2.09	0.51
2:H:136:VAL:HG13	2:H:183:VAL:CG2	2.36	0.51
2:H:155:ASN:O	2:H:156:SER:C	2.53	0.51
3:Y:120:VAL:C	3:Y:122:ALA:N	2.68	0.51
1:L:28:SER:O	1:L:30:GLY:N	2.43	0.51
2:H:5:GLN:HE22	2:H:25:THR:HG23	1.76	0.51
1:L:89:GLN:HB2	1:L:98:PHE:CD2	2.46	0.51
3:Y:10:ALA:CA	3:Y:129:LEU:HD23	2.41	0.51
2:H:134:SER:C	2:H:185:SER:HB2	2.36	0.50
1:L:47:LEU:CD2	1:L:58:ILE:HD12	2.36	0.50
1:L:117:ILE:C	1:L:118:PHE:CD2	2.90	0.50
1:L:124:GLN:HG2	1:L:124:GLN:O	2.11	0.50
2:H:40:PHE:HB3	2:H:41:PRO:CD	2.40	0.50
1:L:150:ILE:HG22	1:L:192:TYR:HD1	1.77	0.50
2:H:40:PHE:CB	2:H:41:PRO:HD2	2.38	0.50
1:L:160:LEU:C	1:L:160:LEU:HD12	2.37	0.49
2:H:67:ILE:HG12	2:H:68:SER:H	1.77	0.49
1:L:190:ASN:ND2	1:L:211:ARG:N	2.61	0.49
1:L:131:SER:OG	1:L:180:THR:HG22	2.13	0.49
3:Y:63:TRP:CZ3	3:Y:75:LEU:HD12	2.48	0.49
2:H:188:ARG:HG2	2:H:212:PRO:HG2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:142:LYS:HD3	1:L:173:TYR:CZ	2.47	0.49
2:H:188:ARG:HE	2:H:212:PRO:HB3	1.77	0.49
3:Y:121:GLN:OE1	3:Y:125:ARG:NH1	2.45	0.49
3:Y:18:ASP:OD1	3:Y:19:ASN:ND2	2.46	0.49
3:Y:45:ARG:HH12	3:Y:68:ARG:NH2	2.09	0.49
3:Y:76:CYS:O	3:Y:78:ILE:N	2.46	0.49
3:Y:45:ARG:HB2	3:Y:45:ARG:NH1	2.12	0.49
3:Y:53:TYR:HE2	3:Y:60:SER:OG	1.96	0.49
3:Y:98:ILE:C	3:Y:100:SER:H	2.21	0.49
2:H:59:TYR:CE1	2:H:69:ILE:HG13	2.48	0.48
3:Y:88:ILE:O	3:Y:89:THR:C	2.55	0.48
1:L:123:GLU:H	1:L:123:GLU:CD	2.21	0.48
1:L:133:VAL:HG21	2:H:124:LEU:HD11	1.95	0.48
2:H:53:TYR:O	3:Y:101:ASP:OD1	2.31	0.48
2:H:188:ARG:CB	2:H:189:PRO:CD	2.63	0.48
1:L:194:CYS:O	1:L:194:CYS:SG	2.71	0.48
2:H:138:LEU:HD23	2:H:210:ILE:HG13	1.95	0.48
3:Y:41:GLN:O	3:Y:42:ALA:C	2.57	0.48
1:L:141:PRO:O	1:L:143:ASP:N	2.47	0.48
3:Y:109:VAL:O	3:Y:112:ARG:N	2.47	0.48
1:L:115:VAL:HG22	1:L:136:LEU:CD2	2.43	0.48
3:Y:74:ASN:CG	3:Y:77:ASN:HA	2.38	0.48
2:H:209:LYS:O	2:H:209:LYS:HG2	2.11	0.47
2:H:88:GLU:C	2:H:90:THR:H	2.22	0.47
2:H:114:ALA:HB3	2:H:146:PHE:CE1	2.49	0.47
3:Y:61:ARG:HG2	3:Y:62:TRP:CD1	2.48	0.47
2:H:184:PRO:O	2:H:187:PRO:HB2	2.14	0.47
2:H:132:THR:O	2:H:133:ASN:CB	2.52	0.47
2:H:186:SER:HA	2:H:187:PRO:C	2.38	0.47
2:H:166:PHE:CD2	2:H:166:PHE:N	2.79	0.47
2:H:184:PRO:HB2	2:H:187:PRO:HB2	1.97	0.47
2:H:197:VAL:HG22	2:H:198:ALA:N	2.29	0.47
1:L:133:VAL:HG22	1:L:178:THR:HG23	1.96	0.47
3:Y:46:ASN:HB2	3:Y:50:SER:OG	2.14	0.47
3:Y:95:ALA:C	3:Y:97:LYS:N	2.69	0.47
1:L:14:THR:HA	1:L:15:PRO:HD2	1.84	0.47
2:H:41:PRO:C	2:H:43:ASN:H	2.22	0.47
1:L:144:ILE:HG23	1:L:144:ILE:O	2.14	0.47
2:H:210:ILE:C	2:H:210:ILE:HD12	2.40	0.47
3:Y:52:ASP:HB3	3:Y:57:GLN:HB3	1.96	0.47
1:L:142:LYS:O	1:L:163:TRP:CZ3	2.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:29:ILE:C	2:H:31:SER:N	2.73	0.47
2:H:35:SER:O	2:H:78:TYR:OH	2.26	0.47
3:Y:61:ARG:HD3	3:Y:62:TRP:CZ2	2.49	0.47
2:H:86:THR:C	2:H:111:VAL:HG11	2.40	0.46
1:L:140:TYR:O	1:L:198:HIS:HE1	1.98	0.46
1:L:192:TYR:HB2	1:L:209:PHE:CE2	2.51	0.46
3:Y:109:VAL:O	3:Y:113:ASN:N	2.39	0.46
2:H:42:GLY:O	2:H:43:ASN:OD1	2.34	0.46
2:H:52:SER:HB2	3:Y:101:ASP:HB2	1.97	0.46
3:Y:43:THR:C	3:Y:44:ASN:HD22	2.23	0.46
1:L:50:TYR:CE1	3:Y:96:LYS:HD3	2.50	0.46
3:Y:6:CYS:O	3:Y:7:GLU:C	2.58	0.46
3:Y:51:THR:H	3:Y:60:SER:HB2	1.81	0.46
2:H:18:LEU:CD1	2:H:109:VAL:HG11	2.45	0.46
2:H:177:LEU:C	2:H:177:LEU:CD1	2.87	0.46
1:L:190:ASN:O	1:L:211:ARG:N	2.46	0.46
2:H:29:ILE:CG2	2:H:76:ASN:OD1	2.64	0.46
1:L:175:MET:HE2	1:L:176:SER:O	2.15	0.45
2:H:5:GLN:NE2	2:H:25:THR:CG2	2.78	0.45
1:L:173:TYR:O	1:L:174:SER:CB	2.64	0.45
1:L:173:TYR:HB3	1:L:174:SER:H	1.52	0.45
3:Y:4:GLY:O	3:Y:6:CYS:N	2.49	0.45
1:L:120:PRO:HG2	1:L:186:TYR:CZ	2.51	0.45
2:H:146:PHE:CD2	2:H:147:PRO:CA	2.81	0.45
3:Y:109:VAL:HG13	3:Y:110:ALA:N	2.31	0.45
1:L:30:GLY:O	1:L:31:ASN:CB	2.39	0.45
1:L:141:PRO:O	1:L:142:LYS:C	2.59	0.45
1:L:151:ASP:OD1	1:L:189:HIS:ND1	2.43	0.45
3:Y:125:ARG:HG2	3:Y:125:ARG:HH21	1.82	0.45
1:L:139:PHE:CE1	1:L:144:ILE:HG21	2.52	0.45
2:H:67:ILE:HG12	2:H:68:SER:N	2.32	0.45
3:Y:78:ILE:HG13	3:Y:82:ALA:HB3	1.99	0.45
3:Y:109:VAL:HG13	3:Y:110:ALA:H	1.81	0.45
1:L:14:THR:O	1:L:15:PRO:C	2.60	0.44
1:L:144:ILE:O	1:L:144:ILE:CG2	2.65	0.44
3:Y:30:CYS:HB2	3:Y:123:TRP:CD1	2.52	0.44
3:Y:45:ARG:HA	3:Y:51:THR:HA	1.99	0.44
1:L:6:GLN:HE21	1:L:35:TRP:HZ3	1.65	0.44
2:H:197:VAL:CG2	2:H:198:ALA:N	2.81	0.44
1:L:76:ASN:O	1:L:77:SER:HB3	2.17	0.44
2:H:30:THR:C	2:H:31:SER:OG	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:16:GLN:H	2:H:85:VAL:CG2	2.30	0.44
1:L:157:ASN:C	1:L:159:VAL:H	2.25	0.44
1:L:154:GLU:O	1:L:155:ARG:NE	2.50	0.44
3:Y:3:PHE:HB3	3:Y:8:LEU:HB2	2.00	0.44
2:H:197:VAL:CG2	2:H:198:ALA:H	2.31	0.44
1:L:49:LYS:O	1:L:50:TYR:C	2.60	0.43
1:L:81:GLU:HG3	1:L:81:GLU:O	2.17	0.43
2:H:97:ASN:O	2:H:99:ASP:N	2.50	0.43
2:H:188:ARG:HG2	2:H:212:PRO:CG	2.47	0.43
1:L:8:PRO:HG2	1:L:11:LEU:HG	2.00	0.43
1:L:186:TYR:CE2	1:L:192:TYR:CE2	3.06	0.43
1:L:61:ARG:HG2	1:L:76:ASN:O	2.18	0.43
1:L:96:TYR:HH	2:H:98:TRP:HH2	1.63	0.43
1:L:1:ASP:HB2	1:L:95:PRO:HD2	2.00	0.43
1:L:150:ILE:HD11	1:L:155:ARG:NH1	2.09	0.43
1:L:166:GLN:HG2	1:L:171:SER:HA	2.00	0.43
2:H:16:GLN:N	2:H:85:VAL:HG22	2.33	0.43
3:Y:58:ILE:HG23	3:Y:63:TRP:CB	2.49	0.43
2:H:67:ILE:CG1	2:H:68:SER:H	2.31	0.43
1:L:39:LYS:O	1:L:40:SER:C	2.62	0.43
2:H:188:ARG:HE	2:H:212:PRO:HB2	1.82	0.43
1:L:2:ILE:CD1	1:L:29:ILE:HG21	2.49	0.42
1:L:115:VAL:HB	1:L:207:LYS:HG2	2.00	0.42
1:L:155:ARG:HA	1:L:155:ARG:NE	2.09	0.42
1:L:48:ILE:HD12	1:L:54:SER:HA	2.01	0.42
1:L:89:GLN:HB2	1:L:98:PHE:CE2	2.55	0.42
2:H:150:VAL:HG23	2:H:151:THR:N	2.35	0.42
3:Y:109:VAL:O	3:Y:110:ALA:C	2.62	0.42
2:H:166:PHE:H	2:H:166:PHE:HD2	1.63	0.42
2:H:211:VAL:O	2:H:213:ARG:HB3	2.18	0.42
3:Y:31:ALA:O	3:Y:35:GLU:HB3	2.20	0.42
2:H:2:VAL:HG13	2:H:27:ASP:HB3	2.01	0.42
2:H:78:TYR:OH	2:H:95:CYS:HB2	2.20	0.42
2:H:97:ASN:O	2:H:98:TRP:C	2.62	0.42
3:Y:63:TRP:CZ2	3:Y:98:ILE:HG12	2.55	0.42
1:L:1:ASP:CB	1:L:95:PRO:HD2	2.50	0.41
1:L:120:PRO:HB3	1:L:130:ALA:CA	2.49	0.41
2:H:4:LEU:HD21	2:H:34:TRP:HZ3	1.85	0.41
2:H:159:LEU:HD13	2:H:181:VAL:HG21	2.02	0.41
3:Y:84:LEU:N	3:Y:84:LEU:CD1	2.81	0.41
3:Y:121:GLN:O	3:Y:122:ALA:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:18:LEU:HD13	2:H:109:VAL:HG11	2.02	0.41
2:H:88:GLU:C	2:H:90:THR:N	2.77	0.41
3:Y:45:ARG:HH12	3:Y:68:ARG:CZ	2.32	0.41
1:L:3:VAL:O	1:L:25:ALA:HA	2.20	0.41
3:Y:46:ASN:C	3:Y:48:ASP:N	2.76	0.41
2:H:52:SER:HG	2:H:56:SER:HB3	1.84	0.41
1:L:50:TYR:HB2	1:L:53:GLN:HG3	2.02	0.41
2:H:98:TRP:HB3	2:H:99:ASP:H	1.62	0.41
3:Y:12:MET:HG2	3:Y:17:LEU:CD1	2.41	0.41
1:L:198:HIS:CG	1:L:199:LYS:H	2.39	0.41
2:H:153:THR:O	2:H:196:ASN:N	2.44	0.41
2:H:48:MET:O	2:H:60:ASN:HB2	2.20	0.41
3:Y:71:GLY:O	3:Y:72:SER:C	2.64	0.41
3:Y:88:ILE:HG13	3:Y:92:VAL:CG2	2.50	0.41
3:Y:79:PRO:O	3:Y:82:ALA:HB3	2.20	0.41
1:L:11:LEU:HA	1:L:11:LEU:HD23	1.70	0.41
1:L:61:ARG:HH11	1:L:82:ASP:CG	2.23	0.41
1:L:119:PRO:O	1:L:120:PRO:C	2.64	0.41
2:H:64:LYS:HB2	2:H:66:ARG:HG2	1.99	0.41
2:H:145:TYR:CE2	2:H:175:TYR:HB3	2.55	0.41
3:Y:121:GLN:CB	3:Y:125:ARG:HE	2.16	0.41
1:L:150:ILE:O	1:L:151:ASP:HB2	2.21	0.41
1:L:187:GLU:H	1:L:187:GLU:HG3	1.76	0.41
2:H:102:TYR:O	2:H:103:TRP:CD1	2.74	0.41
1:L:108:ARG:NH2	1:L:109:ALA:O	2.52	0.40
2:H:6:GLU:H	2:H:6:GLU:HG2	1.54	0.40
2:H:20:LEU:N	2:H:20:LEU:HD12	2.36	0.40
3:Y:31:ALA:O	3:Y:35:GLU:CB	2.69	0.40
2:H:18:LEU:HD22	2:H:85:VAL:HG12	2.03	0.40
2:H:59:TYR:HE1	2:H:69:ILE:CG1	2.33	0.40
2:H:188:ARG:NE	2:H:212:PRO:HB2	2.36	0.40
1:L:82:ASP:O	1:L:104:LEU:HD22	2.22	0.40
1:L:118:PHE:CE2	1:L:135:PHE:HD1	2.40	0.40
3:Y:53:TYR:HB2	3:Y:83:LEU:HD12	2.03	0.40
1:L:61:ARG:NH1	1:L:82:ASP:CG	2.79	0.40
1:L:118:PHE:HA	1:L:119:PRO:HD3	1.92	0.40
2:H:121:VAL:CG2	2:H:197:VAL:HG11	2.38	0.40
2:H:155:ASN:O	2:H:156:SER:O	2.40	0.40
3:Y:8:LEU:O	3:Y:9:ALA:C	2.65	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	212/214 (99%)	162 (76%)	33 (16%)	17 (8%)	1	3
2	H	213/215 (99%)	155 (73%)	38 (18%)	20 (9%)	0	2
3	Y	127/129 (98%)	86 (68%)	24 (19%)	17 (13%)	0	1
All	All	552/558 (99%)	403 (73%)	95 (17%)	54 (10%)	0	2

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	29	ILE
1	L	50	TYR
1	L	130	ALA
1	L	144	ILE
1	L	154	GLU
1	L	156	GLN
1	L	174	SER
2	H	30	THR
2	H	54	SER
2	H	64	LYS
2	H	76	ASN
2	H	133	ASN
2	H	156	SER
2	H	157	GLY
2	H	187	PRO
2	H	192	THR
3	Y	5	ARG
3	Y	77	ASN
3	Y	82	ALA
3	Y	85	SER
1	L	40	SER
1	L	67	SER
1	L	142	LYS
2	H	68	SER

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Mol	Chain	Res	Type
2	H	98	TRP
2	H	173	ASP
2	H	188	ARG
2	H	210	ILE
3	Y	48	ASP
3	Y	72	SER
3	Y	99	VAL
3	Y	116	LYS
1	L	44	PRO
1	L	168	SER
2	H	100	GLY
2	H	155	ASN
2	H	161	SER
2	H	212	PRO
3	Y	7	GLU
3	Y	33	LYS
3	Y	36	SER
3	Y	42	ALA
3	Y	47	THR
3	Y	96	LYS
1	L	15	PRO
1	L	162	SER
2	H	31	SER
2	H	172	SER
1	L	151	ASP
1	L	177	SER
1	L	213	GLU
3	Y	57	GLN
3	Y	70	PRO
3	Y	102	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	L	192/192 (100%)	139 (72%)	53 (28%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	192/192 (100%)	138 (72%)	54 (28%)	0	2
3	Y	105/105 (100%)	89 (85%)	16 (15%)	3	14
All	All	489/489 (100%)	366 (75%)	123 (25%)	0	3

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	ILE
1	L	7	SER
1	L	12	SER
1	L	14	THR
1	L	17	ASN
1	L	18	SER
1	L	19	VAL
1	L	21	LEU
1	L	28	SER
1	L	29	ILE
1	L	32	ASN
1	L	33	LEU
1	L	34	HIS
1	L	41	HIS
1	L	43	SER
1	L	45	ARG
1	L	56	SER
1	L	58	ILE
1	L	69	THR
1	L	72	THR
1	L	73	LEU
1	L	77	SER
1	L	78	VAL
1	L	81	GLU
1	L	90	GLN
1	L	93	SER
1	L	104	LEU
1	L	107	LYS
1	L	123	GLU
1	L	126	THR
1	L	127	SER
1	L	132	VAL
1	L	143	ASP
1	L	145	ASN

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Mol	Chain	Res	Type
1	L	147	LYS
1	L	155	ARG
1	L	160	LEU
1	L	165	ASP
1	L	168	SER
1	L	171	SER
1	L	172	THR
1	L	178	THR
1	L	184	ASP
1	L	187	GLU
1	L	191	SER
1	L	193	THR
1	L	197	THR
1	L	200	THR
1	L	202	THR
1	L	203	SER
1	L	211	ARG
1	L	212	ASN
1	L	213	GLU
2	H	4	LEU
2	H	5	GLN
2	H	6	GLU
2	H	11	LEU
2	H	15	SER
2	H	16	GLN
2	H	18	LEU
2	H	19	SER
2	H	28	SER
2	H	29	ILE
2	H	31	SER
2	H	33	TYR
2	H	38	ARG
2	H	43	ASN
2	H	51	VAL
2	H	54	SER
2	H	70	THR
2	H	80	LEU
2	H	86	THR
2	H	87	THR
2	H	94	TYR
2	H	98	TRP
2	H	110	THR

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Mol	Chain	Res	Type
2	H	117	THR
2	H	120	SER
2	H	131	GLN
2	H	137	THR
2	H	138	LEU
2	H	142	VAL
2	H	150	VAL
2	H	152	VAL
2	H	153	THR
2	H	155	ASN
2	H	166	PHE
2	H	170	LEU
2	H	171	GLN
2	H	176	THR
2	H	177	LEU
2	H	180	SER
2	H	182	THR
2	H	185	SER
2	H	187	PRO
2	H	190	SER
2	H	191	GLU
2	H	192	THR
2	H	193	VAL
2	H	196	ASN
2	H	197	VAL
2	H	207	ASP
2	H	209	LYS
2	H	210	ILE
2	H	211	VAL
2	H	213	ARG
2	H	215	CYS
3	Y	12	MET
3	Y	44	ASN
3	Y	45	ARG
3	Y	50	SER
3	Y	55	ILE
3	Y	56	LEU
3	Y	58	ILE
3	Y	68	ARG
3	Y	70	PRO
3	Y	86	SER
3	Y	88	ILE

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Mol	Chain	Res	Type
3	Y	97	LYS
3	Y	101	ASP
3	Y	120	VAL
3	Y	128	ARG
3	Y	129	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	34	HIS
1	L	138	ASN
1	L	156	GLN
1	L	190	ASN
1	L	210	ASN
2	H	5	GLN
2	H	16	GLN
2	H	83	ASN
2	H	105	GLN
2	H	164	HIS
2	H	171	GLN
3	Y	15	HIS
3	Y	57	GLN
3	Y	59	ASN
3	Y	74	ASN
3	Y	113	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 oligosaccharides 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 [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	214/214 (100%)	-0.26	2 (0%) 81 61	11, 16, 20, 26	0
2	H	215/215 (100%)	-0.01	8 (3%) 45 25	14, 18, 23, 26	0
3	Y	129/129 (100%)	-0.25	0 100 100	11, 16, 20, 21	0
All	All	558/558 (100%)	-0.16	10 (1%) 67 44	11, 17, 22, 26	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	133	ASN	3.8
2	H	130	ALA	3.3
2	H	212	PRO	3.1
1	L	214	CYS	2.9
2	H	190	SER	2.8
2	H	132	THR	2.3
1	L	213	GLU	2.2
2	H	192	THR	2.2
2	H	185	SER	2.2
2	H	191	GLU	2.0

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.