



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 08:43 AM EDT

PDB ID : 4YXH / pdb_00004yxh
Title : Crystal structure of Deer prion protein complexed with POM1 FAB
Authors : Baral, P.K.; Swayampakula, M.; James, M.N.G.
Deposited on : 2015-03-23
Resolution : 2.70 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

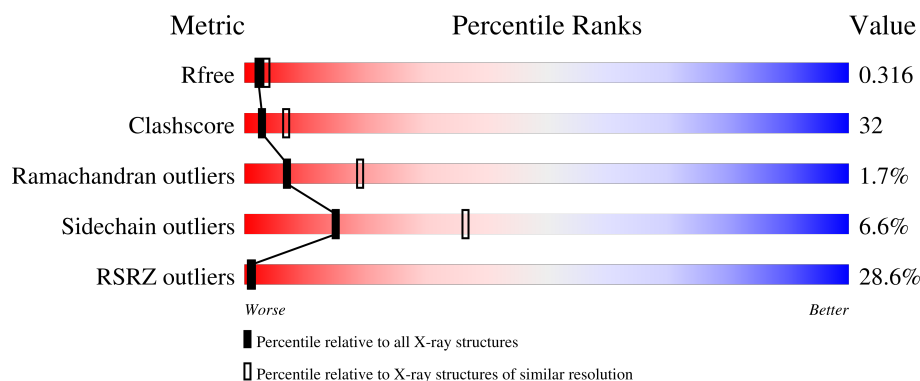
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	A	135	9% 47% 26% 25%
2	H	218	25% 66% 24% 10%
3	L	213	40% 53% 28% 15%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4223 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 Major prion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	101	Total	C	N	O	S	0	0	0
			851	530	148	165	8			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	MET	-	expression tag	UNP P47852
A	87	GLY	-	expression tag	UNP P47852
A	88	SER	-	expression tag	UNP P47852
A	89	SER	-	expression tag	UNP P47852
A	90	HIS	-	expression tag	UNP P47852
A	91	HIS	-	expression tag	UNP P47852
A	92	HIS	-	expression tag	UNP P47852
A	93	HIS	-	expression tag	UNP P47852
A	94	HIS	-	expression tag	UNP P47852
A	95	HIS	-	expression tag	UNP P47852
A	96	SER	-	expression tag	UNP P47852
A	97	SER	-	expression tag	UNP P47852
A	98	GLY	-	expression tag	UNP P47852
A	99	LEU	-	expression tag	UNP P47852
A	100	VAL	-	expression tag	UNP P47852
A	101	PRO	-	expression tag	UNP P47852
A	102	ARG	-	expression tag	UNP P47852
A	103	GLY	-	expression tag	UNP P47852
A	104	SER	-	expression tag	UNP P47852
A	105	HIS	-	expression tag	UNP P47852
A	106	MET	-	expression tag	UNP P47852
A	107	LEU	-	expression tag	UNP P47852
A	108	GLU	-	expression tag	UNP P47852
A	109	ASP	-	expression tag	UNP P47852
A	110	PRO	-	expression tag	UNP P47852
A	111	HIS	-	expression tag	UNP P47852
A	112	MET	-	expression tag	UNP P47852

- Molecule 2 is a protein called POM1 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1642	1037	265	330	10			

- Molecule 3 is a protein called POM1 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1652	1022	280	345	5			

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	1	Total	Na	0	0
			1	1		

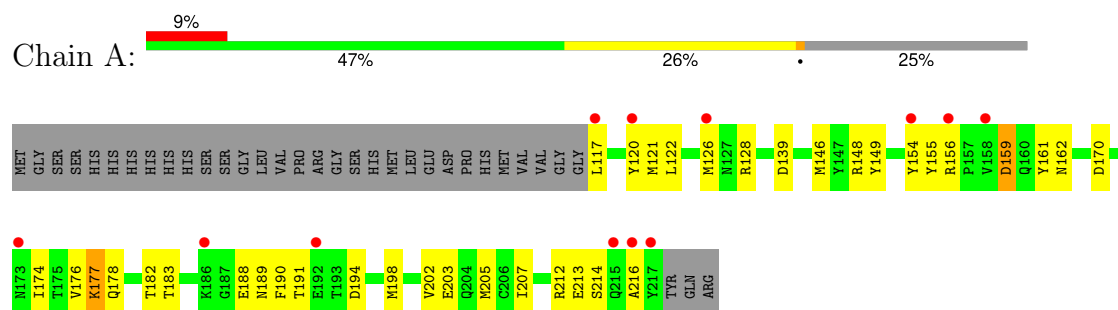
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	18	Total	O	0	0
			18	18		
5	H	30	Total	O	0	0
			30	30		
5	L	29	Total	O	0	0
			29	29		

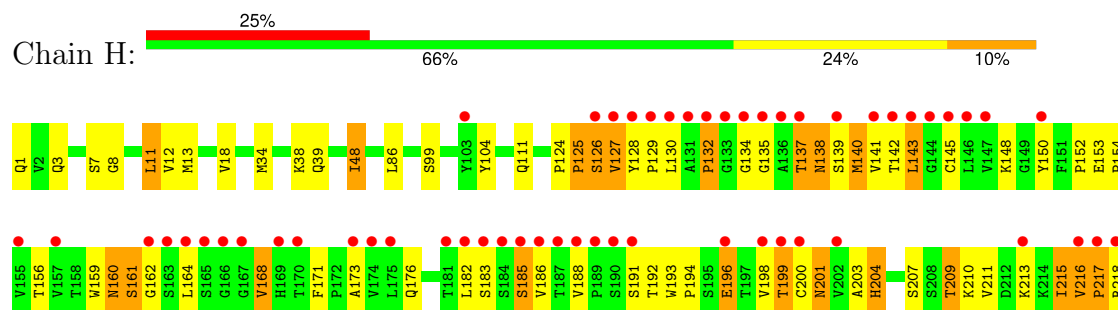
3 Residue-property plots

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.

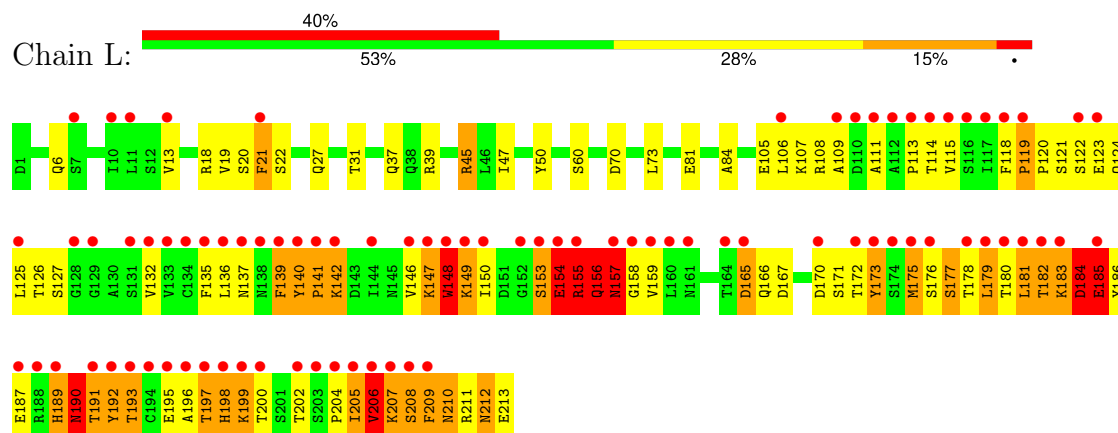
• Molecule 1: Major prion protein



• Molecule 2: POM1 FAB HEAVY CHAIN



• Molecule 3: POM1 FAB LIGHT CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	84.28Å 106.58Å 75.78Å 90.00° 95.81° 90.00°	Depositor
Resolution (Å)	38.33 – 2.70 38.33 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (38.33-2.70) 92.4 (38.33-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.242 , 0.288 0.279 , 0.316	Depositor DCC
R_{free} test set	932 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4223	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.89	0/870	1.21	4/1177 (0.3%)
2	H	0.91	2/1688 (0.1%)	1.35	17/2306 (0.7%)
3	L	1.04	8/1687 (0.5%)	1.90	68/2291 (3.0%)
All	All	0.96	10/4245 (0.2%)	1.57	89/5774 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	L	0	3
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	205	ILE	C-O	-7.33	1.16	1.24
3	L	148	TRP	CA-C	6.96	1.61	1.52
3	L	190	ASN	CA-C	6.66	1.60	1.52
3	L	154	GLU	N-CA	6.17	1.54	1.46
3	L	141	PRO	N-CD	5.91	1.56	1.47
3	L	147	LYS	C-O	-5.79	1.17	1.24
3	L	183	LYS	C-O	-5.68	1.17	1.24
2	H	188	VAL	CA-CB	5.50	1.62	1.54
2	H	48	ILE	CA-CB	-5.39	1.49	1.55
3	L	139	PHE	CA-C	5.17	1.58	1.52

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	210	ASN	N-CA-C	13.72	133.13	109.80
2	H	134	GLY	N-CA-C	13.28	125.02	111.21
3	L	142	LYS	N-CA-C	12.74	125.24	111.36
3	L	208	SER	N-CA-C	12.35	126.63	108.60
3	L	148	TRP	O-C-N	-11.13	110.30	123.10
3	L	204	PRO	CA-C-N	10.54	136.08	120.69
3	L	204	PRO	C-N-CA	10.54	136.08	120.69
3	L	141	PRO	CA-N-CD	-10.43	96.90	111.50
3	L	183	LYS	N-CA-C	10.08	123.30	111.71
3	L	190	ASN	CB-CA-C	9.78	126.07	109.65
3	L	179	LEU	CA-CB-CG	9.67	150.16	116.30
3	L	148	TRP	CA-C-O	-9.51	110.06	121.28
3	L	206	VAL	N-CA-C	9.22	120.90	108.27
3	L	210	ASN	CA-C-N	9.00	132.34	120.28
3	L	210	ASN	C-N-CA	9.00	132.34	120.28
3	L	147	LYS	CA-C-N	8.99	137.93	122.64
3	L	147	LYS	C-N-CA	8.99	137.93	122.64
3	L	190	ASN	N-CA-C	-8.98	102.11	113.43
3	L	127	SER	N-CA-C	8.91	124.20	113.16
3	L	208	SER	CA-C-N	7.64	136.13	121.54
3	L	208	SER	C-N-CA	7.64	136.13	121.54
3	L	185	GLU	N-CA-C	-7.56	103.04	111.28
3	L	146	VAL	CA-C-N	7.56	133.64	122.99
3	L	146	VAL	C-N-CA	7.56	133.64	122.99
3	L	207	LYS	N-CA-C	-7.46	97.24	109.40
2	H	160	ASN	N-CA-C	-7.46	101.10	111.39
3	L	173	TYR	N-CA-C	7.40	121.55	109.85
3	L	205	ILE	O-C-N	-7.32	115.69	122.79
1	A	216	ALA	N-CA-C	-7.27	95.32	110.80
2	H	143	LEU	CA-C-N	-7.25	113.79	121.48
2	H	143	LEU	C-N-CA	-7.25	113.79	121.48
2	H	217	PRO	N-CA-C	7.25	127.40	112.47
3	L	156	GLN	N-CA-C	7.05	125.82	110.80
3	L	153	SER	N-CA-C	-7.02	100.06	110.46
2	H	126	SER	N-CA-C	-6.88	98.04	109.46
3	L	189	HIS	N-CA-C	-6.78	99.04	109.14
3	L	157	ASN	N-CA-C	6.73	119.77	110.35
3	L	183	LYS	CA-C-N	-6.59	110.78	120.28
3	L	183	LYS	C-N-CA	-6.59	110.78	120.28
3	L	199	LYS	N-CA-C	6.59	119.46	111.82
3	L	165	ASP	N-CA-C	-6.58	102.05	110.53
3	L	165	ASP	N-CA-CB	6.51	119.74	110.44
3	L	147	LYS	N-CA-CB	-6.48	99.80	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	171	PHE	N-CA-C	6.45	119.19	110.29
3	L	204	PRO	N-CA-C	6.38	121.10	111.14
3	L	202	THR	N-CA-C	-6.35	105.39	113.01
3	L	193	THR	N-CA-C	6.34	120.16	109.76
1	A	214	SER	CA-C-N	-6.32	113.50	122.41
1	A	214	SER	C-N-CA	-6.32	113.50	122.41
2	H	162	GLY	N-CA-C	6.26	123.96	115.32
3	L	210	ASN	CB-CA-C	-6.21	103.38	113.37
3	L	207	LYS	CA-CB-CG	-6.20	101.70	114.10
3	L	192	TYR	CA-C-N	6.18	131.85	122.65
3	L	192	TYR	C-N-CA	6.18	131.85	122.65
3	L	183	LYS	CA-C-O	-6.17	113.13	120.10
2	H	199	THR	N-CA-C	6.12	119.47	109.24
3	L	158	GLY	N-CA-C	6.11	127.65	113.18
2	H	204	HIS	CA-C-N	6.10	126.28	119.32
2	H	204	HIS	C-N-CA	6.10	126.28	119.32
3	L	21	PHE	CA-C-N	-5.99	113.41	122.81
3	L	21	PHE	C-N-CA	-5.99	113.41	122.81
3	L	180	THR	N-CA-C	5.94	118.63	109.07
3	L	182	THR	N-CA-C	-5.87	102.23	110.50
3	L	147	LYS	CA-CB-CG	5.87	125.83	114.10
2	H	125	PRO	CA-C-N	-5.72	114.12	122.19
2	H	125	PRO	C-N-CA	-5.72	114.12	122.19
3	L	149	LYS	CA-C-O	-5.72	114.08	120.66
2	H	188	VAL	N-CA-CB	-5.70	105.60	111.87
3	L	154	GLU	N-CA-C	5.69	122.93	110.80
3	L	190	ASN	CA-CB-CG	5.61	118.21	112.60
1	A	214	SER	N-CA-C	5.50	117.28	111.28
3	L	181	LEU	N-CA-C	-5.49	101.02	109.52
2	H	8	GLY	N-CA-C	5.43	118.80	112.50
3	L	119	PRO	CA-C-N	5.43	125.44	119.90
3	L	119	PRO	C-N-CA	5.43	125.44	119.90
3	L	146	VAL	CA-C-O	5.42	126.22	120.48
3	L	47	ILE	N-CA-C	-5.42	107.57	112.12
3	L	118	PHE	N-CA-C	5.41	118.89	108.45
3	L	191	THR	N-CA-C	5.39	117.74	109.07
3	L	184	ASP	N-CA-C	-5.29	105.62	111.71
3	L	177	SER	CA-C-N	-5.23	115.39	122.77
3	L	177	SER	C-N-CA	-5.23	115.39	122.77
3	L	205	ILE	CB-CA-C	-5.21	103.48	111.71
3	L	146	VAL	O-C-N	5.19	128.63	123.18
3	L	142	LYS	CB-CA-C	-5.18	102.04	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	216	VAL	CA-C-N	5.14	126.26	119.84
2	H	216	VAL	C-N-CA	5.14	126.26	119.84
3	L	140	TYR	N-CA-C	5.11	118.88	107.95
3	L	205	ILE	CA-C-O	-5.03	114.65	120.99

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	189	ASN	Sidechain
3	L	148	TRP	Mainchain
3	L	155	ARG	Mainchain
3	L	45	ARG	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	A	851	0	793	28	0
2	H	1642	0	1580	84	0
3	L	1652	0	1573	157	0
4	L	1	0	0	0	0
5	A	18	0	0	5	0
5	H	30	0	0	2	0
5	L	29	0	0	4	0
All	All	4223	0	3946	261	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 32.

All (261) 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)
3:L:141:PRO:HG2	3:L:199:LYS:NZ	1.42	1.31
3:L:154:GLU:O	3:L:155:ARG:HG3	1.37	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:150:ILE:HG13	3:L:154:GLU:OE2	1.40	1.21
3:L:198:HIS:CE1	3:L:205:ILE:HD11	1.81	1.16
2:H:138:ASN:HB2	2:H:140:MET:HG3	1.31	1.13
3:L:196:ALA:HB3	3:L:205:ILE:CG1	1.81	1.11
3:L:196:ALA:HB3	3:L:205:ILE:HG13	1.18	1.11
3:L:198:HIS:CE1	3:L:205:ILE:CD1	2.34	1.09
3:L:196:ALA:CB	3:L:205:ILE:HG13	1.83	1.08
3:L:141:PRO:HG2	3:L:199:LYS:HZ3	0.95	1.03
3:L:198:HIS:HE1	3:L:205:ILE:HG12	1.23	1.02
3:L:198:HIS:CE1	3:L:205:ILE:HG12	1.95	1.01
3:L:150:ILE:HG13	3:L:154:GLU:CD	1.87	0.97
3:L:198:HIS:CE1	3:L:205:ILE:CG1	2.48	0.97
2:H:138:ASN:HB2	2:H:140:MET:CG	1.96	0.95
3:L:198:HIS:ND1	3:L:205:ILE:HD11	1.81	0.94
3:L:150:ILE:HG13	3:L:154:GLU:CG	1.99	0.92
3:L:196:ALA:HB3	3:L:205:ILE:CB	1.99	0.92
2:H:143:LEU:HD22	2:H:198:VAL:HG11	1.50	0.92
3:L:141:PRO:CD	3:L:199:LYS:HD2	2.01	0.91
2:H:159:TRP:CZ2	2:H:200:CYS:SG	2.65	0.90
3:L:150:ILE:CG1	3:L:154:GLU:HG3	2.02	0.89
2:H:211:VAL:HG11	2:H:213:LYS:HE2	1.53	0.89
2:H:168:VAL:HG12	2:H:186:VAL:HG12	1.56	0.88
2:H:138:ASN:CB	2:H:140:MET:HG3	2.03	0.88
3:L:141:PRO:CG	3:L:199:LYS:NZ	2.35	0.88
3:L:150:ILE:HG13	3:L:154:GLU:HG3	1.54	0.88
2:H:159:TRP:CH2	2:H:200:CYS:SG	2.68	0.87
3:L:141:PRO:CG	3:L:199:LYS:HZ3	1.86	0.87
2:H:161:SER:H	2:H:201:ASN:HD21	1.22	0.87
3:L:148:TRP:CD2	3:L:179:LEU:HD23	2.10	0.86
3:L:149:LYS:HE3	3:L:195:GLU:OE2	1.74	0.86
2:H:159:TRP:CE2	2:H:200:CYS:SG	2.70	0.84
2:H:138:ASN:O	2:H:139:SER:OG	1.98	0.81
3:L:150:ILE:CG1	3:L:154:GLU:OE2	2.27	0.81
3:L:147:LYS:HZ1	3:L:149:LYS:HG2	1.46	0.80
3:L:183:LYS:HA	3:L:186:TYR:HB3	1.64	0.80
2:H:211:VAL:CG1	2:H:213:LYS:HE2	2.13	0.79
3:L:141:PRO:HD2	3:L:199:LYS:HD2	1.66	0.78
3:L:149:LYS:HG3	3:L:195:GLU:OE1	1.84	0.77
3:L:191:THR:OG1	3:L:209:PHE:HA	1.85	0.76
3:L:196:ALA:HB3	3:L:205:ILE:HB	1.68	0.76
2:H:203:ALA:HB2	2:H:210:LYS:HD3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:13:VAL:HG11	3:L:19:VAL:HG11	1.68	0.74
2:H:161:SER:H	2:H:201:ASN:ND2	1.85	0.74
3:L:141:PRO:HG2	3:L:199:LYS:HZ2	1.44	0.74
2:H:159:TRP:CZ3	2:H:200:CYS:SG	2.80	0.73
3:L:148:TRP:CE2	3:L:179:LEU:HD23	2.24	0.73
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.69	0.72
2:H:125:PRO:HB3	2:H:150:TYR:HB3	1.72	0.72
2:H:173:ALA:HB2	2:H:182:LEU:HD11	1.72	0.71
3:L:183:LYS:HG3	3:L:186:TYR:HD2	1.55	0.71
3:L:198:HIS:HE1	3:L:205:ILE:CG1	1.95	0.71
3:L:189:HIS:CD2	3:L:191:THR:H	2.09	0.71
3:L:154:GLU:O	3:L:155:ARG:CG	2.29	0.71
2:H:153:GLU:HG3	2:H:154:PRO:HA	1.72	0.70
3:L:108:ARG:NE	3:L:109:ALA:O	2.24	0.70
2:H:12:VAL:HG11	2:H:86:LEU:HD12	1.73	0.70
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.73	0.70
3:L:147:LYS:HZ1	3:L:149:LYS:CG	2.03	0.70
3:L:148:TRP:CD2	3:L:179:LEU:CD2	2.75	0.70
2:H:128:TYR:CE1	3:L:123:GLU:HG2	2.29	0.68
2:H:143:LEU:CD2	2:H:198:VAL:HG11	2.25	0.67
2:H:159:TRP:CD2	2:H:200:CYS:SG	2.87	0.67
3:L:120:PRO:HD2	3:L:211:ARG:HH21	1.60	0.67
2:H:130:LEU:HD22	3:L:119:PRO:O	1.95	0.66
2:H:138:ASN:C	2:H:140:MET:H	2.02	0.66
2:H:128:TYR:CE2	3:L:124:GLN:HG3	2.31	0.66
3:L:148:TRP:CE3	3:L:179:LEU:CD2	2.78	0.66
3:L:175:MET:CE	3:L:177:SER:HB2	2.26	0.66
2:H:127:VAL:HG22	2:H:213:LYS:HE3	1.78	0.66
3:L:183:LYS:HG2	3:L:187:GLU:HG3	1.79	0.65
3:L:108:ARG:NH2	3:L:172:THR:CG2	2.59	0.65
3:L:111:ALA:O	3:L:139:PHE:HD1	1.80	0.65
3:L:181:LEU:HB3	3:L:185:GLU:HB3	1.79	0.64
2:H:138:ASN:HB2	2:H:140:MET:SD	2.37	0.64
2:H:132:PRO:O	2:H:218:ARG:N	2.25	0.64
3:L:191:THR:HG1	3:L:209:PHE:HA	1.61	0.64
3:L:190:ASN:CG	3:L:212:ASN:HD21	2.06	0.64
2:H:128:TYR:HE1	3:L:123:GLU:HG2	1.64	0.63
3:L:190:ASN:HD21	3:L:212:ASN:ND2	1.96	0.63
2:H:138:ASN:OD1	2:H:139:SER:N	2.31	0.63
2:H:192:THR:HA	2:H:196:GLU:OE2	1.99	0.62
3:L:175:MET:HE3	3:L:177:SER:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:143:LEU:HD23	2:H:215:ILE:CD1	2.29	0.62
3:L:195:GLU:HG2	3:L:196:ALA:N	2.14	0.62
2:H:128:TYR:HD1	3:L:123:GLU:CD	2.08	0.61
2:H:159:TRP:CE3	2:H:200:CYS:SG	2.93	0.61
2:H:143:LEU:HB3	2:H:215:ILE:HD12	1.82	0.61
3:L:115:VAL:O	3:L:207:LYS:NZ	2.22	0.61
3:L:150:ILE:CB	3:L:154:GLU:HG3	2.30	0.61
1:A:120:TYR:CZ	1:A:174:ILE:HD13	2.36	0.60
3:L:189:HIS:NE2	3:L:191:THR:HG22	2.16	0.60
2:H:159:TRP:HZ3	2:H:215:ILE:HD11	1.67	0.60
2:H:128:TYR:CD1	3:L:123:GLU:CD	2.80	0.59
3:L:37:GLN:OE1	3:L:45:ARG:NH1	2.36	0.59
3:L:150:ILE:O	3:L:153:SER:N	2.31	0.59
3:L:150:ILE:CG1	3:L:154:GLU:CG	2.70	0.59
3:L:122:SER:O	3:L:126:THR:HG23	2.03	0.59
1:A:212:ARG:CD	5:A:303:HOH:O	2.50	0.59
2:H:129:PRO:HB2	2:H:215:ILE:HG22	1.85	0.58
3:L:183:LYS:HG3	3:L:186:TYR:CD2	2.38	0.58
3:L:159:VAL:HA	3:L:178:THR:O	2.04	0.58
3:L:167:ASP:OD1	3:L:172:THR:N	2.33	0.57
3:L:190:ASN:ND2	3:L:212:ASN:ND2	2.53	0.57
3:L:205:ILE:O	3:L:206:VAL:HG23	2.04	0.57
1:A:191:THR:HG23	1:A:194:ASP:H	1.68	0.57
1:A:161:TYR:OH	1:A:170:ASP:OD2	2.24	0.56
1:A:203:GLU:O	1:A:207:ILE:HG13	2.06	0.56
3:L:198:HIS:ND1	3:L:205:ILE:CG1	2.68	0.56
2:H:161:SER:N	2:H:201:ASN:HD21	1.98	0.56
3:L:108:ARG:HH21	3:L:172:THR:HG23	1.71	0.56
3:L:148:TRP:CB	3:L:154:GLU:OE1	2.54	0.56
2:H:145:CYS:HG	2:H:200:CYS:CB	2.16	0.56
3:L:148:TRP:CE3	3:L:179:LEU:HD21	2.40	0.56
3:L:150:ILE:N	3:L:153:SER:O	2.28	0.55
2:H:153:GLU:CG	2:H:154:PRO:HA	2.35	0.55
3:L:141:PRO:HG2	3:L:199:LYS:CE	2.30	0.55
3:L:195:GLU:HG2	3:L:196:ALA:H	1.71	0.55
3:L:210:ASN:HD21	3:L:212:ASN:ND2	2.05	0.54
3:L:183:LYS:HA	3:L:186:TYR:CB	2.35	0.54
3:L:198:HIS:ND1	3:L:205:ILE:CD1	2.56	0.54
3:L:166:GLN:HG3	3:L:171:SER:C	2.33	0.54
3:L:183:LYS:O	3:L:187:GLU:HG3	2.08	0.54
3:L:27:GLN:NE2	5:L:404:HOH:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ARG:HD2	5:A:301:HOH:O	2.08	0.53
3:L:148:TRP:HB3	3:L:154:GLU:OE1	2.09	0.53
2:H:128:TYR:CD2	3:L:124:GLN:HG3	2.44	0.53
1:A:159:ASP:OD1	1:A:159:ASP:N	2.43	0.52
3:L:148:TRP:CE3	3:L:179:LEU:HD23	2.42	0.52
2:H:126:SER:HB3	2:H:128:TYR:CZ	2.45	0.52
3:L:183:LYS:CA	3:L:186:TYR:HB3	2.37	0.52
1:A:120:TYR:CE1	1:A:174:ILE:HD13	2.45	0.51
3:L:190:ASN:ND2	3:L:212:ASN:HD21	2.08	0.51
1:A:162:ASN:O	1:A:162:ASN:ND2	2.44	0.51
3:L:108:ARG:NH2	3:L:172:THR:HG23	2.26	0.51
3:L:154:GLU:C	3:L:155:ARG:HG3	2.28	0.51
3:L:111:ALA:O	3:L:139:PHE:HA	2.11	0.51
3:L:139:PHE:HE1	3:L:200:THR:HG23	1.76	0.51
3:L:186:TYR:HA	3:L:192:TYR:OH	2.10	0.50
3:L:196:ALA:HB1	3:L:205:ILE:HG13	1.88	0.50
2:H:168:VAL:CG1	2:H:186:VAL:HG12	2.36	0.50
3:L:167:ASP:OD2	3:L:170:ASP:HB2	2.11	0.50
2:H:1:GLN:CD	2:H:1:GLN:N	2.69	0.50
2:H:138:ASN:C	2:H:140:MET:N	2.70	0.50
3:L:115:VAL:HA	3:L:135:PHE:O	2.13	0.49
3:L:153:SER:O	3:L:154:GLU:HB2	2.13	0.49
2:H:198:VAL:HG12	2:H:215:ILE:HD11	1.95	0.49
3:L:139:PHE:CE1	3:L:200:THR:HG23	2.48	0.49
2:H:142:THR:HA	2:H:186:VAL:O	2.13	0.49
2:H:173:ALA:HB2	2:H:182:LEU:CD1	2.41	0.49
1:A:202:VAL:HA	1:A:205:MET:HE3	1.94	0.48
2:H:99:SER:HB2	2:H:104:TYR:HA	1.96	0.48
3:L:140:TYR:CD2	3:L:141:PRO:HA	2.49	0.48
3:L:111:ALA:O	3:L:139:PHE:CD1	2.62	0.48
3:L:107:LYS:NZ	3:L:108:ARG:O	2.36	0.48
1:A:183:THR:HG21	1:A:190:PHE:CZ	2.48	0.48
2:H:143:LEU:CD2	2:H:198:VAL:CG1	2.92	0.48
3:L:20:SER:HA	3:L:73:LEU:O	2.14	0.48
2:H:168:VAL:HA	2:H:185:SER:O	2.13	0.48
3:L:142:LYS:HE2	3:L:173:TYR:CE1	2.49	0.48
3:L:210:ASN:HD21	3:L:212:ASN:HD21	1.60	0.47
2:H:124:PRO:HG3	2:H:207:SER:HB2	1.96	0.47
3:L:175:MET:SD	3:L:176:SER:N	2.87	0.47
2:H:161:SER:N	2:H:201:ASN:ND2	2.58	0.47
3:L:159:VAL:HA	3:L:179:LEU:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3:GLN:NE2	5:H:309:HOH:O	2.46	0.47
2:H:137:THR:O	2:H:137:THR:OG1	2.22	0.47
3:L:141:PRO:HD3	3:L:199:LYS:HD2	1.91	0.47
2:H:159:TRP:CE2	2:H:186:VAL:HG13	2.49	0.47
3:L:115:VAL:HB	3:L:207:LYS:HE2	1.96	0.47
1:A:146:MET:HA	1:A:149:TYR:CD2	2.50	0.47
3:L:189:HIS:CD2	3:L:191:THR:N	2.79	0.47
3:L:195:GLU:CG	3:L:196:ALA:N	2.77	0.47
2:H:150:TYR:OH	2:H:182:LEU:HD13	2.14	0.47
3:L:147:LYS:NZ	3:L:149:LYS:CG	2.76	0.47
3:L:170:ASP:O	3:L:172:THR:HG23	2.15	0.47
1:A:120:TYR:CD1	1:A:156:ARG:HG2	2.50	0.46
1:A:177:LYS:HA	1:A:177:LYS:HD3	1.41	0.46
2:H:34:MET:HE2	2:H:34:MET:HB2	1.80	0.46
3:L:183:LYS:HG2	3:L:183:LYS:O	2.15	0.46
3:L:31:THR:O	3:L:50:TYR:HA	2.16	0.46
3:L:166:GLN:HG3	3:L:171:SER:O	2.16	0.46
2:H:156:THR:OG1	2:H:203:ALA:HB3	2.15	0.46
3:L:156:GLN:OE1	3:L:157:ASN:HA	2.15	0.46
3:L:196:ALA:CB	3:L:205:ILE:HB	2.42	0.46
3:L:196:ALA:CB	3:L:205:ILE:CB	2.85	0.46
1:A:188:GLU:HB3	5:A:308:HOH:O	2.16	0.45
3:L:139:PHE:CG	3:L:140:TYR:N	2.84	0.45
3:L:141:PRO:HG2	3:L:199:LYS:CD	2.46	0.45
3:L:148:TRP:NE1	3:L:159:VAL:HG11	2.32	0.45
1:A:128:ARG:NH1	1:A:146:MET:O	2.50	0.45
2:H:138:ASN:CG	2:H:140:MET:HG3	2.41	0.45
1:A:178:GLN:O	1:A:182:THR:HG23	2.16	0.45
1:A:212:ARG:NE	5:A:303:HOH:O	2.49	0.45
2:H:138:ASN:C	2:H:139:SER:HG	2.10	0.45
2:H:143:LEU:HD23	2:H:215:ILE:HD12	1.99	0.45
3:L:166:GLN:HG2	3:L:171:SER:HA	1.98	0.45
3:L:183:LYS:O	3:L:183:LYS:CG	2.64	0.45
3:L:195:GLU:CG	3:L:196:ALA:H	2.28	0.45
2:H:148:LYS:HE3	2:H:176:GLN:NE2	2.31	0.45
2:H:159:TRP:HB3	2:H:164:LEU:HD12	1.99	0.44
1:A:154:TYR:CE2	1:A:178:GLN:HG2	2.53	0.44
3:L:141:PRO:CG	3:L:199:LYS:HZ2	2.14	0.44
3:L:70:ASP:HB2	5:L:402:HOH:O	2.17	0.44
3:L:150:ILE:HB	3:L:154:GLU:HG3	1.98	0.44
1:A:139:ASP:OD2	2:H:104:TYR:OH	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:175:MET:HE1	3:L:177:SER:HB2	1.97	0.44
3:L:125:LEU:HD23	3:L:125:LEU:HA	1.86	0.44
3:L:193:THR:HG22	3:L:208:SER:OG	2.17	0.44
3:L:211:ARG:C	3:L:213:GLU:H	2.25	0.44
1:A:122:LEU:HD13	1:A:154:TYR:CE1	2.53	0.43
3:L:159:VAL:HB	3:L:179:LEU:HB3	1.99	0.43
3:L:205:ILE:HG12	3:L:205:ILE:H	1.37	0.43
2:H:193:TRP:CG	2:H:194:PRO:HA	2.53	0.43
3:L:18:ARG:HD2	5:L:422:HOH:O	2.19	0.43
3:L:197:THR:O	3:L:198:HIS:O	2.36	0.43
2:H:13:MET:HE3	2:H:13:MET:HB3	1.84	0.43
3:L:183:LYS:O	3:L:186:TYR:HB3	2.18	0.43
2:H:152:PRO:O	2:H:204:HIS:NE2	2.41	0.43
3:L:39:ARG:HG2	3:L:84:ALA:HB2	2.00	0.43
1:A:191:THR:HG22	1:A:194:ASP:OD2	2.19	0.43
3:L:108:ARG:HD2	3:L:171:SER:OG	2.19	0.43
3:L:108:ARG:HD2	3:L:171:SER:HG	1.83	0.43
2:H:210:LYS:HA	2:H:210:LYS:HD2	1.69	0.42
3:L:208:SER:OG	3:L:209:PHE:N	2.51	0.42
1:A:212:ARG:HD2	5:A:303:HOH:O	2.16	0.42
2:H:18:VAL:HG12	2:H:86:LEU:HD11	2.00	0.42
3:L:108:ARG:HH21	3:L:172:THR:CG2	2.27	0.42
1:A:121:MET:O	1:A:154:TYR:HA	2.19	0.42
1:A:191:THR:HG22	1:A:194:ASP:CG	2.45	0.42
2:H:160:ASN:OD1	2:H:199:THR:N	2.33	0.42
3:L:60:SER:N	5:L:409:HOH:O	2.53	0.42
3:L:148:TRP:HB2	3:L:154:GLU:OE1	2.20	0.42
2:H:216:VAL:HG13	2:H:217:PRO:HD2	2.02	0.42
3:L:6:GLN:HA	3:L:22:SER:O	2.20	0.42
2:H:203:ALA:CB	2:H:210:LYS:HD3	2.44	0.42
3:L:211:ARG:C	3:L:213:GLU:N	2.77	0.42
2:H:127:VAL:HG22	2:H:213:LYS:CE	2.49	0.41
2:H:209:THR:HG23	2:H:211:VAL:HG23	2.03	0.41
1:A:162:ASN:ND2	1:A:162:ASN:C	2.78	0.41
1:A:176:VAL:HG22	1:A:198:MET:HG2	2.02	0.41
3:L:182:THR:O	3:L:185:GLU:HB2	2.21	0.41
3:L:113:PRO:HA	3:L:137:ASN:O	2.20	0.41
2:H:11:LEU:HD22	2:H:12:VAL:N	2.35	0.41
3:L:165:ASP:OD1	3:L:166:GLN:N	2.38	0.41
3:L:184:ASP:HA	3:L:187:GLU:HB2	2.02	0.41
2:H:39:GLN:HA	5:H:308:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:215:ILE:H	2:H:215:ILE:HG12	1.61	0.41
3:L:150:ILE:CD1	3:L:154:GLU:CG	2.98	0.41
3:L:13:VAL:O	3:L:106:LEU:HA	2.21	0.40
2:H:129:PRO:CB	2:H:215:ILE:HG22	2.51	0.40
2:H:159:TRP:CD2	2:H:186:VAL:HG11	2.56	0.40
3:L:136:LEU:HD12	3:L:136:LEU:N	2.37	0.40
3:L:183:LYS:O	3:L:187:GLU:N	2.52	0.40
3:L:197:THR:O	3:L:198:HIS:CG	2.74	0.40
1:A:155:TYR:OH	1:A:213:GLU:OE2	2.37	0.40
2:H:111:GLN:H	2:H:111:GLN:HG3	1.71	0.40
2:H:193:TRP:CZ2	2:H:217:PRO:HD3	2.56	0.40
3:L:148:TRP:NE1	3:L:159:VAL:HG21	2.37	0.40
3:L:150:ILE:CD1	3:L:154:GLU:HG3	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	99/135 (73%)	97 (98%)	2 (2%)	0	100	100
2	H	216/218 (99%)	207 (96%)	6 (3%)	3 (1%)	9	23
3	L	211/213 (99%)	192 (91%)	13 (6%)	6 (3%)	4	9
All	All	526/566 (93%)	496 (94%)	21 (4%)	9 (2%)	7	19

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	135	GLY
3	L	154	GLU
3	L	198	HIS
2	H	138	ASN

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Mol	Chain	Res	Type
3	L	155	ARG
3	L	156	GLN
3	L	197	THR
3	L	209	PHE
2	H	132	PRO

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	A	94/123 (76%)	90 (96%)	4 (4%)	26	54
2	H	187/187 (100%)	172 (92%)	15 (8%)	11	28
3	L	191/191 (100%)	179 (94%)	12 (6%)	16	39
All	All	472/501 (94%)	441 (93%)	31 (7%)	15	36

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	LEU
1	A	126	MET
1	A	159	ASP
1	A	177	LYS
2	H	7	SER
2	H	11	LEU
2	H	127	VAL
2	H	137	THR
2	H	140	MET
2	H	141	VAL
2	H	161	SER
2	H	168	VAL
2	H	183	SER
2	H	185	SER
2	H	191	SER
2	H	196	GLU
2	H	201	ASN

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Mol	Chain	Res	Type
2	H	209	THR
2	H	215	ILE
3	L	21	PHE
3	L	81	GLU
3	L	105	GLU
3	L	114	THR
3	L	121	SER
3	L	157	ASN
3	L	175	MET
3	L	184	ASP
3	L	185	GLU
3	L	190	ASN
3	L	206	VAL
3	L	212	ASN

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

Mol	Chain	Res	Type
1	A	162	ASN
1	A	209	GLN
2	H	201	ASN
3	L	189	HIS
3	L	198	HIS
3	L	212	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

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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	A	101/135 (74%)	0.87	12 (11%)	9 7	45, 65, 95, 107	0
2	H	218/218 (100%)	1.14	55 (25%)	1 1	39, 61, 132, 146	0
3	L	213/213 (100%)	1.63	85 (39%)	1 0	43, 78, 147, 155	0
All	All	532/566 (93%)	1.29	152 (28%)	1 1	39, 68, 140, 155	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	116	SER	9.0
2	H	144	GLY	7.3
3	L	135	PHE	7.1
2	H	130	LEU	6.4
3	L	193	THR	6.2
2	H	134	GLY	6.0
3	L	133	VAL	5.7
3	L	148	TRP	5.5
2	H	184	SER	5.4
3	L	119	PRO	5.1
3	L	200	THR	5.1
3	L	115	VAL	4.9
2	H	147	VAL	4.8
3	L	192	TYR	4.5
2	H	188	VAL	4.5
3	L	155	ARG	4.4
3	L	206	VAL	4.4
2	H	183	SER	4.4
2	H	142	THR	4.4
2	H	174	VAL	4.3
3	L	118	PHE	4.3
3	L	208	SER	4.2
3	L	132	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
2	H	145	CYS	4.2
2	H	175	LEU	4.1
2	H	128	TYR	4.1
3	L	128	GLY	4.1
3	L	199	LYS	4.0
2	H	157	VAL	3.9
1	A	216	ALA	3.9
3	L	117	ILE	3.9
3	L	114	THR	3.9
2	H	186	VAL	3.9
2	H	127	VAL	3.8
2	H	143	LEU	3.8
2	H	187	THR	3.7
3	L	173	TYR	3.7
3	L	159	VAL	3.7
3	L	175	MET	3.7
3	L	179	LEU	3.6
2	H	182	LEU	3.6
2	H	190	SER	3.6
1	A	217	TYR	3.5
3	L	146	VAL	3.5
1	A	215	GLN	3.5
3	L	178	THR	3.4
2	H	199	THR	3.4
3	L	144	ILE	3.4
3	L	149	LYS	3.4
3	L	207	LYS	3.4
2	H	189	PRO	3.3
2	H	216	VAL	3.3
1	A	192	GLU	3.3
3	L	136	LEU	3.3
3	L	139	PHE	3.3
3	L	194	CYS	3.3
2	H	135	GLY	3.3
3	L	137	ASN	3.3
2	H	200	CYS	3.2
2	H	202	VAL	3.2
2	H	137	THR	3.2
2	H	133	GLY	3.2
2	H	131	ALA	3.2
1	A	120	TYR	3.2
3	L	202	THR	3.2

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Mol	Chain	Res	Type	RSRZ
3	L	131	SER	3.2
3	L	106	LEU	3.1
3	L	196	ALA	3.1
2	H	129	PRO	3.1
3	L	198	HIS	3.1
2	H	166	GLY	3.1
2	H	136	ALA	3.1
3	L	183	LYS	3.1
3	L	157	ASN	3.0
3	L	205	ILE	3.0
3	L	112	ALA	3.0
1	A	117	LEU	3.0
3	L	174	SER	3.0
3	L	111	ALA	3.0
3	L	142	LYS	3.0
2	H	146	LEU	2.9
2	H	173	ALA	2.9
2	H	191	SER	2.9
1	A	154	TYR	2.9
3	L	129	GLY	2.9
2	H	141	VAL	2.9
3	L	11	LEU	2.9
3	L	123	GLU	2.8
3	L	134	CYS	2.8
2	H	132	PRO	2.8
2	H	185	SER	2.8
2	H	213	LYS	2.8
3	L	140	TYR	2.8
3	L	10	ILE	2.7
2	H	164	LEU	2.7
3	L	161	ASN	2.7
3	L	154	GLU	2.7
1	A	158	VAL	2.7
3	L	165	ASP	2.7
1	A	186	LYS	2.7
3	L	7	SER	2.7
3	L	204	PRO	2.7
2	H	217	PRO	2.6
3	L	113	PRO	2.6
3	L	182	THR	2.6
3	L	147	LYS	2.6
3	L	172	THR	2.6

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Mol	Chain	Res	Type	RSRZ
3	L	150	ILE	2.6
3	L	195	GLU	2.5
2	H	167	GLY	2.5
3	L	209	PHE	2.5
2	H	169	HIS	2.5
3	L	158	GLY	2.5
2	H	196	GLU	2.5
3	L	138	ASN	2.5
3	L	197	THR	2.5
2	H	218	ARG	2.4
3	L	160	LEU	2.4
3	L	180	THR	2.4
2	H	126	SER	2.4
3	L	110	ASP	2.3
2	H	155	VAL	2.3
3	L	21	PHE	2.3
3	L	187	GLU	2.3
2	H	139	SER	2.3
3	L	176	SER	2.3
3	L	185	GLU	2.3
3	L	170	ASP	2.3
1	A	173	ASN	2.3
3	L	181	LEU	2.3
3	L	109	ALA	2.2
1	A	126	MET	2.2
3	L	153	SER	2.2
3	L	125	LEU	2.2
3	L	191	THR	2.2
2	H	103	TYR	2.2
3	L	122	SER	2.2
3	L	13	VAL	2.2
2	H	181	THR	2.1
2	H	165	SER	2.1
3	L	203	SER	2.1
2	H	162	GLY	2.1
3	L	188	ARG	2.1
3	L	164	THR	2.1
3	L	141	PRO	2.1
3	L	152	GLY	2.1
2	H	150	TYR	2.1
2	H	163	SER	2.0
3	L	189	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	156	ARG	2.0
2	H	170	THR	2.0
2	H	198	VAL	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	L	301	1/1	0.59	0.28	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.