



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:48 AM UTC

PDB ID : 3D9A / pdb_00003d9a
Title : High Resolution Crystal Structure Structure of HyHel10 Fab Complexed to Hen Egg Lysozyme
Authors : DeSantis, M.E.; Li, M.; Shanmuganathan, A.; Acchione, M.; Walter, R.; Wlodawer, A.; Smith-Gill, S.
Deposited on : 2008-05-27
Resolution : 1.20 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

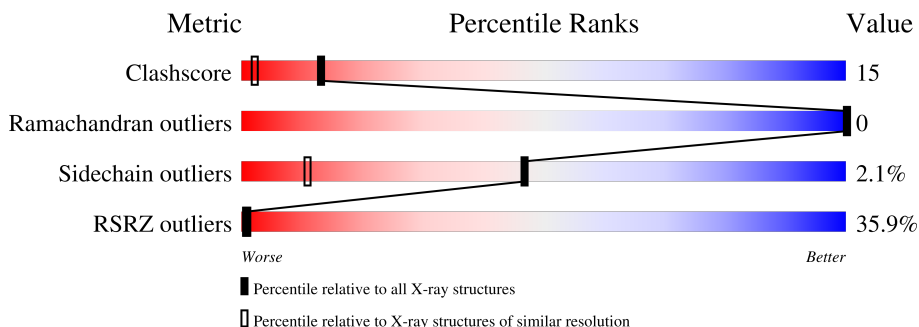
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 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	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)
RSRZ outliers	180081	1214 (1.20-1.20)

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	C	129	33% 79% 21%
2	L	213	36% 86% 12% .
3	H	210	37% 81% 16% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4947 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 Lysozyme C.

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

- Molecule 2 is a protein called Light Chain of HyHel10 Antibody Fragment (Fab).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	2	0
			1655	1029	280	340	6			

- Molecule 3 is a protein called Heavy Chain of HyHel10 Antibody Fragment (Fab).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	210	Total	C	N	O	S	0	1	0
			1608	1016	256	330	6			

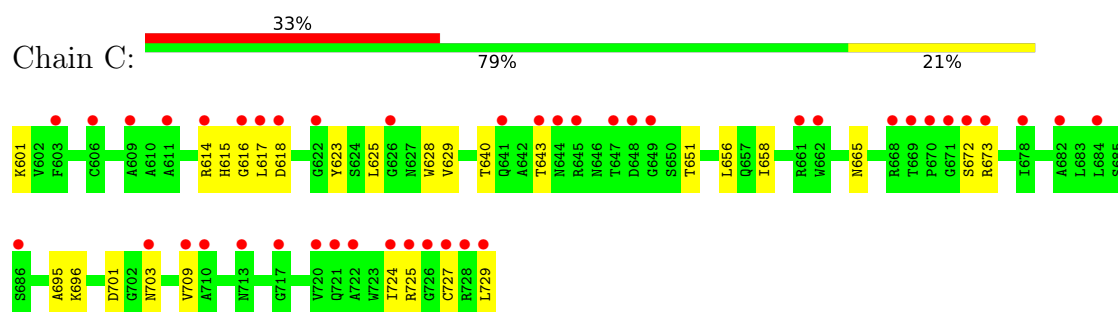
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	155	Total	O	0	0
			155	155		
4	L	268	Total	O	0	0
			268	268		
4	H	260	Total	O	0	0
			260	260		

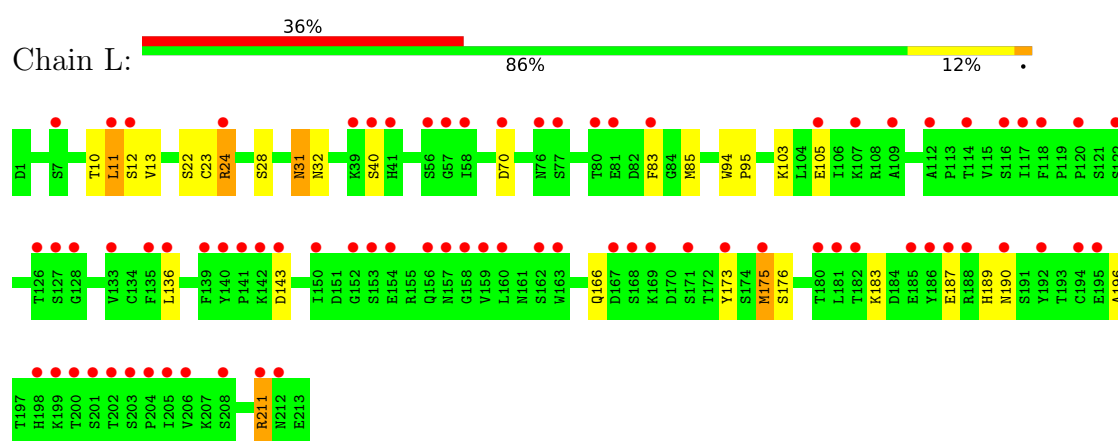
3 Residue-property plots

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.

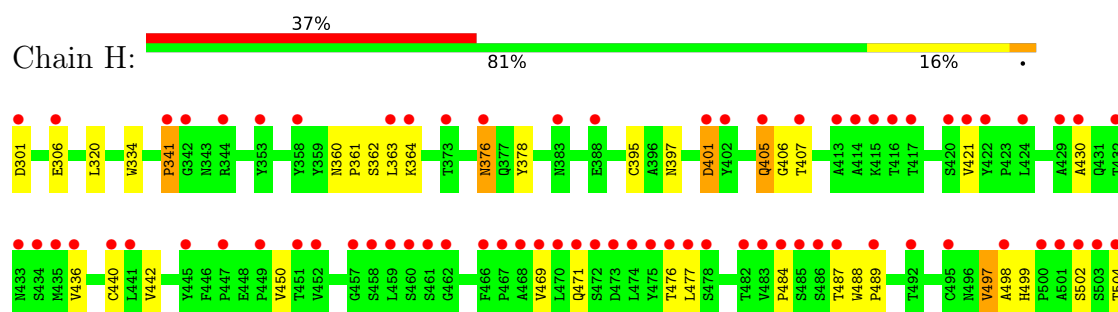
• Molecule 1: Lysozyme C

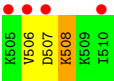


• Molecule 2: Light Chain of HyHel10 Antibody Fragment (Fab)



• Molecule 3: Heavy Chain of HyHel10 Antibody Fragment (Fab)





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	39.84Å 77.39Å 89.11Å 90.00° 96.66° 90.00°	Depositor
Resolution (Å)	50.00 – 1.20 50.00 – 1.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-1.20) 94.3 (50.00-1.20)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 1.20Å)	Xtriage
Refinement program	REFMAC 5.4.0057	Depositor
R, R_{free}	0.190 , 0.205 0.197 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.0	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 40.4	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	0.95	EDS
Total number of atoms	4947	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% 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

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	C	0.67	0/1021	0.81	0/1379
2	L	0.62	0/1699	0.75	1/2308 (0.0%)
3	H	0.65	0/1655	0.82	3/2272 (0.1%)
All	All	0.64	0/4375	0.79	4/5959 (0.1%)

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
3	H	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	498	ALA	N-CA-C	11.56	129.38	109.96
3	H	405	GLN	N-CA-C	6.30	120.22	112.54
2	L	211	ARG	NE-CZ-NH2	5.44	124.09	119.20
3	H	341	PRO	N-CA-C	5.36	123.51	112.47

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	497	VAL	Peptide

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	C	1001	0	956	38	0
2	L	1655	0	1582	37	0
3	H	1608	0	1546	53	0
4	C	155	0	0	30	0
4	H	260	0	0	31	1
4	L	268	0	0	16	1
All	All	4947	0	4084	124	1

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 15.

All (124) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:176:SER:HB3	4:L:454:HOH:O	1.09	1.26
3:H:406:GLY:N	4:H:644:HOH:O	1.61	1.24
3:H:376:ASN:HB2	4:H:721:HOH:O	1.34	1.20
1:C:625:LEU:HD12	4:C:814:HOH:O	1.46	1.13
3:H:497:VAL:HG11	4:H:757:HOH:O	1.50	1.09
1:C:617:LEU:O	4:C:805:HOH:O	1.72	1.08
3:H:362:SER:OG	3:H:363:LEU:CD1	2.06	1.04
2:L:189:HIS:O	2:L:211:ARG:HD3	1.56	1.03
3:H:306:GLU:OE1	4:H:644:HOH:O	1.80	1.00
3:H:405:GLN:O	4:H:605:HOH:O	1.87	0.93
3:H:397:ASN:ND2	3:H:401:ASP:OD2	2.04	0.90
3:H:362:SER:OG	3:H:363:LEU:HD12	1.72	0.89
2:L:70:ASP:HB3	4:L:291:HOH:O	1.71	0.89
2:L:28:SER:OG	4:L:366:HOH:O	1.92	0.88
1:C:703:ASN:ND2	4:C:782:HOH:O	2.07	0.87
3:H:484:PRO:O	3:H:487:THR:HG22	1.77	0.84
2:L:176:SER:CB	4:L:454:HOH:O	1.82	0.82
2:L:189:HIS:O	2:L:211:ARG:CD	2.27	0.82
1:C:618:ASP:OD1	4:C:806:HOH:O	1.97	0.81
2:L:11:LEU:HD22	2:L:13:VAL:HG22	1.60	0.80
1:C:703:ASN:OD1	4:C:749:HOH:O	2.00	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:10:THR:HG23	4:L:434:HOH:O	1.83	0.78
3:H:499:HIS:HB3	3:H:504:THR:OG1	1.84	0.78
1:C:703:ASN:CG	4:C:749:HOH:O	2.26	0.78
1:C:724:ILE:CG2	4:C:789:HOH:O	2.31	0.77
1:C:665:ASN:OD1	4:C:868:HOH:O	2.04	0.76
1:C:623:TYR:OH	4:C:872:HOH:O	2.01	0.75
3:H:301:ASP:O	4:H:647:HOH:O	2.03	0.75
3:H:407[A]:THR:HG22	4:H:533:HOH:O	1.86	0.75
1:C:703:ASN:ND2	4:C:749:HOH:O	2.18	0.75
1:C:629:VAL:CG2	4:C:789:HOH:O	2.34	0.74
1:C:625:LEU:HD22	4:C:815:HOH:O	1.87	0.73
3:H:376:ASN:CB	4:H:721:HOH:O	2.07	0.72
1:C:614:ARG:HD3	4:C:847:HOH:O	1.88	0.72
3:H:361:PRO:HA	3:H:364:LYS:HG3	1.70	0.71
3:H:376:ASN:CG	4:H:721:HOH:O	2.31	0.71
2:L:190:ASN:OD1	4:L:346:HOH:O	2.08	0.70
3:H:306:GLU:CG	4:H:533:HOH:O	2.38	0.70
3:H:360:ASN:HB3	3:H:363:LEU:HD13	1.76	0.68
1:C:709:VAL:HG23	4:C:849:HOH:O	1.93	0.67
3:H:320:LEU:HD13	4:H:729:HOH:O	1.93	0.67
2:L:22:SER:OG	2:L:24:ARG:NE	2.23	0.67
2:L:85:MET:SD	2:L:103:LYS:HD3	2.35	0.67
3:H:476:THR:HG23	4:H:603:HOH:O	1.94	0.67
3:H:442:VAL:HG13	4:H:757:HOH:O	1.95	0.66
3:H:362:SER:C	3:H:363:LEU:HD12	2.20	0.66
3:H:363:LEU:HD12	3:H:363:LEU:N	2.11	0.64
1:C:629:VAL:HG23	4:C:789:HOH:O	1.98	0.62
3:H:421:VAL:HG21	3:H:506:VAL:HG21	1.82	0.62
3:H:405:GLN:HG2	4:H:519:HOH:O	1.99	0.62
1:C:696:LYS:NZ	2:L:32:ASN:HD21	1.98	0.61
1:C:656:LEU:HD12	4:C:869:HOH:O	2.01	0.61
3:H:306:GLU:HG2	4:H:533:HOH:O	1.99	0.60
3:H:430:ALA:HB1	4:H:634:HOH:O	2.01	0.60
3:H:421:VAL:HG22	4:H:757:HOH:O	2.01	0.60
3:H:306:GLU:CD	4:H:533:HOH:O	2.45	0.58
3:H:306:GLU:HG3	3:H:395:CYS:SG	2.43	0.57
1:C:696:LYS:NZ	2:L:31:ASN:HD21	2.02	0.57
1:C:629:VAL:HG21	4:C:789:HOH:O	2.03	0.57
2:L:10:THR:CG2	4:L:447:HOH:O	2.52	0.57
1:C:701:ASP:OD2	1:C:703:ASN:ND2	2.37	0.56
2:L:105:GLU:OE2	2:L:173:TYR:OH	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:421:VAL:HG21	3:H:506:VAL:CG2	2.36	0.55
1:C:673:ARG:HG3	4:C:864:HOH:O	2.07	0.54
3:H:469:VAL:HG23	4:H:746:HOH:O	2.06	0.54
3:H:421:VAL:CG2	4:H:757:HOH:O	2.56	0.54
1:C:658:ILE:HD11	4:C:869:HOH:O	2.06	0.54
3:H:364:LYS:CG	4:H:624:HOH:O	2.55	0.53
2:L:166:GLN:NE2	4:L:426:HOH:O	2.37	0.53
1:C:696:LYS:HZ3	2:L:31:ASN:HD21	1.56	0.53
2:L:83:PHE:CE1	2:L:166:GLN:HB3	2.44	0.53
1:C:615:HIS:HD2	4:C:738:HOH:O	1.92	0.53
2:L:23:CYS:C	2:L:24:ARG:HD3	2.34	0.53
3:H:476:THR:HG21	4:H:701:HOH:O	2.09	0.53
3:H:301:ASP:HA	4:H:572:HOH:O	2.08	0.52
3:H:363:LEU:CD1	3:H:363:LEU:N	2.72	0.52
2:L:83:PHE:CZ	2:L:166:GLN:HB3	2.45	0.52
1:C:724:ILE:HG21	4:C:789:HOH:O	2.05	0.52
2:L:10:THR:HG22	4:L:447:HOH:O	2.08	0.52
3:H:502:SER:OG	3:H:504:THR:HG23	2.10	0.52
1:C:618:ASP:O	4:C:745:HOH:O	2.19	0.51
2:L:183:LYS:O	2:L:187:GLU:HG3	2.11	0.50
2:L:94:TRP:CD2	2:L:95:PRO:HA	2.46	0.50
3:H:334:TRP:HB3	3:H:378:TYR:CZ	2.47	0.50
1:C:643:THR:CG2	1:C:651:THR:CG2	2.90	0.49
2:L:40:SER:O	4:L:441:HOH:O	2.19	0.49
1:C:625:LEU:HG	4:C:789:HOH:O	2.12	0.49
1:C:729:LEU:N	1:C:729:LEU:HD23	2.27	0.49
3:H:421:VAL:CG2	3:H:506:VAL:HG21	2.44	0.48
1:C:672:SER:CB	4:C:868:HOH:O	2.61	0.48
3:H:407[B]:THR:HG23	4:H:533:HOH:O	2.14	0.48
2:L:24:ARG:NE	4:L:311:HOH:O	2.47	0.47
2:L:10:THR:HG21	4:L:447:HOH:O	2.14	0.47
1:C:616:GLY:HA3	2:L:31:ASN:ND2	2.30	0.46
1:C:623:TYR:O	4:C:805:HOH:O	2.20	0.46
3:H:450:VAL:CG2	3:H:477:LEU:HD13	2.46	0.46
3:H:362:SER:OG	3:H:363:LEU:HD13	2.07	0.45
2:L:12:SER:OG	4:L:447:HOH:O	2.20	0.45
3:H:306:GLU:CD	4:H:644:HOH:O	2.49	0.44
2:L:136:LEU:CD2	2:L:196:ALA:HB2	2.48	0.44
2:L:31:ASN:H	2:L:31:ASN:HD22	1.65	0.44
1:C:727:CYS:HB3	4:C:787:HOH:O	2.17	0.43
3:H:471:GLN:NE2	4:H:701:HOH:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:136:LEU:HD23	2:L:196:ALA:HB2	1.99	0.43
3:H:362:SER:OG	3:H:363:LEU:HD11	2.10	0.43
3:H:436:VAL:HB	4:H:645:HOH:O	2.18	0.43
1:C:601:LYS:N	1:C:640:THR:HG1	2.17	0.42
1:C:628:TRP:HB2	4:C:814:HOH:O	2.19	0.42
2:L:105:GLU:CD	4:L:426:HOH:O	2.62	0.42
2:L:24:ARG:HD3	2:L:24:ARG:N	2.34	0.42
3:H:487:THR:HG21	4:H:752:HOH:O	2.19	0.42
1:C:695:ALA:HB2	4:C:869:HOH:O	2.18	0.42
3:H:362:SER:CB	3:H:363:LEU:HD12	2.48	0.42
3:H:488:TRP:CD1	3:H:489:PRO:HA	2.54	0.42
3:H:507:ASP:O	3:H:508:LYS:HD2	2.19	0.42
1:C:725:ARG:NE	4:C:764:HOH:O	2.49	0.42
1:C:672:SER:HB3	4:C:868:HOH:O	2.20	0.42
2:L:103:LYS:HD2	4:L:303:HOH:O	2.19	0.42
2:L:11:LEU:CD2	2:L:13:VAL:HG22	2.42	0.41
3:H:477:LEU:HA	4:H:655:HOH:O	2.21	0.41
3:H:487:THR:HG23	4:H:577:HOH:O	2.21	0.41
3:H:364:LYS:HG2	4:H:624:HOH:O	2.19	0.40
2:L:136:LEU:HD13	2:L:175:MET:HG2	2.04	0.40
2:L:187:GLU:HG2	4:L:362:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:469:HOH:O	4:H:538:HOH:O[2_656]	1.98	0.22

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	C	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
2	L	213/213 (100%)	210 (99%)	3 (1%)	0	100	100
3	H	209/210 (100%)	205 (98%)	4 (2%)	0	100	100
All	All	549/552 (100%)	540 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	C	105/105 (100%)	105 (100%)	0	100	100
2	L	193/191 (101%)	188 (97%)	5 (3%)	40	7
3	H	188/187 (100%)	183 (97%)	5 (3%)	39	6
All	All	486/483 (101%)	476 (98%)	10 (2%)	47	11

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	11	LEU
2	L	24	ARG
2	L	31	ASN
2	L	143	ASP
2	L	175	MET
3	H	341	PRO
3	H	376	ASN
3	H	401	ASP
3	H	440	CYS
3	H	508	LYS

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

Mol	Chain	Res	Type
1	C	615	HIS
1	C	637	ASN
1	C	641	GLN
1	C	644	ASN
1	C	646	ASN
1	C	693	ASN
1	C	713	ASN
1	C	721	GLN
2	L	31	ASN
2	L	32	ASN
2	L	53	GLN
2	L	92	ASN
2	L	190	ASN
2	L	210	ASN
3	H	377	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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 ⓘ

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	C	129/129 (100%)	1.71	43 (33%) 1 1	12, 16, 25, 39	0
2	L	213/213 (100%)	1.76	77 (36%) 1 1	10, 19, 27, 31	2 (0%)
3	H	210/210 (100%)	1.86	78 (37%) 1 1	11, 19, 27, 34	1 (0%)
All	All	552/552 (100%)	1.79	198 (35%) 1 1	10, 18, 27, 39	3 (0%)

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	649	GLY	7.1
2	L	41	HIS	6.9
3	H	469	VAL	6.5
2	L	163	TRP	6.0
1	C	703	ASN	5.9
2	L	83	PHE	5.8
2	L	157	ASN	5.7
3	H	413	ALA	5.6
3	H	440	CYS	5.5
1	C	670	PRO	5.4
3	H	341	PRO	5.4
3	H	504	THR	5.1
3	H	503	SER	5.1
2	L	40	SER	5.0
3	H	498	ALA	5.0
2	L	156	GLN	4.9
1	C	662	TRP	4.8
3	H	462	GLY	4.8
2	L	11	LEU	4.5
3	H	500	PRO	4.4
3	H	415	LYS	4.4
1	C	709	VAL	4.3
1	C	729	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
3	H	363	LEU	4.2
3	H	473	ASP	4.1
1	C	726	GLY	4.1
2	L	142	LYS	4.1
3	H	373	THR	4.1
2	L	182	THR	4.0
3	H	461	SER	3.9
3	H	436	VAL	3.9
2	L	24	ARG	3.8
3	H	301	ASP	3.8
1	C	725	ARG	3.8
3	H	505	LYS	3.8
1	C	622	GLY	3.7
2	L	169	LYS	3.7
2	L	202	THR	3.7
3	H	433	ASN	3.7
1	C	672	SER	3.7
2	L	160	LEU	3.7
3	H	487	THR	3.6
2	L	208	SER	3.6
2	L	188	ARG	3.6
3	H	388	GLU	3.6
2	L	181	LEU	3.6
1	C	669	THR	3.6
1	C	645	ARG	3.5
3	H	472	SER	3.5
3	H	405	GLN	3.5
3	H	364	LYS	3.5
3	H	470	LEU	3.5
2	L	168	SER	3.5
3	H	353	TYR	3.4
3	H	475	TYR	3.4
3	H	342	GLY	3.4
3	H	501	ALA	3.4
2	L	143	ASP	3.3
3	H	466	PHE	3.3
2	L	133	VAL	3.3
2	L	136	LEU	3.3
2	L	139	PHE	3.3
2	L	212	ASN	3.3
2	L	7	SER	3.2
2	L	112	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
2	L	128	GLY	3.2
3	H	476	THR	3.2
2	L	211	ARG	3.2
3	H	507	ASP	3.2
1	C	713	ASN	3.1
3	H	414	ALA	3.1
1	C	617	LEU	3.1
1	C	684	LEU	3.1
3	H	445	TYR	3.1
2	L	194	CYS	3.0
3	H	471	GLN	3.0
2	L	70	ASP	3.0
3	H	506	VAL	3.0
1	C	644	ASN	3.0
3	H	449	PRO	3.0
2	L	206	VAL	3.0
3	H	421	VAL	3.0
2	L	122	SER	3.0
3	H	458	SER	3.0
3	H	468	ALA	3.0
3	H	306	GLU	2.9
2	L	175	MET	2.9
2	L	152	GLY	2.9
2	L	80	THR	2.9
1	C	728	ARG	2.9
3	H	510	ILE	2.9
1	C	661	ARG	2.8
2	L	205	ILE	2.8
2	L	204	PRO	2.8
3	H	430	ALA	2.8
1	C	720	VAL	2.8
2	L	159	VAL	2.8
3	H	447	PRO	2.8
3	H	429	ALA	2.8
1	C	643	THR	2.8
1	C	721	GLN	2.8
1	C	727	CYS	2.8
2	L	127	SER	2.7
3	H	416	THR	2.7
2	L	199	LYS	2.7
3	H	484	PRO	2.7
3	H	477	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	686	SER	2.7
2	L	167	ASP	2.7
2	L	180	THR	2.7
2	L	39	LYS	2.7
2	L	57	GLY	2.7
2	L	81	GLU	2.7
2	L	12	SER	2.7
3	H	434	SER	2.7
3	H	478	SER	2.7
1	C	668	ARG	2.6
2	L	135	PHE	2.6
3	H	457	GLY	2.6
2	L	120	PRO	2.6
3	H	483	VAL	2.6
3	H	376	ASN	2.6
3	H	401	ASP	2.6
2	L	192	TYR	2.6
3	H	474	LEU	2.6
3	H	485	SER	2.6
1	C	724	ILE	2.6
2	L	190	ASN	2.6
3	H	344	ARG	2.5
3	H	402	TYR	2.5
1	C	606	CYS	2.5
3	H	495	CYS	2.5
3	H	467	PRO	2.5
2	L	150	ILE	2.5
2	L	171	SER	2.5
3	H	486	SER	2.5
1	C	673	ARG	2.5
2	L	186	TYR	2.5
2	L	117	ILE	2.5
3	H	383	ASN	2.5
1	C	648	ASP	2.5
1	C	611	ALA	2.5
2	L	195	GLU	2.5
3	H	420	SER	2.4
2	L	76	ASN	2.4
3	H	417	THR	2.4
2	L	187	GLU	2.4
2	L	116	SER	2.4
2	L	198	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
3	H	459	LEU	2.4
1	C	722	ALA	2.4
1	C	647	THR	2.3
1	C	682	ALA	2.3
2	L	203	SER	2.3
3	H	460	SER	2.3
2	L	126	THR	2.3
3	H	482	THR	2.3
3	H	492	THR	2.3
1	C	614	ARG	2.3
1	C	717	GLY	2.3
3	H	407[A]	THR	2.3
1	C	603	PHE	2.3
3	H	435	MET	2.3
1	C	678	ILE	2.3
2	L	140	TYR	2.3
2	L	173	TYR	2.3
2	L	56	SER	2.2
2	L	114	THR	2.2
2	L	200	THR	2.2
2	L	158	GLY	2.2
2	L	141	PRO	2.2
2	L	153	SER	2.2
1	C	671	GLY	2.2
2	L	77	SER	2.2
2	L	58	ILE	2.2
1	C	609	ALA	2.2
2	L	201	SER	2.2
1	C	618	ASP	2.1
2	L	105	GLU	2.1
3	H	358	TYR	2.1
3	H	432	THR	2.1
2	L	109	ALA	2.1
3	H	452	VAL	2.1
3	H	502	SER	2.1
3	H	424	LEU	2.1
2	L	118	PHE	2.1
3	H	451	THR	2.1
1	C	641	GLN	2.1
2	L	154	GLU	2.1
3	H	489	PRO	2.1
2	L	107	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	L	162	SER	2.0
1	C	616	GLY	2.0
1	C	626	GLY	2.0
3	H	441	LEU	2.0
1	C	710	ALA	2.0
2	L	185	GLU	2.0
3	H	422	TYR	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.