



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:31 AM EDT

PDB ID : 2G60 / pdb_00002g60
Title : Structure of anti-FLAG M2 Fab domain
Authors : Roosild, T.P.
Deposited on : 2006-02-23
Resolution : 1.85 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

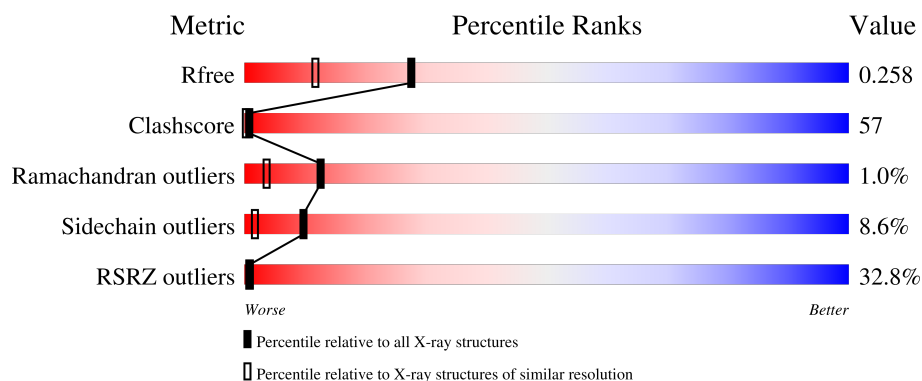
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	216	
2	H	215	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3518 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 anti-FLAG M2 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1635	1026	275	328	6			

- Molecule 2 is a protein called anti-FLAG M2 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	208	Total	C	N	O	S	0	0	0
			1499	949	245	298	7			

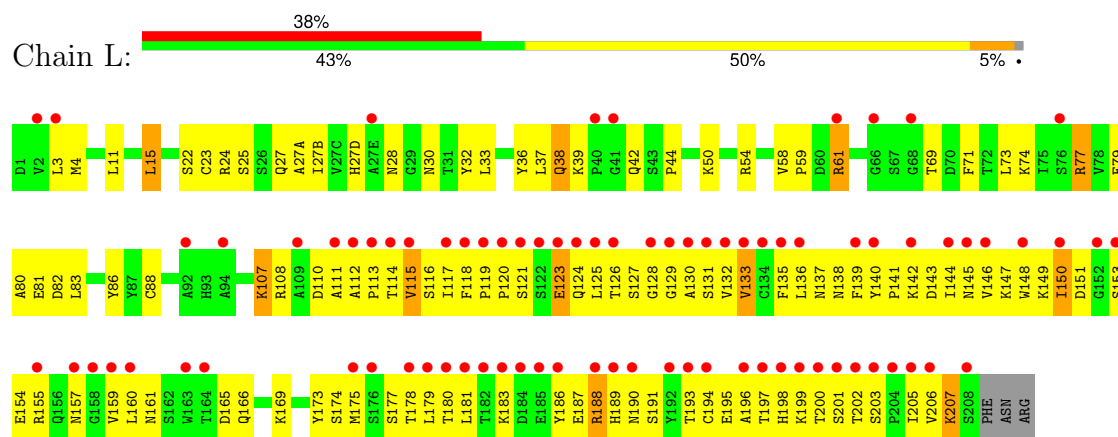
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	175	Total	O	0	0
			175	175		
3	H	209	Total	O	0	0
			209	209		

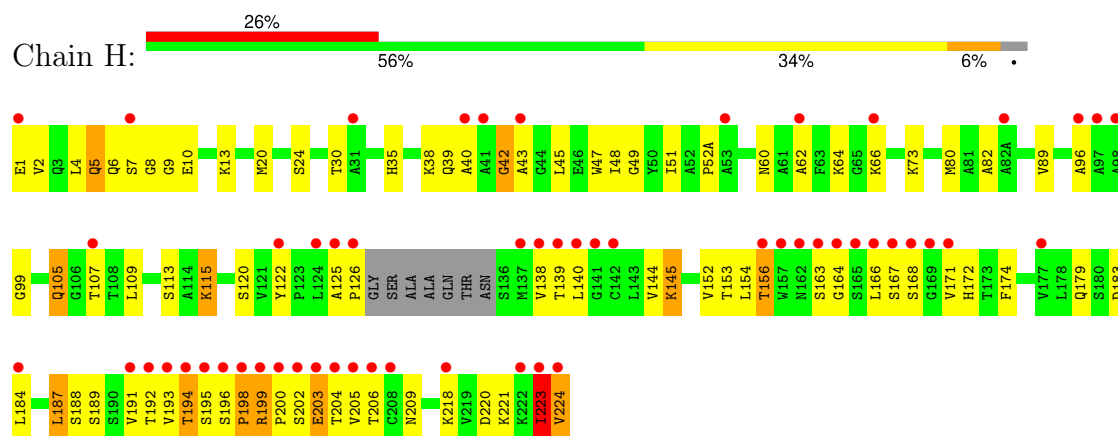
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: anti-FLAG M2 Fab light chain



• Molecule 2: anti-FLAG M2 Fab heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	87.36Å 133.76Å 41.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.85 50.00 – 1.86	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.85) 95.7 (50.00-1.86)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 1.86Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.278 0.254 , 0.258	Depositor DCC
R_{free} test set	2008 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.552	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 73.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3518	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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	L	0.95	2/1673 (0.1%)	1.15	5/2274 (0.2%)
2	H	1.24	5/1535 (0.3%)	1.32	5/2097 (0.2%)
All	All	1.10	7/3208 (0.2%)	1.23	10/4371 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	62	ALA	CA-CB	7.52	1.66	1.53
2	H	224	VAL	C-OXT	6.11	1.35	1.23
1	L	38	GLN	C-O	5.78	1.30	1.23
2	H	144	VAL	CA-CB	5.65	1.60	1.53
2	H	5	GLN	CD-OE1	5.56	1.34	1.23
2	H	80	MET	SD-CE	5.21	1.92	1.79
1	L	32	TYR	CA-C	-5.12	1.47	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	133	VAL	N-CA-C	8.59	120.64	108.36
1	L	138	ASN	N-CA-C	8.29	122.68	111.24
2	H	99	GLY	N-CA-C	-7.50	97.96	111.16
2	H	60	ASN	N-CA-C	-7.37	97.98	109.25
2	H	174	PHE	N-CA-C	6.60	119.40	110.29
1	L	165	ASP	N-CA-C	-6.52	102.12	110.53
1	L	115	VAL	N-CA-C	6.17	117.18	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	145	LYS	N-CA-C	6.11	119.42	109.59
1	L	88	CYS	N-CA-C	-5.87	102.08	110.59
2	H	120	SER	N-CA-C	-5.25	100.68	109.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	36	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1635	0	1579	184	0
2	H	1499	0	1473	173	0
3	H	209	0	0	104	1
3	L	175	0	0	86	1
All	All	3518	0	3052	355	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 57.

All (355) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:9:GLY:HA3	3:H:414:HOH:O	1.34	1.27
1:L:61:ARG:HD2	3:L:372:HOH:O	1.45	1.12
1:L:108:ARG:HD3	3:L:371:HOH:O	1.48	1.09
2:H:1:GLU:HG2	2:H:2:VAL:N	1.60	1.08
2:H:198:PRO:HA	3:H:428:HOH:O	1.53	1.08
2:H:206:THR:HB	3:H:418:HOH:O	1.54	1.07
2:H:105:GLN:HB3	3:H:416:HOH:O	1.57	1.04
2:H:194:THR:O	2:H:198:PRO:HD2	1.58	1.04
2:H:8:GLY:HA3	3:H:385:HOH:O	1.54	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:27(A):ALA:HB1	3:L:378:HOH:O	1.59	1.03
1:L:150:ILE:HD11	1:L:189:HIS:HB3	1.40	1.03
2:H:39:GLN:HB3	3:H:417:HOH:O	1.58	1.03
1:L:174:SER:HB3	3:L:380:HOH:O	1.60	1.02
1:L:61:ARG:NH2	1:L:79:GLU:HB2	1.75	1.01
2:H:199:ARG:HG2	3:H:421:HOH:O	1.59	1.01
2:H:199:ARG:HB3	2:H:199:ARG:HH11	1.23	1.01
1:L:131:SER:HA	3:L:317:HOH:O	1.59	1.00
2:H:1:GLU:CG	2:H:2:VAL:N	2.24	0.99
2:H:89:VAL:HB	3:H:417:HOH:O	1.62	0.99
2:H:154:LEU:HB2	3:H:432:HOH:O	1.64	0.98
1:L:159:VAL:HG22	1:L:179:LEU:HB2	1.43	0.98
2:H:138:VAL:HG12	3:H:415:HOH:O	1.62	0.97
2:H:223:ILE:H	2:H:223:ILE:HD12	1.28	0.97
1:L:80:ALA:HB1	3:L:373:HOH:O	1.63	0.96
2:H:223:ILE:HG22	2:H:224:VAL:H	1.27	0.95
2:H:188:SER:HB2	3:H:430:HOH:O	1.65	0.95
2:H:1:GLU:HB3	3:H:296:HOH:O	1.67	0.95
1:L:27:GLN:HG3	3:L:375:HOH:O	1.65	0.94
1:L:107:LYS:HD2	1:L:140:TYR:OH	1.68	0.94
1:L:120:PRO:HB2	1:L:125:LEU:HD21	1.48	0.92
2:H:30:THR:HA	3:H:424:HOH:O	1.69	0.92
2:H:7:SER:N	3:H:246:HOH:O	2.04	0.90
2:H:194:THR:C	2:H:198:PRO:HD2	1.96	0.90
1:L:202:THR:HA	3:L:294:HOH:O	1.72	0.89
2:H:1:GLU:CG	2:H:2:VAL:H	1.87	0.88
3:L:383:HOH:O	2:H:139:THR:HG21	1.74	0.88
1:L:38:GLN:HG2	3:L:381:HOH:O	1.74	0.86
1:L:207:LYS:HG3	3:L:323:HOH:O	1.74	0.86
1:L:118:PHE:HD2	3:H:423:HOH:O	1.58	0.85
2:H:154:LEU:HD12	2:H:156:THR:H	1.41	0.84
2:H:204:THR:HA	3:H:397:HOH:O	1.78	0.83
2:H:154:LEU:HD23	2:H:189:SER:CB	2.08	0.82
2:H:223:ILE:HD12	2:H:223:ILE:N	1.95	0.81
1:L:179:LEU:O	3:L:317:HOH:O	1.97	0.81
2:H:140:LEU:N	3:H:429:HOH:O	2.12	0.81
2:H:193:VAL:HG12	3:H:413:HOH:O	1.81	0.81
2:H:223:ILE:H	2:H:223:ILE:CD1	1.93	0.80
1:L:133:VAL:HA	3:L:334:HOH:O	1.81	0.80
2:H:115:LYS:CE	2:H:115:LYS:H	1.95	0.80
2:H:138:VAL:HG13	3:H:413:HOH:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:164:GLY:CA	3:H:431:HOH:O	2.29	0.80
1:L:157:ASN:HB2	3:L:382:HOH:O	1.80	0.80
1:L:83:LEU:HD21	1:L:166:GLN:OE1	1.81	0.80
2:H:20:MET:HE1	2:H:109:LEU:HD22	1.63	0.79
2:H:115:LYS:H	2:H:115:LYS:HE3	1.47	0.79
1:L:178:THR:HA	3:L:334:HOH:O	1.81	0.79
1:L:118:PHE:CD2	3:H:423:HOH:O	2.32	0.79
2:H:154:LEU:HD12	2:H:156:THR:N	1.97	0.79
2:H:52(A):PRO:CG	3:H:424:HOH:O	2.31	0.78
1:L:142:LYS:HD2	1:L:173:TYR:CE2	2.18	0.78
2:H:40:ALA:O	3:H:313:HOH:O	2.01	0.78
1:L:147:LYS:HE3	3:L:386:HOH:O	1.83	0.78
2:H:7:SER:O	2:H:107:THR:HG23	1.83	0.78
1:L:140:TYR:HB3	3:L:384:HOH:O	1.82	0.78
2:H:8:GLY:CA	3:H:385:HOH:O	2.21	0.78
1:L:140:TYR:CB	3:L:384:HOH:O	2.30	0.77
1:L:150:ILE:HB	3:L:332:HOH:O	1.83	0.77
2:H:191:VAL:HG13	2:H:191:VAL:O	1.85	0.77
2:H:10:GLU:OE1	2:H:20:MET:HG2	1.85	0.76
2:H:66:LYS:HD3	3:H:373:HOH:O	1.85	0.76
1:L:108:ARG:CD	3:L:371:HOH:O	2.14	0.76
1:L:149:LYS:HG2	1:L:154:GLU:HA	1.66	0.76
1:L:159:VAL:HG23	1:L:179:LEU:HD13	1.67	0.76
2:H:139:THR:HG22	2:H:192:THR:OG1	1.86	0.75
1:L:132:VAL:HG13	3:L:341:HOH:O	1.85	0.75
2:H:6:GLN:C	3:H:246:HOH:O	2.27	0.75
1:L:61:ARG:HH22	1:L:79:GLU:HB2	1.47	0.75
2:H:66:LYS:HG3	3:H:422:HOH:O	1.86	0.75
1:L:116:SER:C	3:L:379:HOH:O	2.29	0.74
2:H:20:MET:CE	2:H:109:LEU:HD22	2.16	0.74
1:L:180:THR:HG23	3:L:226:HOH:O	1.88	0.74
2:H:40:ALA:C	3:H:313:HOH:O	2.31	0.73
2:H:195:SER:HB2	3:H:271:HOH:O	1.88	0.73
2:H:140:LEU:HG	3:H:429:HOH:O	1.88	0.73
2:H:199:ARG:HB3	2:H:199:ARG:NH1	2.01	0.73
1:L:22:SER:HB3	3:L:374:HOH:O	1.87	0.73
2:H:139:THR:C	3:H:429:HOH:O	2.32	0.73
2:H:188:SER:CB	3:H:430:HOH:O	2.27	0.73
2:H:115:LYS:HE3	2:H:115:LYS:N	2.05	0.72
2:H:183:ASP:C	2:H:184:LEU:HD22	2.14	0.72
1:L:3:LEU:HB2	3:L:352:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:43:ALA:N	3:H:313:HOH:O	2.23	0.71
2:H:1:GLU:HG3	2:H:2:VAL:H	1.55	0.71
1:L:114:THR:HA	3:L:329:HOH:O	1.89	0.71
1:L:15:LEU:HD23	3:L:259:HOH:O	1.90	0.71
1:L:38:GLN:CG	3:L:381:HOH:O	2.35	0.71
1:L:155:ARG:HD2	1:L:179:LEU:HD21	1.71	0.71
2:H:96:ALA:N	3:H:362:HOH:O	2.22	0.71
1:L:147:LYS:N	3:L:344:HOH:O	2.25	0.70
2:H:52(A):PRO:HG2	3:H:424:HOH:O	1.90	0.70
2:H:10:GLU:HB2	3:H:312:HOH:O	1.92	0.70
2:H:223:ILE:HG22	2:H:224:VAL:N	2.04	0.70
1:L:111:ALA:HB3	3:L:384:HOH:O	1.89	0.70
2:H:125:ALA:CB	2:H:224:VAL:HG21	2.22	0.70
2:H:1:GLU:N	3:H:296:HOH:O	2.26	0.69
2:H:189:SER:N	3:H:430:HOH:O	2.24	0.69
1:L:54:ARG:HG2	1:L:58:VAL:HB	1.74	0.68
1:L:159:VAL:HG22	1:L:179:LEU:CB	2.20	0.68
2:H:198:PRO:O	3:H:428:HOH:O	2.10	0.68
1:L:150:ILE:CD1	1:L:189:HIS:HB3	2.22	0.68
1:L:188:ARG:HG2	1:L:188:ARG:HH11	1.57	0.68
2:H:156:THR:HG22	2:H:209:ASN:OD1	1.93	0.68
2:H:218:LYS:NZ	2:H:220:ASP:OD1	2.27	0.68
1:L:61:ARG:HB3	3:L:372:HOH:O	1.92	0.68
1:L:160:LEU:CD1	3:L:358:HOH:O	2.42	0.67
1:L:77:ARG:HD2	3:L:319:HOH:O	1.95	0.67
1:L:22:SER:CB	3:L:374:HOH:O	2.43	0.66
1:L:83:LEU:CD2	1:L:166:GLN:OE1	2.44	0.66
1:L:108:ARG:CB	3:L:371:HOH:O	2.42	0.66
1:L:161:ASN:HD22	1:L:177:SER:HA	1.60	0.66
1:L:111:ALA:C	1:L:200:THR:HG21	2.20	0.66
2:H:42:GLY:C	3:H:420:HOH:O	2.39	0.65
1:L:27(A):ALA:O	3:L:375:HOH:O	2.13	0.65
1:L:161:ASN:ND2	1:L:177:SER:OG	2.29	0.65
2:H:42:GLY:N	3:H:420:HOH:O	2.30	0.65
2:H:164:GLY:HA2	3:H:431:HOH:O	1.95	0.65
1:L:180:THR:HA	3:L:317:HOH:O	1.96	0.64
2:H:167:SER:N	3:H:338:HOH:O	2.30	0.64
2:H:1:GLU:CB	3:H:296:HOH:O	2.35	0.64
2:H:167:SER:O	2:H:171:VAL:HG22	1.97	0.64
2:H:138:VAL:N	3:H:415:HOH:O	2.29	0.64
2:H:125:ALA:HB2	2:H:224:VAL:CG2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:145:LYS:HE3	3:H:335:HOH:O	1.97	0.63
2:H:138:VAL:HG22	3:H:429:HOH:O	1.97	0.63
2:H:154:LEU:CA	3:H:432:HOH:O	2.46	0.63
1:L:159:VAL:CG2	1:L:179:LEU:HD13	2.28	0.63
2:H:35:HIS:HD2	2:H:47:TRP:HE1	1.46	0.63
1:L:149:LYS:HG2	1:L:154:GLU:HG3	1.81	0.63
1:L:38:GLN:CD	3:L:381:HOH:O	2.42	0.62
1:L:61:ARG:CD	3:L:372:HOH:O	2.22	0.62
1:L:200:THR:N	3:L:385:HOH:O	2.31	0.62
2:H:188:SER:CA	3:H:430:HOH:O	2.45	0.62
2:H:10:GLU:CD	3:H:297:HOH:O	2.42	0.62
2:H:205:VAL:HB	2:H:223:ILE:HD13	1.82	0.62
2:H:52(A):PRO:HB2	3:H:424:HOH:O	2.00	0.61
1:L:116:SER:HB3	3:L:379:HOH:O	1.99	0.61
1:L:181:LEU:CD1	1:L:186:TYR:HB2	2.30	0.61
2:H:66:LYS:NZ	3:H:422:HOH:O	2.33	0.61
1:L:128:GLY:HA2	1:L:183:LYS:HD3	1.82	0.61
2:H:199:ARG:CD	3:H:427:HOH:O	2.47	0.61
1:L:203:SER:HB3	3:L:270:HOH:O	2.00	0.61
1:L:206:VAL:O	1:L:207:LYS:HD2	2.01	0.61
2:H:125:ALA:HA	3:H:377:HOH:O	2.00	0.61
1:L:193:THR:HA	3:L:335:HOH:O	2.00	0.61
2:H:30:THR:HG21	2:H:73:LYS:HE2	1.82	0.61
1:L:195:GLU:HG3	1:L:206:VAL:HG22	1.83	0.60
1:L:136:LEU:HB2	1:L:175:MET:HG3	1.84	0.60
1:L:147:LYS:HG2	3:L:386:HOH:O	2.02	0.60
2:H:139:THR:HA	3:H:266:HOH:O	2.02	0.60
1:L:61:ARG:NH2	1:L:79:GLU:CB	2.60	0.60
1:L:140:TYR:N	3:L:384:HOH:O	2.34	0.59
2:H:66:LYS:CD	3:H:373:HOH:O	2.47	0.59
2:H:66:LYS:CG	3:H:373:HOH:O	2.50	0.59
1:L:128:GLY:HA2	1:L:183:LYS:CE	2.32	0.59
2:H:196:SER:N	2:H:198:PRO:CD	2.65	0.59
2:H:30:THR:CG2	2:H:73:LYS:HE2	2.32	0.58
1:L:38:GLN:NE2	1:L:42:GLN:O	2.37	0.58
1:L:205:ILE:HG22	3:L:338:HOH:O	2.03	0.58
2:H:66:LYS:HG2	3:H:373:HOH:O	2.02	0.58
1:L:112:ALA:N	1:L:200:THR:HG21	2.19	0.58
1:L:115:VAL:HB	1:L:207:LYS:HD3	1.86	0.58
2:H:199:ARG:CG	3:H:427:HOH:O	2.51	0.58
1:L:130:ALA:HB3	1:L:181:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:196:SER:HB3	3:H:330:HOH:O	2.04	0.57
2:H:125:ALA:HB1	2:H:224:VAL:HG21	1.85	0.57
1:L:121:SER:HB2	1:L:123:GLU:OE2	2.03	0.57
1:L:169:LYS:HA	1:L:169:LYS:HE2	1.85	0.57
2:H:191:VAL:C	3:H:266:HOH:O	2.48	0.57
2:H:193:VAL:CG1	3:H:413:HOH:O	2.44	0.57
2:H:203:GLU:HG3	3:H:428:HOH:O	2.04	0.57
2:H:7:SER:O	2:H:107:THR:CG2	2.51	0.57
1:L:194:CYS:HA	3:L:233:HOH:O	2.05	0.56
2:H:140:LEU:N	3:H:266:HOH:O	2.38	0.56
1:L:188:ARG:HH11	1:L:188:ARG:CG	2.18	0.56
1:L:119:PRO:HG2	3:L:340:HOH:O	2.04	0.56
2:H:52(A):PRO:HD2	3:H:424:HOH:O	2.05	0.56
1:L:27:GLN:CG	3:L:375:HOH:O	2.39	0.56
1:L:117:ILE:HD12	3:L:335:HOH:O	2.05	0.56
2:H:126:PRO:HD2	3:H:377:HOH:O	2.06	0.56
1:L:149:LYS:HG2	1:L:154:GLU:CA	2.37	0.55
1:L:107:LYS:HD2	1:L:140:TYR:HH	1.71	0.55
1:L:199:LYS:HB2	3:L:345:HOH:O	2.07	0.55
1:L:108:ARG:HG2	3:L:230:HOH:O	2.07	0.55
2:H:35:HIS:CD2	2:H:47:TRP:HE1	2.24	0.55
2:H:154:LEU:HD23	2:H:189:SER:OG	2.07	0.55
2:H:166:LEU:HB2	3:H:349:HOH:O	2.06	0.55
2:H:193:VAL:O	3:H:382:HOH:O	2.18	0.55
2:H:9:GLY:CA	3:H:414:HOH:O	2.15	0.55
2:H:154:LEU:CD2	2:H:189:SER:CB	2.83	0.55
3:L:381:HOH:O	2:H:39:GLN:NE2	2.39	0.54
2:H:164:GLY:N	3:H:431:HOH:O	2.39	0.54
1:L:107:LYS:CD	1:L:140:TYR:OH	2.49	0.54
2:H:13:LYS:HD3	2:H:113:SER:HA	1.90	0.54
2:H:198:PRO:HG3	3:H:378:HOH:O	2.07	0.54
1:L:120:PRO:HB2	1:L:125:LEU:CD2	2.31	0.54
2:H:194:THR:OG1	2:H:198:PRO:HG2	2.07	0.53
1:L:28:ASN:OD1	1:L:30:ASN:HB2	2.08	0.53
2:H:125:ALA:HB2	2:H:224:VAL:HG21	1.89	0.53
1:L:157:ASN:CB	3:L:382:HOH:O	2.47	0.53
1:L:128:GLY:HA2	1:L:183:LYS:CD	2.39	0.53
1:L:198:HIS:HB3	3:L:385:HOH:O	2.09	0.53
2:H:89:VAL:CB	3:H:417:HOH:O	2.38	0.53
2:H:153:THR:C	3:H:432:HOH:O	2.52	0.53
2:H:223:ILE:HB	3:H:427:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:59:PRO:HB2	1:L:61:ARG:HD3	1.90	0.53
1:L:142:LYS:HD2	1:L:173:TYR:CD2	2.44	0.53
1:L:190:ASN:ND2	3:L:295:HOH:O	2.42	0.53
2:H:52(A):PRO:CD	3:H:424:HOH:O	2.54	0.52
2:H:154:LEU:HD12	2:H:209:ASN:O	2.10	0.52
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.91	0.52
1:L:145:ASN:O	1:L:196:ALA:HA	2.09	0.52
2:H:42:GLY:CA	3:H:420:HOH:O	2.57	0.52
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.44	0.52
2:H:52(A):PRO:O	2:H:73:LYS:HE3	2.10	0.52
2:H:193:VAL:HG22	2:H:194:THR:N	2.24	0.52
1:L:201:SER:N	3:L:385:HOH:O	2.42	0.52
1:L:181:LEU:HD13	1:L:186:TYR:HB2	1.90	0.52
1:L:195:GLU:CG	1:L:206:VAL:HG22	2.38	0.52
1:L:155:ARG:HD3	1:L:179:LEU:HD11	1.92	0.52
1:L:61:ARG:HH21	1:L:79:GLU:HB2	1.67	0.52
2:H:167:SER:C	3:H:338:HOH:O	2.53	0.52
2:H:125:ALA:CB	2:H:224:VAL:CG2	2.88	0.51
1:L:125:LEU:HD13	1:L:129:GLY:O	2.09	0.51
2:H:187:LEU:HD23	2:H:187:LEU:C	2.35	0.51
2:H:7:SER:HB2	3:H:246:HOH:O	2.11	0.51
2:H:166:LEU:C	3:H:338:HOH:O	2.53	0.51
1:L:27(B):ILE:HD11	1:L:71:PHE:CE1	2.45	0.51
1:L:206:VAL:C	1:L:207:LYS:HD2	2.35	0.51
2:H:154:LEU:HD23	2:H:189:SER:HB2	1.89	0.51
2:H:164:GLY:C	3:H:431:HOH:O	2.51	0.51
1:L:117:ILE:HG12	3:L:341:HOH:O	2.10	0.51
1:L:136:LEU:HD21	1:L:146:VAL:HG22	1.93	0.51
2:H:172:HIS:CE1	3:H:394:HOH:O	2.63	0.51
2:H:199:ARG:HD3	3:H:427:HOH:O	2.06	0.51
1:L:139:PHE:HB2	1:L:198:HIS:CE1	2.45	0.50
1:L:202:THR:HG22	1:L:202:THR:O	2.11	0.50
2:H:205:VAL:HG12	2:H:223:ILE:HD11	1.92	0.50
1:L:124:GLN:HG3	2:H:122:TYR:CE2	2.47	0.49
1:L:147:LYS:NZ	3:L:309:HOH:O	2.45	0.49
2:H:8:GLY:C	3:H:385:HOH:O	2.53	0.49
2:H:9:GLY:C	3:H:414:HOH:O	2.48	0.49
2:H:126:PRO:CD	3:H:377:HOH:O	2.60	0.49
1:L:24:ARG:HA	1:L:69:THR:O	2.11	0.49
1:L:145:ASN:HB3	1:L:197:THR:HB	1.94	0.49
1:L:125:LEU:O	1:L:126:THR:C	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:198:PRO:CG	3:H:378:HOH:O	2.62	0.48
1:L:175:MET:N	3:L:380:HOH:O	2.47	0.48
1:L:81:GLU:H	1:L:81:GLU:CD	2.22	0.48
2:H:218:LYS:NZ	3:H:319:HOH:O	2.47	0.48
1:L:27:GLN:C	3:L:375:HOH:O	2.57	0.48
1:L:27(D):HIS:HD2	1:L:28:ASN:H	1.62	0.48
1:L:61:ARG:NH2	1:L:82:ASP:OD2	2.47	0.47
1:L:130:ALA:HB3	1:L:181:LEU:CD1	2.43	0.47
1:L:186:TYR:CD2	1:L:187:GLU:OE2	2.68	0.47
1:L:77:ARG:HD2	1:L:77:ARG:H	1.79	0.47
2:H:40:ALA:HB3	3:H:313:HOH:O	2.14	0.47
2:H:154:LEU:CB	3:H:432:HOH:O	2.34	0.47
1:L:113:PRO:HG3	1:L:144:ILE:HD11	1.96	0.47
1:L:146:VAL:HG13	1:L:195:GLU:O	2.15	0.47
2:H:200:PRO:O	2:H:202:SER:C	2.58	0.47
1:L:108:ARG:NE	3:L:371:HOH:O	2.41	0.46
2:H:140:LEU:CG	3:H:429:HOH:O	2.52	0.46
2:H:184:LEU:HD22	2:H:184:LEU:N	2.30	0.46
1:L:108:ARG:HB3	3:L:371:HOH:O	2.11	0.46
1:L:124:GLN:HG3	2:H:122:TYR:CZ	2.50	0.46
1:L:198:HIS:CG	1:L:199:LYS:H	2.33	0.46
2:H:115:LYS:CE	3:H:403:HOH:O	2.62	0.46
1:L:61:ARG:CB	3:L:372:HOH:O	2.57	0.46
1:L:149:LYS:CG	1:L:154:GLU:HG3	2.46	0.46
1:L:27(A):ALA:CB	3:L:378:HOH:O	2.36	0.46
1:L:39:LYS:HE2	1:L:81:GLU:O	2.16	0.46
1:L:193:THR:HG23	1:L:206:VAL:HG13	1.98	0.46
1:L:160:LEU:HD12	3:L:358:HOH:O	2.10	0.46
1:L:178:THR:HG23	3:L:334:HOH:O	2.16	0.45
1:L:50:LYS:NZ	3:L:288:HOH:O	2.49	0.45
1:L:148:TRP:O	1:L:155:ARG:N	2.49	0.45
2:H:199:ARG:HH11	2:H:199:ARG:CB	2.09	0.45
1:L:4:MET:HE3	1:L:23:CYS:SG	2.56	0.45
2:H:7:SER:O	2:H:107:THR:OG1	2.35	0.45
1:L:77:ARG:HD2	1:L:77:ARG:N	2.31	0.45
1:L:27(B):ILE:HD11	1:L:71:PHE:CZ	2.52	0.45
1:L:37:LEU:CD2	1:L:39:LYS:HE3	2.47	0.45
1:L:161:ASN:ND2	1:L:177:SER:CB	2.79	0.45
1:L:117:ILE:CD1	3:L:335:HOH:O	2.63	0.45
2:H:183:ASP:O	2:H:184:LEU:HD22	2.17	0.45
1:L:150:ILE:HD13	1:L:191:SER:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:188:ARG:CG	1:L:188:ARG:NH1	2.80	0.44
1:L:38:GLN:OE1	1:L:44:PRO:HG3	2.16	0.44
1:L:116:SER:CB	3:L:379:HOH:O	2.61	0.44
1:L:135:PHE:C	1:L:136:LEU:HD12	2.42	0.44
2:H:199:ARG:HA	2:H:200:PRO:HA	1.62	0.44
2:H:20:MET:HE2	2:H:109:LEU:HD13	1.99	0.44
2:H:193:VAL:HG22	2:H:194:THR:H	1.81	0.44
1:L:118:PHE:HE1	3:L:379:HOH:O	2.00	0.44
2:H:204:THR:CA	3:H:397:HOH:O	2.50	0.44
1:L:27(D):HIS:CD2	1:L:28:ASN:H	2.35	0.44
2:H:125:ALA:HB2	2:H:224:VAL:HG22	1.99	0.44
2:H:52(A):PRO:CB	3:H:424:HOH:O	2.51	0.43
1:L:108:ARG:HB2	3:L:371:HOH:O	2.14	0.43
2:H:66:LYS:O	2:H:82:ALA:HA	2.18	0.43
1:L:108:ARG:NH2	1:L:111:ALA:HB2	2.33	0.43
1:L:149:LYS:HA	1:L:153:SER:O	2.17	0.43
1:L:180:THR:CB	3:L:358:HOH:O	2.66	0.43
2:H:154:LEU:N	3:H:432:HOH:O	2.52	0.43
1:L:150:ILE:HD13	1:L:151:ASP:N	2.34	0.43
1:L:38:GLN:OE1	3:L:381:HOH:O	2.21	0.43
1:L:147:LYS:HD2	1:L:154:GLU:HG2	2.01	0.42
2:H:7:SER:HB3	3:H:336:HOH:O	2.19	0.42
2:H:7:SER:O	2:H:107:THR:CB	2.67	0.42
1:L:147:LYS:C	3:L:233:HOH:O	2.63	0.42
1:L:83:LEU:HD22	3:L:290:HOH:O	2.20	0.42
1:L:160:LEU:HD12	1:L:160:LEU:N	2.34	0.42
1:L:195:GLU:CB	3:L:344:HOH:O	2.67	0.42
2:H:7:SER:CB	3:H:246:HOH:O	2.67	0.42
1:L:137:ASN:HA	3:L:380:HOH:O	2.19	0.42
1:L:180:THR:HA	3:L:226:HOH:O	2.19	0.42
1:L:25:SER:OG	1:L:69:THR:HA	2.20	0.42
1:L:140:TYR:CG	1:L:141:PRO:HA	2.54	0.42
1:L:146:VAL:HA	1:L:195:GLU:O	2.20	0.42
1:L:181:LEU:HD11	1:L:186:TYR:HB2	2.02	0.42
2:H:39:GLN:HB2	2:H:45:LEU:HD23	2.02	0.41
2:H:42:GLY:N	3:H:313:HOH:O	2.50	0.41
2:H:154:LEU:CD2	2:H:189:SER:HB3	2.50	0.41
1:L:196:ALA:HB3	1:L:205:ILE:HB	2.03	0.41
2:H:168:SER:N	3:H:338:HOH:O	2.53	0.41
1:L:150:ILE:N	1:L:153:SER:O	2.50	0.41
2:H:4:LEU:HA	2:H:4:LEU:HD23	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:40:ALA:CA	3:H:313:HOH:O	2.67	0.41
2:H:115:LYS:HE2	3:H:403:HOH:O	2.21	0.41
2:H:203:GLU:CG	3:H:428:HOH:O	2.65	0.41
1:L:155:ARG:CD	1:L:179:LEU:HD21	2.46	0.41
2:H:30:THR:C	3:H:424:HOH:O	2.64	0.41
1:L:37:LEU:HD13	1:L:86:TYR:CZ	2.56	0.41
1:L:54:ARG:HD3	1:L:58:VAL:O	2.20	0.41
1:L:159:VAL:HA	1:L:179:LEU:HA	2.02	0.41
1:L:193:THR:CA	3:L:335:HOH:O	2.66	0.41
1:L:183:LYS:HD2	3:L:280:HOH:O	2.20	0.40
2:H:66:LYS:HD2	3:H:274:HOH:O	2.21	0.40
1:L:27(A):ALA:CA	3:L:378:HOH:O	2.68	0.40
1:L:27:GLN:CB	3:L:375:HOH:O	2.65	0.40
1:L:174:SER:CB	3:L:380:HOH:O	2.41	0.40
1:L:195:GLU:C	3:L:344:HOH:O	2.64	0.40
1:L:126:THR:OG1	1:L:127:SER:N	2.54	0.40
1:L:180:THR:HB	3:L:358:HOH:O	2.22	0.40
2:H:166:LEU:HD23	3:H:338: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)
3:L:212:HOH:O	3:H:227:HOH:O[4_455]	1.79	0.41

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	211/216 (98%)	197 (93%)	14 (7%)	0	100	100
2	H	204/215 (95%)	189 (93%)	11 (5%)	4 (2%)	6	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	415/431 (96%)	386 (93%)	25 (6%)	4 (1%)	12 4

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	223	ILE
2	H	163	SER
2	H	198	PRO
2	H	42	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	183/186 (98%)	169 (92%)	14 (8%)	12 3
2	H	156/160 (98%)	141 (90%)	15 (10%)	8 1
All	All	339/346 (98%)	310 (91%)	29 (9%)	10 2

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	11	LEU
1	L	15	LEU
1	L	33	LEU
1	L	61	ARG
1	L	73	LEU
1	L	74	LYS
1	L	77	ARG
1	L	107	LYS
1	L	110	ASP
1	L	123	GLU
1	L	143	ASP
1	L	150	ILE
1	L	188	ARG
1	L	207	LYS

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Mol	Chain	Res	Type
2	H	5	GLN
2	H	24	SER
2	H	51	ILE
2	H	64	LYS
2	H	105	GLN
2	H	115	LYS
2	H	152	VAL
2	H	156	THR
2	H	179	GLN
2	H	187	LEU
2	H	194	THR
2	H	199	ARG
2	H	203	GLU
2	H	221	LYS
2	H	223	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	27(D)	HIS
1	L	30	ASN
1	L	93	HIS
1	L	157	ASN
1	L	161	ASN
1	L	189	HIS
1	L	198	HIS
2	H	3	GLN
2	H	35	HIS
2	H	172	HIS

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 [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	L	213/216 (98%)	1.65	82 (38%)  	22, 47, 88, 98	0
2	H	208/215 (96%)	1.16	56 (26%)  	19, 32, 76, 87	0
All	All	421/431 (97%)	1.41	138 (32%)  	19, 38, 85, 98	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	134	CYS	6.4
2	H	223	ILE	5.9
1	L	129	GLY	5.4
2	H	200	PRO	5.2
2	H	125	ALA	5.2
1	L	160	LEU	5.1
2	H	126	PRO	5.1
1	L	132	VAL	4.8
2	H	41	ALA	4.8
1	L	208	SER	4.5
1	L	179	LEU	4.5
2	H	224	VAL	4.5
2	H	96	ALA	4.5
2	H	124	LEU	4.4
2	H	140	LEU	4.4
2	H	98	ALA	4.4
2	H	165	SER	4.3
1	L	159	VAL	4.2
2	H	193	VAL	4.1
1	L	158	GLY	4.0
2	H	205	VAL	4.0
1	L	185	GLU	4.0
1	L	189	HIS	3.9
1	L	194	CYS	3.9

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Mol	Chain	Res	Type	RSRZ
2	H	139	THR	3.9
1	L	68	GLY	3.8
1	L	178	THR	3.8
2	H	194	THR	3.7
1	L	130	ALA	3.7
2	H	204	THR	3.7
1	L	125	LEU	3.7
1	L	192	TYR	3.7
1	L	135	PHE	3.7
1	L	204	PRO	3.6
2	H	156	THR	3.6
1	L	198	HIS	3.6
1	L	117	ILE	3.6
1	L	205	ILE	3.6
1	L	163	TRP	3.6
1	L	112	ALA	3.5
2	H	198	PRO	3.5
1	L	27(E)	ALA	3.5
1	L	94	ALA	3.5
1	L	196	ALA	3.4
1	L	197	THR	3.4
2	H	206	THR	3.4
1	L	136	LEU	3.4
1	L	113	PRO	3.4
2	H	31	ALA	3.3
1	L	148	TRP	3.3
1	L	126	THR	3.3
1	L	184	ASP	3.3
1	L	203	SER	3.3
1	L	114	THR	3.3
1	L	118	PHE	3.3
1	L	186	TYR	3.2
2	H	167	SER	3.2
2	H	199	ARG	3.2
2	H	138	VAL	3.2
2	H	163	SER	3.1
2	H	166	LEU	3.1
1	L	200	THR	3.1
2	H	142	CYS	3.1
2	H	192	THR	3.0
2	H	107	THR	3.0
1	L	133	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	40	ALA	2.9
2	H	97	ALA	2.9
1	L	190	ASN	2.9
1	L	183	LYS	2.9
1	L	115	VAL	2.9
1	L	128	GLY	2.9
1	L	182	THR	2.8
2	H	191	VAL	2.8
2	H	43	ALA	2.8
2	H	208	CYS	2.8
1	L	144	ILE	2.8
1	L	206	VAL	2.8
2	H	62	ALA	2.8
1	L	41	GLY	2.8
1	L	66	GLY	2.7
1	L	150	ILE	2.7
1	L	121	SER	2.7
1	L	153	SER	2.7
1	L	123	GLU	2.7
2	H	164	GLY	2.6
1	L	193	THR	2.6
1	L	201	SER	2.6
1	L	140	TYR	2.6
2	H	141	GLY	2.6
2	H	66	LYS	2.6
2	H	171	VAL	2.6
1	L	119	PRO	2.5
1	L	176	SER	2.5
1	L	2	VAL	2.5
1	L	199	LYS	2.5
2	H	222	LYS	2.5
1	L	181	LEU	2.5
1	L	155	ARG	2.5
1	L	111	ALA	2.5
1	L	188	ARG	2.4
2	H	177	VAL	2.4
1	L	152	GLY	2.4
1	L	76	SER	2.4
1	L	131	SER	2.4
2	H	122	TYR	2.4
2	H	137	MET	2.4
1	L	139	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	40	PRO	2.4
1	L	124	GLN	2.4
1	L	180	THR	2.4
1	L	202	THR	2.4
1	L	146	VAL	2.4
2	H	184	LEU	2.3
1	L	92	ALA	2.3
1	L	157	ASN	2.3
1	L	120	PRO	2.3
2	H	168	SER	2.3
1	L	175	MET	2.3
2	H	1	GLU	2.3
1	L	3	LEU	2.3
1	L	145	ASN	2.3
1	L	164	THR	2.3
2	H	169	GLY	2.2
1	L	122	SER	2.2
2	H	195	SER	2.2
2	H	196	SER	2.2
2	H	157	TRP	2.2
1	L	109	ALA	2.2
2	H	82(A)	ALA	2.2
2	H	53	ALA	2.2
2	H	7	SER	2.1
1	L	61	ARG	2.1
1	L	142	LYS	2.1
2	H	203	GLU	2.0
2	H	202	SER	2.0
2	H	218	LYS	2.0
2	H	162	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.