



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:15 AM UTC

PDB ID : 5GZO / pdb_00005gzo
Title : Structure of neutralizing antibody bound to Zika envelope protein
Authors : Wang, Q.; Yang, H.; Liu, X.; Dai, L.; Ma, T.; Qi, J.; Wong, G.; Peng, R.; Liu, S.; Li, J.; Li, S.; Song, J.; Liu, J.; He, J.; Yuan, H.; Xiong, Y.; Liao, Y.; Li, J.; Yang, J.; Tong, Z.; Griffin, B.; Bi, Y.; Liang, M.; Xu, X.; Cheng, G.; Wang, P.; Qiu, X.; Kobinger, G.; Shi, Y.; Yan, J.; Gao, G.F.
Deposited on : 2016-09-29
Resolution : 2.75 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

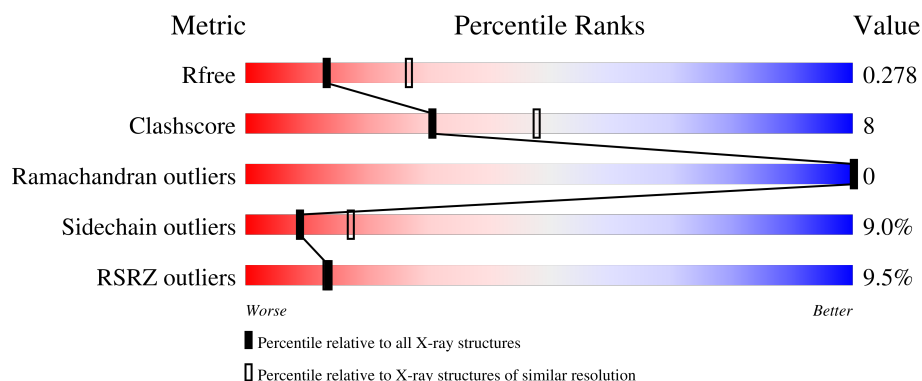
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	409	8% 80% 13% • 5%
1	B	409	19% 76% 18% • 5%
2	C	220	9% 75% 21% • •
2	H	220	2% 76% 17% • •
3	D	215	7% 79% 18% • •

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Mol	Chain	Length	Quality of chain
3	L	215	3% 76% 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12422 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 Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			2976	1861	519	571	25			
1	B	390	Total	C	N	O	S	0	0	0
			2976	1861	519	571	25			

- Molecule 2 is a protein called Antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total	C	N	O	S	0	0	0
			1599	1009	268	318	4			
2	C	214	Total	C	N	O	S	0	0	0
			1599	1009	268	318	4			

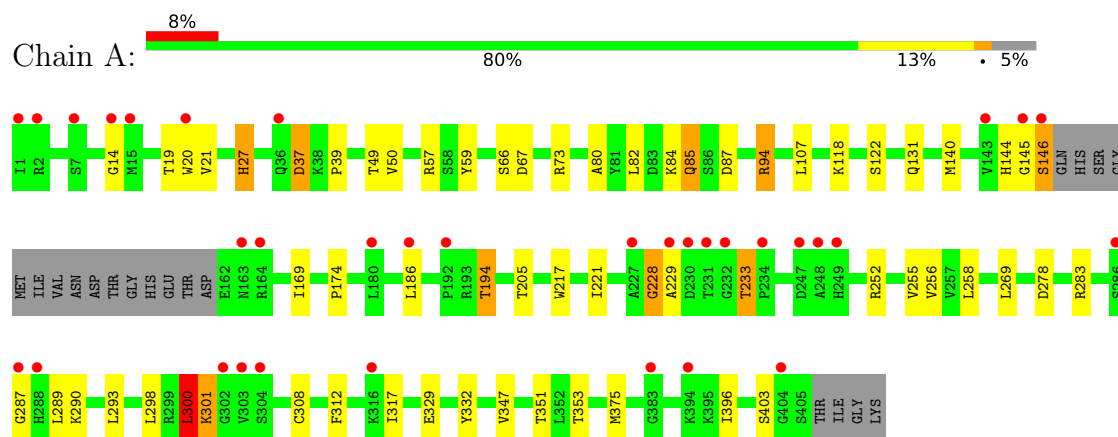
- Molecule 3 is a protein called Antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1636	1019	282	330	5			
3	D	213	Total	C	N	O	S	0	0	0
			1636	1019	282	330	5			

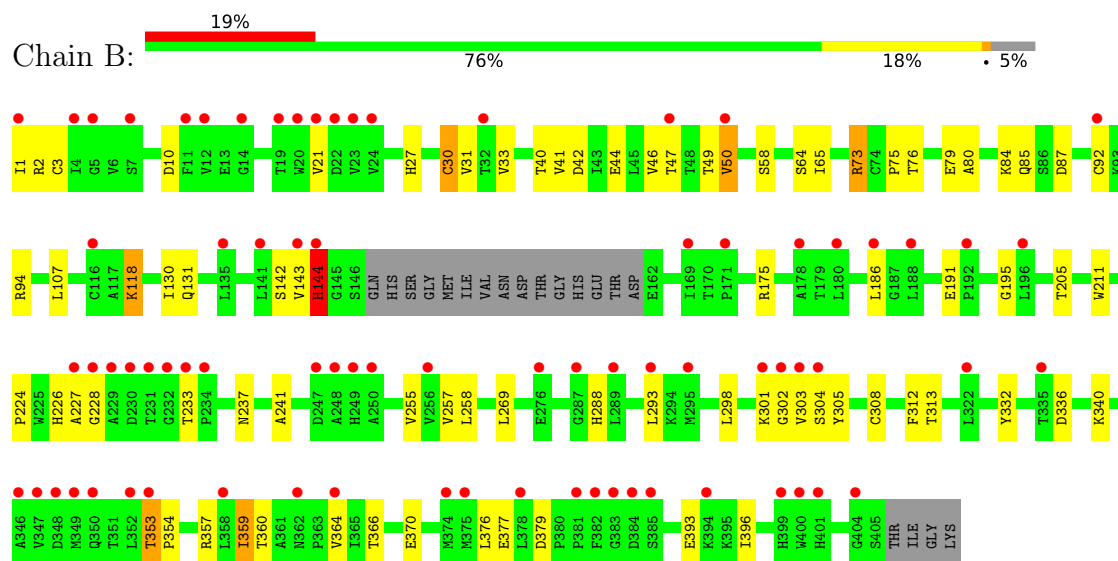
3 Residue-property plots [i](#)

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.

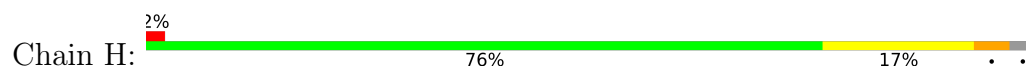
• Molecule 1: Genome polypeptide

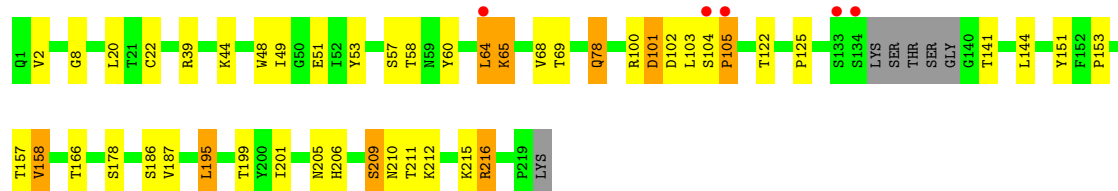


• Molecule 1: Genome polypeptide

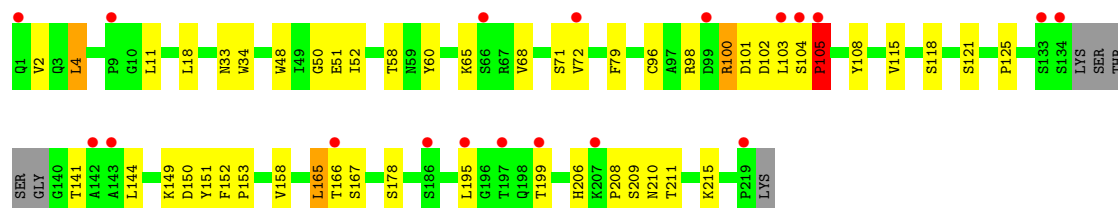
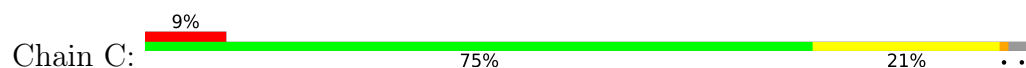


• Molecule 2: Antibody heavy chain

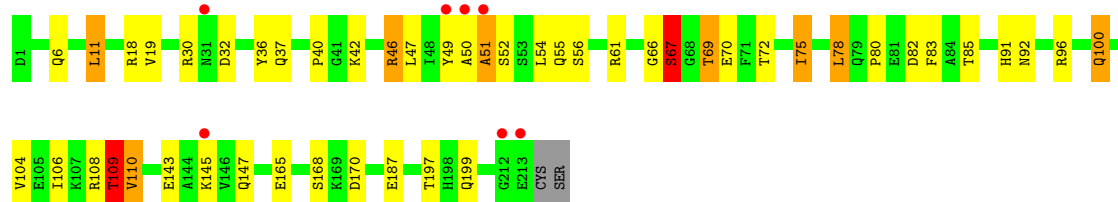
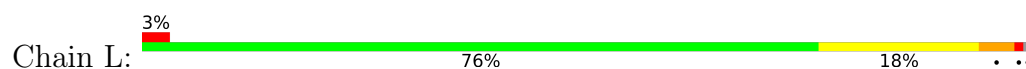




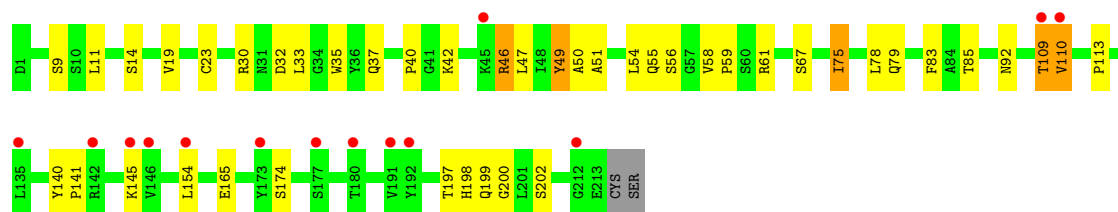
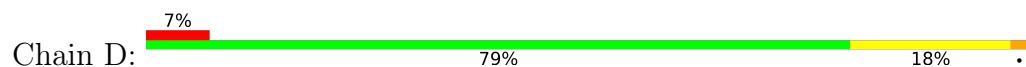
• Molecule 2: Antibody heavy chain



• Molecule 3: Antibody light chain



• Molecule 3: Antibody 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	128.67Å 97.50Å 165.75Å 90.00° 91.52° 90.00°	Depositor
Resolution (Å)	44.68 – 2.75 44.68 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.68-2.75) 99.8 (44.68-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.231 , 0.277 0.236 , 0.278	Depositor DCC
R_{free} test set	2593 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	54.3	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12422	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.27% 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	A	0.38	0/3038	0.82	5/4114 (0.1%)
1	B	0.32	0/3038	0.83	5/4114 (0.1%)
2	C	0.45	1/1640 (0.1%)	0.84	2/2242 (0.1%)
2	H	0.49	0/1640	0.87	5/2242 (0.2%)
3	D	0.38	0/1670	0.85	5/2264 (0.2%)
3	L	0.50	1/1670 (0.1%)	1.07	6/2264 (0.3%)
All	All	0.41	2/12696 (0.0%)	0.87	28/17240 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	105	PRO	N-CD	5.23	1.55	1.47
3	L	67	SER	C-O	-5.06	1.18	1.24

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	49	TYR	N-CA-C	30.11	150.14	113.41
3	D	49	TYR	N-CA-C	11.98	128.52	113.43
2	H	65	LYS	N-CA-CB	-11.27	94.14	110.81
1	A	228	GLY	N-CA-C	10.16	126.78	114.69
2	H	65	LYS	N-CA-C	-9.99	101.65	114.04
1	B	143	VAL	CB-CA-C	9.59	124.35	111.21
3	L	49	TYR	CB-CA-C	-9.21	93.13	109.24
2	C	101	ASP	N-CA-C	9.17	122.11	111.11
1	A	300	LEU	N-CA-C	-8.13	99.04	110.50
1	B	144	HIS	N-CA-C	7.90	120.66	111.02
3	L	51	ALA	CB-CA-C	-7.71	95.07	110.42
1	B	359	ILE	CB-CA-C	-7.66	102.29	111.94
1	B	143	VAL	N-CA-C	-7.57	97.36	108.87
3	D	110	VAL	N-CA-C	-7.41	99.33	109.55
3	L	110	VAL	N-CA-CB	-7.18	97.59	110.95
3	L	110	VAL	N-CA-C	-7.10	97.90	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	110	VAL	N-CA-CB	-7.01	98.22	110.49
2	H	105	PRO	CB-CA-C	-6.79	100.36	111.56
1	A	301	LYS	N-CA-C	-6.73	99.93	109.96
3	D	109	THR	N-CA-C	-6.34	100.45	109.96
3	D	30	ARG	CB-CA-C	-5.99	109.08	117.23
3	L	109	THR	N-CA-C	-5.74	102.41	110.50
1	A	301	LYS	CB-CA-C	5.44	118.00	110.16
1	A	194	THR	CB-CA-C	-5.36	100.45	110.36
2	H	101	ASP	N-CA-C	5.33	119.49	112.89
2	H	166	THR	N-CA-C	-5.16	106.92	114.39
1	B	144	HIS	CB-CA-C	-5.12	102.79	110.92
2	C	50	GLY	N-CA-C	5.06	118.52	111.19

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	A	2976	0	2919	33	1
1	B	2976	0	2919	79	0
2	C	1599	0	1566	28	0
2	H	1599	0	1566	27	0
3	D	1636	0	1597	21	0
3	L	1636	0	1597	32	1
All	All	12422	0	12164	203	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 8.

All (203) 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:B:301:LYS:HZ1	1:B:366:THR:CG2	1.53	1.22
1:B:301:LYS:NZ	1:B:366:THR:CG2	2.12	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:LYS:NZ	1:B:366:THR:HG21	1.67	1.08
1:B:301:LYS:HZ1	1:B:366:THR:HG21	0.87	1.00
2:C:60:TYR:CD1	2:C:65:LYS:HD3	1.98	0.98
1:B:301:LYS:HE3	1:B:364:VAL:CG1	1.97	0.95
1:B:144:HIS:HD2	1:B:360:THR:HA	1.33	0.94
1:B:144:HIS:HD2	1:B:360:THR:CA	1.84	0.91
3:L:6:GLN:HB2	3:L:100:GLN:OE1	1.74	0.87
1:B:301:LYS:NZ	1:B:366:THR:HG22	1.89	0.86
1:B:144:HIS:CD2	1:B:360:THR:HA	2.12	0.85
1:B:302:GLY:O	1:B:303:VAL:HG23	1.79	0.83
1:A:145:GLY:O	1:A:146:SER:OG	1.98	0.81
1:B:58:SER:HB2	1:B:226:HIS:CE1	2.17	0.79
1:A:118:LYS:NZ	2:H:51:GLU:OE2	2.16	0.77
1:B:308:CYS:SG	1:B:340:LYS:O	2.42	0.77
1:B:144:HIS:CD2	1:B:360:THR:CA	2.69	0.74
1:B:301:LYS:HZ2	1:B:366:THR:HG22	1.51	0.74
1:B:144:HIS:CD2	1:B:360:THR:CG2	2.70	0.74
1:B:46:VAL:HG12	1:B:47:THR:HG23	1.70	0.72
1:B:1:ILE:CD1	1:B:144:HIS:O	2.37	0.71
2:H:105:PRO:CB	3:L:36:TYR:OH	2.39	0.70
1:B:301:LYS:HE3	1:B:364:VAL:HB	1.72	0.70
1:B:301:LYS:CD	1:B:364:VAL:HG11	2.21	0.70
2:H:105:PRO:HB2	3:L:36:TYR:OH	1.92	0.69
1:B:144:HIS:NE2	1:B:359:ILE:HG22	2.08	0.69
1:B:301:LYS:HE3	1:B:364:VAL:CB	2.21	0.69
1:A:37:ASP:C	1:A:300:LEU:HD21	2.18	0.68
3:L:108:ARG:NH2	3:L:170:ASP:O	2.26	0.67
1:B:144:HIS:CD2	1:B:360:THR:HG23	2.29	0.67
1:A:145:GLY:O	1:A:146:SER:CB	2.42	0.66
1:B:144:HIS:HD2	1:B:360:THR:N	1.93	0.66
2:C:100:ARG:HB3	2:C:104:SER:OG	1.96	0.65
3:L:6:GLN:CB	3:L:100:GLN:OE1	2.44	0.65
1:B:302:GLY:O	1:B:303:VAL:CG2	2.44	0.65
3:D:40:PRO:HG2	3:D:165:GLU:HG2	1.78	0.64
3:D:19:VAL:HB	3:D:75:ILE:HG23	1.79	0.63
2:H:206:HIS:ND1	2:H:209:SER:HB3	2.13	0.63
2:C:48:TRP:HZ2	2:C:51:GLU:HB2	1.62	0.63
3:D:37:GLN:HB2	3:D:47:LEU:HD11	1.82	0.62
3:D:50:ALA:O	3:D:51:ALA:HB3	1.98	0.62
2:H:201:ILE:HG12	2:H:216:ARG:HG3	1.81	0.62
1:B:301:LYS:HE3	1:B:364:VAL:HG11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:40:PRO:HG2	3:L:165:GLU:HG2	1.82	0.61
3:L:19:VAL:HB	3:L:75:ILE:HG23	1.82	0.61
3:D:145:LYS:HB2	3:D:197:THR:HB	1.82	0.61
3:L:6:GLN:N	3:L:100:GLN:OE1	2.32	0.61
2:C:125:PRO:HB3	2:C:151:TYR:HB3	1.82	0.61
1:B:301:LYS:CE	1:B:364:VAL:HB	2.30	0.60
1:B:144:HIS:CD2	1:B:360:THR:N	2.70	0.60
2:C:18:LEU:HD12	2:C:115:VAL:HG11	1.84	0.60
1:A:300:LEU:H	1:A:300:LEU:CD2	2.16	0.59
3:L:6:GLN:CA	3:L:100:GLN:OE1	2.51	0.59
1:A:57:ARG:NH1	1:A:59:TYR:OH	2.35	0.59
1:B:85:GLN:OE1	1:B:94:ARG:NH2	2.32	0.59
3:L:83:PHE:HZ	3:L:165:GLU:HG3	1.67	0.59
1:A:186:LEU:HD21	1:A:298:LEU:HD22	1.84	0.59
1:A:194:THR:HG21	1:A:290:LYS:HE2	1.85	0.59
2:H:105:PRO:HB3	3:L:36:TYR:OH	2.04	0.58
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.85	0.58
3:D:49:TYR:HB2	3:D:55:GLN:NE2	2.18	0.58
1:A:145:GLY:C	1:A:146:SER:OG	2.47	0.58
2:H:48:TRP:HZ2	2:H:51:GLU:HB2	1.67	0.58
1:B:301:LYS:HD3	1:B:305:TYR:CE2	2.39	0.58
2:C:60:TYR:HD1	2:C:65:LYS:HD3	1.65	0.58
1:B:65:ILE:HA	2:C:103:LEU:HD12	1.87	0.57
1:B:301:LYS:HD2	1:B:364:VAL:HG21	1.86	0.57
1:B:186:LEU:HD21	1:B:298:LEU:HD22	1.87	0.56
1:B:227:ALA:O	1:B:228:GLY:C	2.49	0.56
1:B:118:LYS:NZ	2:C:51:GLU:OE2	2.37	0.55
3:L:80:PRO:HA	3:L:106:ILE:HD13	1.88	0.55
1:B:301:LYS:CE	1:B:364:VAL:HG11	2.35	0.55
3:L:83:PHE:CZ	3:L:165:GLU:HG3	2.41	0.55
1:B:50:VAL:HG11	1:B:130:ILE:HG23	1.88	0.55
2:C:166:THR:HG23	2:C:167:SER:N	2.20	0.55
3:D:46:ARG:NH2	3:D:56:SER:O	2.39	0.55
2:C:165:LEU:C	2:C:165:LEU:HD12	2.32	0.54
1:A:85:GLN:OE1	1:A:94:ARG:NH2	2.41	0.54
1:B:144:HIS:CG	1:B:360:THR:HG22	2.43	0.54
1:A:300:LEU:H	1:A:300:LEU:HD23	1.72	0.54
1:A:308:CYS:HB3	1:A:332:TYR:CZ	2.42	0.54
1:B:301:LYS:HE3	1:B:364:VAL:HG12	1.85	0.53
1:B:144:HIS:CD2	1:B:360:THR:HG22	2.44	0.53
3:L:61:ARG:HH21	3:L:82:ASP:CG	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:THR:HB	1:B:144:HIS:HB2	1.90	0.53
3:L:61:ARG:NH2	3:L:82:ASP:OD1	2.33	0.52
1:B:1:ILE:HD12	1:B:144:HIS:O	2.07	0.52
1:A:312:PHE:C	1:A:396:ILE:HD11	2.35	0.52
2:C:4:LEU:HD11	2:C:108:TYR:HB3	1.92	0.52
2:H:8:GLY:HA3	2:H:20:LEU:HD23	1.92	0.51
1:B:30:CYS:SG	1:B:31:VAL:N	2.83	0.51
1:B:312:PHE:C	1:B:396:ILE:HD11	2.35	0.51
1:A:27:HIS:HB2	1:A:287:GLY:H	1.75	0.51
1:A:300:LEU:CD2	1:A:300:LEU:N	2.73	0.51
1:B:301:LYS:CE	1:B:364:VAL:CG1	2.79	0.50
2:C:11:LEU:HD11	2:C:118:SER:HB3	1.91	0.50
3:L:40:PRO:CG	3:L:165:GLU:HG2	2.40	0.50
1:B:118:LYS:HB3	2:C:103:LEU:HD13	1.94	0.50
3:L:6:GLN:O	3:L:100:GLN:OE1	2.29	0.50
3:L:32:ASP:HB2	3:L:92:ASN:HB2	1.93	0.50
2:C:52:ILE:HD12	2:C:58:THR:HG22	1.94	0.50
2:C:206:HIS:CD2	2:C:208:PRO:HD2	2.45	0.50
3:D:59:PRO:HB2	3:D:61:ARG:HG2	1.94	0.49
1:B:302:GLY:C	1:B:303:VAL:HG23	2.35	0.49
3:D:40:PRO:CG	3:D:165:GLU:HG2	2.43	0.49
1:A:67:ASP:OD2	3:L:96:ARG:NH2	2.42	0.49
1:A:84:LYS:NZ	2:H:58:THR:O	2.45	0.49
1:A:228:GLY:O	1:A:229:ALA:HB3	2.13	0.49
3:D:50:ALA:O	3:D:51:ALA:CB	2.61	0.49
3:L:145:LYS:HB2	3:L:197:THR:HB	1.93	0.48
2:C:79:PHE:CZ	2:C:96:CYS:HB2	2.48	0.48
2:C:33:ASN:HD22	2:C:98:ARG:HD2	1.79	0.48
2:H:39:ARG:HB3	2:H:49:ILE:HD11	1.96	0.48
1:B:1:ILE:HD11	1:B:144:HIS:O	2.13	0.48
1:B:73:ARG:HD3	1:B:80:ALA:HA	1.94	0.48
1:B:308:CYS:HB3	1:B:332:TYR:CZ	2.48	0.48
3:L:11:LEU:HD11	3:L:19:VAL:HG13	1.96	0.47
1:B:336:ASP:OD1	1:B:336:ASP:N	2.43	0.47
1:A:82:LEU:O	1:A:85:GLN:HB2	2.14	0.47
2:H:100:ARG:HB3	2:H:104:SER:OG	2.14	0.47
1:B:40:THR:OG1	1:B:359:ILE:O	2.31	0.47
1:A:67:ASP:OD2	1:A:118:LYS:NZ	2.40	0.47
1:B:65:ILE:CA	2:C:103:LEU:HD12	2.44	0.47
1:B:305:TYR:HB2	1:B:340:LYS:HG3	1.98	0.46
1:B:144:HIS:NE2	1:B:359:ILE:CG2	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:PRO:O	1:B:76:THR:OG1	2.30	0.46
1:A:87:ASP:OD2	2:H:57:SER:OG	2.29	0.46
2:H:102:ASP:C	2:H:104:SER:H	2.23	0.46
1:B:79:GLU:HB3	1:B:94:ARG:NH1	2.31	0.46
1:B:85:GLN:HA	1:B:92:CYS:SG	2.56	0.46
1:B:301:LYS:CE	1:B:366:THR:CG2	2.90	0.46
3:D:83:PHE:CZ	3:D:165:GLU:HG3	2.51	0.46
1:B:118:LYS:HE3	2:C:34:TRP:CD1	2.51	0.45
3:D:198:HIS:CD2	3:D:200:GLY:H	2.34	0.45
2:H:60:TYR:HB2	2:H:65:LYS:HD2	1.99	0.45
1:B:359:ILE:HD11	1:B:379:ASP:HB2	1.99	0.45
1:A:73:ARG:HD3	1:A:80:ALA:HA	1.99	0.45
3:L:108:ARG:HG3	3:L:109:THR:O	2.17	0.44
1:B:144:HIS:CD2	1:B:359:ILE:C	2.95	0.44
1:A:169:ILE:HG23	1:A:174:PRO:HA	1.99	0.44
3:L:50:ALA:O	3:L:51:ALA:CB	2.65	0.44
1:B:195:GLY:O	1:B:288:HIS:HB3	2.18	0.44
1:B:353:THR:HA	1:B:354:PRO:HD3	1.84	0.44
3:L:66:GLY:C	3:L:67:SER:OG	2.61	0.43
1:A:19:THR:HG1	1:A:20:TRP:CD1	2.36	0.43
2:H:157:THR:OG1	2:H:205:ASN:HB3	2.19	0.43
1:B:84:LYS:HA	1:B:87:ASP:HB2	1.99	0.43
3:D:49:TYR:HB2	3:D:55:GLN:HE21	1.83	0.43
1:B:2:ARG:HE	1:B:44:GLU:CD	2.26	0.43
1:B:224:PRO:HD3	1:B:241:ALA:HB3	2.00	0.43
1:B:186:LEU:HG	1:B:298:LEU:HD13	1.99	0.43
1:B:211:TRP:CD2	1:B:269:LEU:HD13	2.53	0.43
1:B:224:PRO:HA	1:B:237:ASN:O	2.18	0.43
2:C:166:THR:CG2	2:C:167:SER:N	2.81	0.43
3:D:23:CYS:HB2	3:D:35:TRP:CH2	2.54	0.43
3:D:140:TYR:CG	3:D:141:PRO:HA	2.54	0.43
1:B:359:ILE:HB	1:B:377:GLU:HB3	2.01	0.43
1:A:39:PRO:HD3	1:A:300:LEU:HD22	2.00	0.42
2:H:102:ASP:OD2	2:H:102:ASP:N	2.49	0.42
2:H:64:LEU:O	2:H:68:VAL:HG22	2.18	0.42
2:C:79:PHE:HZ	2:C:96:CYS:HB2	1.84	0.42
1:B:301:LYS:HD3	1:B:364:VAL:HG11	1.98	0.42
1:B:33:VAL:HB	1:B:41:VAL:HG23	2.01	0.42
2:C:102:ASP:OD2	2:C:102:ASP:N	2.38	0.42
3:L:11:LEU:HD22	3:L:104:VAL:HG22	2.01	0.42
1:A:300:LEU:O	1:A:301:LYS:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:32:ASP:HB2	3:D:92:ASN:HB2	2.02	0.42
2:H:101:ASP:C	2:H:103:LEU:H	2.27	0.42
1:A:118:LYS:HB3	2:H:103:LEU:HD13	2.02	0.42
1:A:329:GLU:HG3	1:A:375:MET:HG2	2.01	0.42
3:D:54:LEU:HD11	3:D:58:VAL:O	2.20	0.42
1:A:217:TRP:CZ3	1:A:221:ILE:HD11	2.55	0.41
1:A:217:TRP:CH2	1:A:269:LEU:HD21	2.55	0.41
3:L:46:ARG:NH2	3:L:56:SER:O	2.53	0.41
3:L:50:ALA:O	3:L:51:ALA:HB3	2.20	0.41
2:C:105:PRO:O	2:C:105:PRO:HG2	2.20	0.41
3:D:113:PRO:HD3	3:D:198:HIS:CD2	2.55	0.41
2:H:100:ARG:NH2	3:L:55:GLN:OE1	2.53	0.41
3:D:61:ARG:CZ	3:D:79:GLN:HG3	2.50	0.41
3:L:100:GLN:H	3:L:100:GLN:HG3	1.50	0.41
1:B:3:CYS:SG	1:B:42:ASP:HB3	2.61	0.41
1:B:144:HIS:HD2	1:B:359:ILE:C	2.28	0.41
2:C:65:LYS:HA	2:C:68:VAL:HG22	2.02	0.41
1:B:64:SER:HA	1:B:257:VAL:HG11	2.02	0.41
1:B:94:ARG:HE	1:B:94:ARG:HB3	1.63	0.41
1:A:66:SER:HB2	3:L:91:HIS:HD2	1.86	0.41
3:L:78:LEU:HD23	3:L:78:LEU:HA	1.76	0.41
1:B:65:ILE:HA	2:C:103:LEU:CD1	2.49	0.41
1:A:233:THR:HG21	2:H:53:TYR:HE2	1.86	0.41
1:B:42:ASP:HB2	1:B:142:SER:OG	2.20	0.41
2:C:149:LYS:HG2	2:C:150:ASP:CG	2.45	0.41
3:D:78:LEU:HD23	3:D:78:LEU:HA	1.85	0.41
2:H:48:TRP:CZ2	2:H:51:GLU:HB2	2.51	0.40
2:H:158:VAL:HG11	2:H:186:SER:HB2	2.02	0.40
2:H:195:LEU:HD12	2:H:195:LEU:HA	1.89	0.40
2:C:100:ARG:HD2	2:C:102:ASP:OD2	2.21	0.40
2:C:152:PHE:HA	2:C:153:PRO:HA	1.90	0.40
1:A:14:GLY:HA2	1:A:21:VAL:HG11	2.03	0.40
2:H:22:CYS:O	2:H:78:GLN:HB2	2.22	0.40
2:H:125:PRO:HB3	2:H:151:TYR:HB3	2.03	0.40
1:B:301:LYS:HZ2	1:B:366:THR:CG2	2.08	0.40
2:H:122:THR:HG22	2:H:153:PRO:HD3	2.03	0.40
3:D:83:PHE:HZ	3:D:165:GLU:HG3	1.85	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)
1:A:278:ASP:OD1	3:L:69:THR:OG1[2_758]	2.00	0.20

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	386/409 (94%)	375 (97%)	11 (3%)	0	100	100
1	B	386/409 (94%)	359 (93%)	27 (7%)	0	100	100
2	C	210/220 (96%)	201 (96%)	9 (4%)	0	100	100
2	H	210/220 (96%)	203 (97%)	7 (3%)	0	100	100
3	D	211/215 (98%)	202 (96%)	9 (4%)	0	100	100
3	L	211/215 (98%)	203 (96%)	8 (4%)	0	100	100
All	All	1614/1688 (96%)	1543 (96%)	71 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	325/341 (95%)	298 (92%)	27 (8%)	10	19
1	B	325/341 (95%)	300 (92%)	25 (8%)	12	22
2	C	185/190 (97%)	167 (90%)	18 (10%)	8	15
2	H	185/190 (97%)	167 (90%)	18 (10%)	8	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	186/188 (99%)	171 (92%)	15 (8%)	11	20
3	L	186/188 (99%)	164 (88%)	22 (12%)	5	9
All	All	1392/1438 (97%)	1267 (91%)	125 (9%)	9	17

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	37	ASP
1	A	49	THR
1	A	50	VAL
1	A	85	GLN
1	A	94	ARG
1	A	107	LEU
1	A	122	SER
1	A	131	GLN
1	A	140	MET
1	A	144	HIS
1	A	146	SER
1	A	205	THR
1	A	233	THR
1	A	252	ARG
1	A	255	VAL
1	A	256	VAL
1	A	258	LEU
1	A	283	ARG
1	A	289	LEU
1	A	293	LEU
1	A	300	LEU
1	A	317	ILE
1	A	347	VAL
1	A	351	THR
1	A	353	THR
1	A	403	SER
2	H	2	VAL
2	H	44	LYS
2	H	64	LEU
2	H	69	THR
2	H	78	GLN
2	H	141	THR
2	H	144	LEU

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Mol	Chain	Res	Type
2	H	158	VAL
2	H	178	SER
2	H	187	VAL
2	H	195	LEU
2	H	199	THR
2	H	209	SER
2	H	210	ASN
2	H	211	THR
2	H	212	LYS
2	H	215	LYS
2	H	216	ARG
3	L	11	LEU
3	L	18	ARG
3	L	30	ARG
3	L	42	LYS
3	L	46	ARG
3	L	52	SER
3	L	54	LEU
3	L	67	SER
3	L	69	THR
3	L	70	GLU
3	L	72	THR
3	L	75	ILE
3	L	78	LEU
3	L	85	THR
3	L	100	GLN
3	L	109	THR
3	L	110	VAL
3	L	143	GLU
3	L	147	GLN
3	L	168	SER
3	L	187	GLU
3	L	199	GLN
1	B	10	ASP
1	B	21	VAL
1	B	27	HIS
1	B	30	CYS
1	B	49	THR
1	B	50	VAL
1	B	73	ARG
1	B	107	LEU
1	B	118	LYS

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Mol	Chain	Res	Type
1	B	131	GLN
1	B	144	HIS
1	B	175	ARG
1	B	191	GLU
1	B	205	THR
1	B	233	THR
1	B	255	VAL
1	B	258	LEU
1	B	293	LEU
1	B	304	SER
1	B	313	THR
1	B	353	THR
1	B	357	ARG
1	B	370	GLU
1	B	376	LEU
1	B	393	GLU
2	C	2	VAL
2	C	4	LEU
2	C	71	SER
2	C	72	VAL
2	C	100	ARG
2	C	105	PRO
2	C	121	SER
2	C	141	THR
2	C	144	LEU
2	C	158	VAL
2	C	165	LEU
2	C	178	SER
2	C	195	LEU
2	C	199	THR
2	C	209	SER
2	C	210	ASN
2	C	211	THR
2	C	215	LYS
3	D	9	SER
3	D	11	LEU
3	D	14	SER
3	D	33	LEU
3	D	42	LYS
3	D	46	ARG
3	D	67	SER
3	D	75	ILE

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Mol	Chain	Res	Type
3	D	85	THR
3	D	109	THR
3	D	110	VAL
3	D	154	LEU
3	D	174	SER
3	D	199	GLN
3	D	202	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	266	HIS
1	A	288	HIS
2	H	59	ASN
2	H	78	GLN
2	H	111	GLN
2	H	198	GLN
3	L	147	GLN
1	B	144	HIS
1	B	226	HIS
2	C	5	GLN
2	C	33	ASN
2	C	198	GLN
3	D	31	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

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	390/409 (95%)	0.51	34 (8%) 16 16	24, 59, 119, 189	0
1	B	390/409 (95%)	1.19	77 (19%) 3 2	49, 82, 159, 199	0
2	C	214/220 (97%)	0.73	19 (8%) 15 15	41, 74, 118, 151	0
2	H	214/220 (97%)	-0.09	5 (2%) 61 59	18, 37, 68, 95	0
3	D	213/215 (99%)	0.68	14 (6%) 24 24	38, 76, 128, 160	0
3	L	213/215 (99%)	0.06	7 (3%) 49 47	23, 48, 84, 118	0
All	All	1634/1688 (96%)	0.59	156 (9%) 14 13	18, 65, 132, 199	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	105	PRO	7.9
1	A	229	ALA	5.4
1	B	248	ALA	5.4
3	L	51	ALA	5.1
1	B	347	VAL	5.1
1	A	230	ASP	4.9
1	B	229	ALA	4.8
1	B	186	LEU	4.6
1	B	304	SER	4.6
2	C	134	SER	4.6
2	C	105	PRO	4.5
1	A	303	VAL	4.5
2	C	66	SER	4.4
1	B	295	MET	4.4
1	A	232	GLY	4.3
1	B	14	GLY	4.3
1	B	169	ILE	4.3
1	A	304	SER	4.3
1	B	303	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
2	C	104	SER	4.3
2	H	134	SER	4.1
1	A	247	ASP	4.0
1	B	301	LYS	4.0
1	B	381	PRO	4.0
1	B	144	HIS	3.9
1	B	1	ILE	3.8
1	B	192	PRO	3.8
1	B	4	ILE	3.7
1	B	227	ALA	3.7
1	B	230	ASP	3.7
1	B	250	ALA	3.7
1	A	192	PRO	3.6
1	B	180	LEU	3.5
1	B	24	VAL	3.5
1	B	349	MET	3.5
3	L	212	GLY	3.4
1	B	399	HIS	3.3
1	A	234	PRO	3.3
3	D	173	TYR	3.3
1	A	1	ILE	3.3
1	B	7	SER	3.3
1	B	23	VAL	3.3
1	B	293	LEU	3.2
1	A	14	GLY	3.2
1	B	249	HIS	3.2
1	B	231	THR	3.2
1	B	353	THR	3.2
3	D	145	LYS	3.1
1	B	11	PHE	3.1
1	A	248	ALA	3.1
1	B	401	HIS	3.1
1	B	116	CYS	3.1
1	B	364	VAL	3.1
3	D	146	VAL	3.1
3	L	49	TYR	3.1
1	B	196	LEU	3.0
1	B	362	ASN	3.0
3	L	50	ALA	3.0
1	B	171	PRO	3.0
2	H	133	SER	2.9
2	C	197	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	20	TRP	2.9
1	A	231	THR	2.9
1	B	394	LYS	2.9
1	B	382	PHE	2.9
1	B	384	ASP	2.8
1	B	234	PRO	2.8
1	B	287	GLY	2.8
1	A	288	HIS	2.8
1	A	302	GLY	2.8
1	B	346	ALA	2.7
1	A	180	LEU	2.7
1	B	232	GLY	2.7
1	B	374	MET	2.7
2	C	186	SER	2.7
1	B	352	LEU	2.7
1	B	21	VAL	2.7
1	B	178	ALA	2.7
1	B	247	ASP	2.7
2	C	219	PRO	2.7
1	B	141	LEU	2.7
3	D	154	LEU	2.7
1	A	287	GLY	2.6
1	B	135	LEU	2.6
1	A	164	ARG	2.6
1	B	233	THR	2.6
1	B	302	GLY	2.6
2	C	199	THR	2.5
1	B	188	LEU	2.5
3	L	213	GLU	2.5
2	C	1	GLN	2.5
2	C	195	LEU	2.5
3	D	110	VAL	2.5
1	B	322	LEU	2.5
3	D	192	TYR	2.5
1	B	5	GLY	2.5
1	A	145	GLY	2.5
1	B	256	VAL	2.5
1	B	50	VAL	2.4
2	C	207	LYS	2.4
1	B	47	THR	2.4
1	A	146	SER	2.4
1	A	404	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	385	SER	2.4
1	A	15	MET	2.4
1	B	383	GLY	2.4
1	A	186	LEU	2.4
1	A	286	SER	2.4
1	B	22	ASP	2.4
1	A	394	LYS	2.4
1	B	12	VAL	2.3
2	H	64	LEU	2.3
1	A	2	ARG	2.3
1	B	350	GLN	2.3
1	B	400	TRP	2.3
2	C	142	ALA	2.3
2	C	166	THR	2.3
3	L	145	LYS	2.3
3	D	45	LYS	2.3
2	C	143	ALA	2.2
1	A	316	LYS	2.2
1	B	378	LEU	2.2
3	D	142	ARG	2.2
1	B	228	GLY	2.2
3	D	177	SER	2.2
1	B	143	VAL	2.2
1	B	276	GLU	2.2
2	C	103	LEU	2.2
1	B	358	LEU	2.2
1	A	143	VAL	2.2
1	B	19	THR	2.1
2	C	9	PRO	2.1
3	L	31	ASN	2.1
1	B	348	ASP	2.1
2	C	133	SER	2.1
3	D	191	VAL	2.1
1	B	92	CYS	2.1
1	A	249	HIS	2.1
1	B	404	GLY	2.1
3	D	212	GLY	2.1
2	C	72	VAL	2.1
3	D	109	THR	2.1
1	B	289	LEU	2.1
1	A	163	ASN	2.1
2	C	99	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	20	TRP	2.0
3	D	180	THR	2.0
1	B	375	MET	2.0
1	A	36	GLN	2.0
1	A	383	GLY	2.0
1	A	227	ALA	2.0
1	A	7	SER	2.0
2	H	104	SER	2.0
1	B	32	THR	2.0
1	B	335	THR	2.0
3	D	135	LEU	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.