



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:18 PM GMT

PDB ID : 3WSQ
Title : Structure of HER2 with an Fab
Authors : Fu, W.Y.; Wang, Y.X.; Zhou, L.J.
Deposited on : 2014-03-20
Resolution : 3.50 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

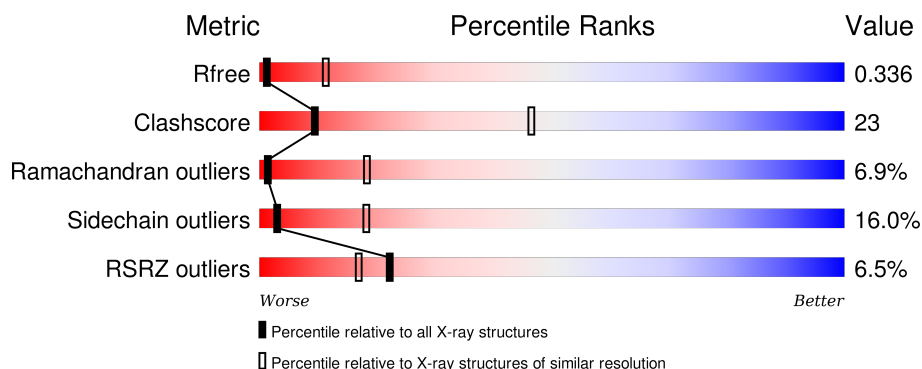
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

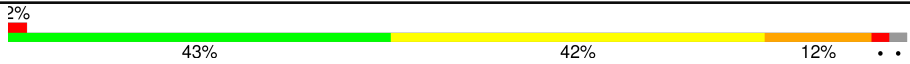


The reported resolution of this entry is 3.50 Å.

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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	564	
2	L	215	
3	H	218	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7475 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 Receptor tyrosine-protein kinase erbB-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4277	2656	769	805	47			

- Molecule 2 is a protein called Antibody Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	215	Total	C	N	O	S	0	0	0
			1584	981	265	333	5			

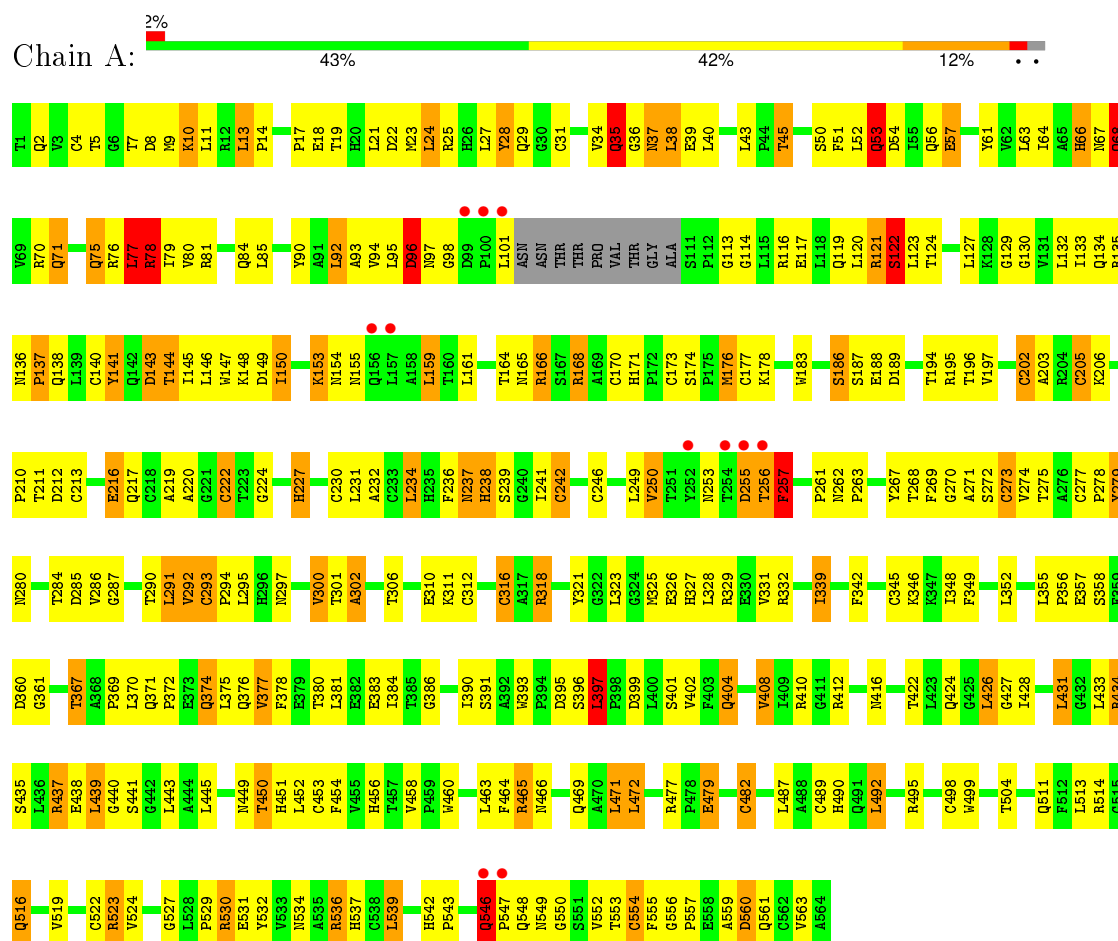
- Molecule 3 is a protein called Antibody Heavy Chain.

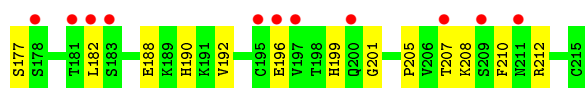
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	218	Total	C	N	O	S	0	0	0
			1614	1011	270	325	8			

3 Residue-property plots

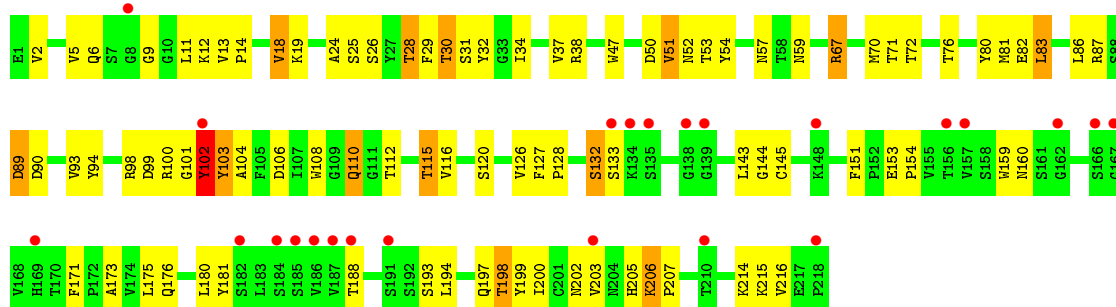
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Receptor tyrosine-protein kinase erbB-2





• Molecule 3: Antibody Heavy Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.56 Å 82.46 Å 110.34 Å 90.00° 90.91° 90.00°	Depositor
Resolution (Å)	38.53 – 3.50 45.85 – 3.39	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.53-3.50) 88.4 (45.85-3.39)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 3.40 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.221 , 0.258 0.263 , 0.336	Depositor DCC
R_{free} test set	750 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.681	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 38.9	EDS
Estimated twinning fraction	0.014 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 18230 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	7475	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.45	0/4374	0.70	2/5950 (0.0%)
2	L	0.32	0/1620	0.64	4/2212 (0.2%)
3	H	0.32	0/1651	0.59	1/2250 (0.0%)
All	All	0.40	0/7645	0.67	7/10412 (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 (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	53	PRO	CA-N-CD	-9.20	98.62	111.50
2	L	96	PRO	CA-N-CD	-8.48	99.63	111.50
3	H	103	TYR	N-CA-C	6.17	127.66	111.00
1	A	38	LEU	CA-CB-CG	5.95	128.99	115.30
2	L	52	ALA	C-N-CD	5.58	140.13	128.40
2	L	32	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	393	TRP	N-CA-C	-5.06	97.33	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	102	TYR	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	A	4277	0	4106	191	0
2	L	1584	0	1514	64	0
3	H	1614	0	1566	87	0
All	All	7475	0	7186	331	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 23.

All (331) 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:H:2:VAL:HA	3:H:26:SER:OG	1.28	1.32
2:L:51:THR:O	2:L:53:PRO:HD3	1.29	1.25
3:H:50:ASP:O	3:H:51:VAL:CG2	1.88	1.22
3:H:11:LEU:CD2	3:H:115:THR:HG23	1.68	1.21
3:H:50:ASP:O	3:H:51:VAL:HG23	1.02	1.19
3:H:11:LEU:HD23	3:H:115:THR:CG2	1.76	1.15
2:L:51:THR:O	2:L:53:PRO:CD	2.03	1.06
3:H:11:LEU:HD23	3:H:115:THR:HG23	1.09	1.05
2:L:20:LEU:HD22	2:L:103:SER:HB2	1.38	1.02
3:H:11:LEU:CD2	3:H:115:THR:CG2	2.34	1.00
3:H:50:ASP:O	3:H:70:MET:CE	2.18	0.90
2:L:20:LEU:HD22	2:L:103:SER:CB	2.03	0.89
3:H:50:ASP:C	3:H:51:VAL:HG23	1.95	0.87
2:L:30:GLY:N	2:L:31:ARG:HA	1.95	0.80
3:H:51:VAL:HG23	3:H:70:MET:CE	2.12	0.80
1:A:560:ASP:N	1:A:560:ASP:OD1	2.15	0.79
3:H:2:VAL:CA	3:H:26:SER:OG	2.23	0.79
1:A:443:LEU:HD13	1:A:472:LEU:HD21	1.66	0.78
2:L:95:VAL:HG13	2:L:96:PRO:HA	1.67	0.76
1:A:554:CYS:SG	1:A:555:PHE:N	2.59	0.76
1:A:148:LYS:O	1:A:195:ARG:NH2	2.18	0.75
2:L:121:PRO:HD3	2:L:133:VAL:HG22	1.67	0.75
2:L:152:ASP:OD2	2:L:190:HIS:ND1	2.18	0.75
3:H:51:VAL:CG2	3:H:70:MET:HE3	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLN:NE2	1:A:117:GLU:O	2.21	0.73
3:H:32:TYR:O	3:H:53:THR:CG2	2.37	0.73
3:H:51:VAL:HG23	3:H:70:MET:HE1	1.67	0.73
1:A:548:GLN:NE2	1:A:552:VAL:O	2.21	0.73
1:A:523:ARG:HB2	1:A:531:GLU:HG3	1.69	0.72
1:A:164:THR:O	1:A:166:ARG:NH1	2.22	0.72
1:A:489:CYS:SG	1:A:498:CYS:N	2.63	0.72
2:L:20:LEU:CD2	2:L:103:SER:HB2	2.20	0.71
1:A:433:LEU:O	1:A:435:SER:N	2.23	0.71
2:L:25:SER:O	2:L:26:ARG:HG3	1.90	0.71
3:H:50:ASP:O	3:H:70:MET:HE1	1.90	0.71
3:H:51:VAL:CG2	3:H:70:MET:CE	2.68	0.71
1:A:375:LEU:O	1:A:377:VAL:N	2.24	0.70
3:H:51:VAL:HG12	3:H:51:VAL:O	1.89	0.70
3:H:32:TYR:O	3:H:53:THR:HG23	1.92	0.70
1:A:404:GLN:HG3	1:A:434:ARG:NH2	2.06	0.70
2:L:77:SER:OG	2:L:78:GLY:N	2.22	0.69
1:A:205:CYS:HB3	1:A:213:CYS:HA	1.76	0.68
1:A:166:ARG:NE	1:A:170:CYS:SG	2.65	0.68
3:H:128:PRO:HA	3:H:145:CYS:HA	1.75	0.68
1:A:378:PHE:HB2	1:A:402:VAL:HG23	1.76	0.67
2:L:48:LEU:O	2:L:56:PRO:HD3	1.94	0.67
1:A:554:CYS:SG	1:A:556:GLY:N	2.66	0.67
1:A:384:ILE:HG22	1:A:386:GLY:H	1.59	0.67
1:A:548:GLN:HG3	1:A:553:THR:HA	1.75	0.67
1:A:390:ILE:HG22	1:A:426:LEU:HD21	1.75	0.67
1:A:256:THR:O	1:A:257:PHE:HB2	1.94	0.66
2:L:35:SER:HB3	2:L:50:SER:HB3	1.78	0.66
1:A:81:ARG:HA	1:A:127:LEU:HB2	1.76	0.66
1:A:272:SER:OG	1:A:273:CYS:N	2.28	0.66
1:A:116:ARG:HG2	1:A:138:GLN:HB3	1.78	0.65
2:L:95:VAL:HG13	3:H:47:TRP:HH2	1.61	0.65
3:H:12:LYS:HB3	3:H:116:VAL:HG22	1.78	0.65
1:A:300:VAL:HG23	1:A:302:ALA:H	1.61	0.65
1:A:250:VAL:HG23	1:A:261:PRO:HA	1.77	0.65
1:A:456:HIS:HB2	1:A:479:GLU:HG3	1.79	0.64
1:A:186:SER:OG	1:A:187:SER:N	2.30	0.64
2:L:96:PRO:HD2	2:L:96:PRO:O	1.97	0.64
1:A:95:LEU:O	1:A:97:ASN:ND2	2.31	0.64
3:H:193:SER:HB2	3:H:197:GLN:HB2	1.80	0.63
1:A:222:CYS:HB2	1:A:224:GLY:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:51:VAL:O	3:H:52:ASN:C	2.34	0.63
1:A:372:PRO:HB3	1:A:397:LEU:HD21	1.81	0.62
3:H:101:GLY:HA3	3:H:102:TYR:HD1	1.63	0.62
1:A:532:TYR:CE1	1:A:539:LEU:HB2	2.35	0.62
1:A:132:LEU:HD12	1:A:161:LEU:HB3	1.82	0.62
2:L:95:VAL:HG13	3:H:47:TRP:CH2	2.35	0.61
3:H:30:THR:HG22	3:H:54:TYR:HA	1.82	0.61
1:A:284:THR:HG22	1:A:286:VAL:H	1.66	0.61
1:A:527:GLY:O	1:A:530:ARG:NH2	2.34	0.60
1:A:428:ILE:HG13	1:A:452:LEU:HD13	1.84	0.60
2:L:56:PRO:HD2	2:L:59:VAL:HB	1.83	0.60
1:A:375:LEU:C	1:A:377:VAL:H	2.05	0.60
1:A:339:ILE:HD13	1:A:370:LEU:HD11	1.83	0.60
3:H:50:ASP:CG	3:H:51:VAL:H	2.06	0.59
3:H:99:ASP:OD1	3:H:99:ASP:N	2.35	0.59
2:L:100:VAL:HG13	2:L:102:GLY:H	1.66	0.59
2:L:95:VAL:CG1	2:L:96:PRO:HA	2.32	0.59
1:A:360:ASP:HB3	3:H:102:TYR:N	2.18	0.59
2:L:2:SER:HA	2:L:98:ALA:HB3	1.83	0.59
1:A:96:ASP:N	1:A:96:ASP:OD1	2.36	0.58
3:H:11:LEU:CD2	3:H:115:THR:HG21	2.30	0.58
3:H:153:GLU:HG3	3:H:154:PRO:HA	1.85	0.58
3:H:30:THR:O	3:H:53:THR:OG1	2.20	0.58
1:A:57:GLU:HG3	1:A:79:ILE:HG23	1.84	0.58
1:A:374:GLN:O	1:A:377:VAL:HG22	2.03	0.58
1:A:404:GLN:HG3	1:A:434:ARG:HH22	1.68	0.58
1:A:408:VAL:HB	1:A:438:GLU:HB3	1.85	0.58
1:A:293:CYS:SG	1:A:294:PRO:HD2	2.42	0.58
1:A:34:VAL:O	1:A:36:GLY:N	2.37	0.58
1:A:316:CYS:O	1:A:318:ARG:NH2	2.37	0.58
1:A:195:ARG:HG3	1:A:203:ALA:O	2.03	0.58
1:A:326:GLU:O	1:A:329:ARG:N	2.24	0.57
3:H:11:LEU:HD22	3:H:115:THR:HG23	1.75	0.57
1:A:78:ARG:NH1	1:A:122:SER:OG	2.37	0.57
3:H:67:ARG:HH22	3:H:90:ASP:CG	2.08	0.57
2:L:38:GLN:HB2	2:L:48:LEU:HD11	1.87	0.57
1:A:85:LEU:HD22	1:A:129:GLY:HA3	1.85	0.56
1:A:487:LEU:H	1:A:487:LEU:HD12	1.70	0.56
1:A:120:LEU:O	1:A:122:SER:N	2.31	0.56
1:A:321:TYR:CE2	1:A:326:GLU:HG3	2.40	0.56
1:A:532:TYR:CZ	1:A:539:LEU:HD12	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:13:VAL:HG13	3:H:14:PRO:HD2	1.86	0.56
2:L:34:VAL:HG21	2:L:67:LYS:HE3	1.87	0.56
2:L:196:GLU:HG3	2:L:207:THR:HB	1.87	0.55
2:L:30:GLY:H	2:L:31:ARG:HG2	1.72	0.55
1:A:401:SER:O	1:A:404:GLN:HB3	2.06	0.55
2:L:39:GLN:NE2	2:L:43:THR:O	2.39	0.55
2:L:95:VAL:HG11	3:H:59:ASN:ND2	2.21	0.55
2:L:86:ASP:HA	2:L:104:GLY:HA2	1.89	0.55
1:A:94:VAL:HB	1:A:133:ILE:HG23	1.88	0.55
1:A:75:GLN:NE2	1:A:119:GLN:OE1	2.40	0.55
3:H:37:VAL:HG22	3:H:47:TRP:HA	1.89	0.55
1:A:267:TYR:N	1:A:274:VAL:O	2.37	0.55
2:L:31:ARG:O	2:L:32:ASP:CG	2.45	0.54
1:A:174:SER:HB3	1:A:177:CYS:SG	2.47	0.54
3:H:200:ILE:HG12	3:H:215:LYS:HA	1.89	0.54
1:A:237:ASN:O	1:A:239:SER:N	2.40	0.54
1:A:360:ASP:HB3	3:H:102:TYR:H	1.72	0.54
3:H:160:ASN:ND2	3:H:198:THR:O	2.41	0.54
1:A:52:LEU:O	1:A:54:ASP:N	2.41	0.53
1:A:140:CYS:HA	1:A:166:ARG:HH21	1.73	0.53
1:A:460:TRP:CE2	1:A:471:LEU:HG	2.44	0.53
2:L:6:GLN:O	2:L:21:SER:OG	2.21	0.53
3:H:51:VAL:CG2	3:H:70:MET:HE1	2.36	0.53
1:A:449:ASN:HB2	1:A:452:LEU:HB2	1.91	0.53
1:A:451:HIS:HA	1:A:477:ARG:HD2	1.90	0.53
2:L:25:SER:O	2:L:26:ARG:CG	2.56	0.53
1:A:523:ARG:O	1:A:531:GLU:N	2.29	0.53
1:A:90:TYR:CZ	1:A:132:LEU:HD13	2.43	0.53
1:A:25:ARG:HG3	1:A:51:PHE:CD2	2.43	0.53
1:A:375:LEU:HB3	1:A:402:VAL:HG21	1.90	0.53
1:A:4:CYS:N	1:A:31:CYS:SG	2.81	0.53
2:L:95:VAL:CG1	3:H:47:TRP:HH2	2.22	0.53
1:A:206:LYS:HG2	1:A:212:ASP:HB3	1.90	0.53
1:A:149:ASP:OD1	1:A:196:THR:N	2.35	0.52
3:H:12:LYS:HZ2	3:H:86:LEU:HD13	1.74	0.52
1:A:479:GLU:HA	1:A:482:CYS:HB2	1.91	0.52
1:A:534:ASN:O	1:A:537:HIS:HB2	2.09	0.52
1:A:81:ARG:HG2	1:A:127:LEU:HD12	1.92	0.52
2:L:28:ASN:HB3	2:L:93:ASP:OD1	2.09	0.52
2:L:143:ARG:HG3	2:L:164:VAL:HG21	1.90	0.52
2:L:62:ARG:O	2:L:76:ILE:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LEU:HD12	1:A:28:TYR:HE2	1.74	0.51
1:A:294:PRO:O	1:A:297:ASN:HB2	2.11	0.51
2:L:28:ASN:ND2	2:L:91:VAL:HG11	2.26	0.51
2:L:95:VAL:HG11	3:H:59:ASN:HD22	1.75	0.50
3:H:71:THR:OG1	3:H:80:TYR:HB2	2.11	0.50
1:A:92:LEU:HD12	1:A:93:ALA:N	2.26	0.50
1:A:279:TYR:CE2	1:A:465:ARG:HG3	2.47	0.50
1:A:216:GLU:HG2	1:A:217:GLN:N	2.25	0.50
1:A:96:ASP:HA	1:A:135:ARG:O	2.10	0.50
1:A:56:GLN:O	1:A:77:LEU:HD23	2.10	0.50
1:A:372:PRO:HB3	1:A:397:LEU:HD11	1.93	0.50
1:A:37:ASN:HB3	1:A:61:TYR:CE1	2.45	0.50
2:L:159:ASN:HD22	2:L:182:LEU:HD21	1.77	0.50
1:A:269:PHE:O	1:A:271:ALA:N	2.45	0.50
1:A:90:TYR:CD1	1:A:132:LEU:HB2	2.47	0.50
1:A:490:HIS:CE1	1:A:492:LEU:HB2	2.47	0.50
1:A:90:TYR:CE2	1:A:132:LEU:HD22	2.47	0.49
1:A:45:THR:HG22	1:A:68:GLN:HB3	1.94	0.49
3:H:151:PHE:HB2	3:H:180:LEU:HD22	1.94	0.49
1:A:141:TYR:HA	1:A:144:THR:OG1	2.11	0.49
1:A:548:GLN:O	1:A:550:GLY:N	2.42	0.49
1:A:280:ASN:ND2	1:A:410:ARG:O	2.45	0.49
1:A:97:ASN:O	1:A:114:GLY:HA2	2.13	0.48
1:A:140:CYS:HA	1:A:166:ARG:NH2	2.28	0.48
2:L:62:ARG:NH2	2:L:83:ASP:OD1	2.46	0.48
1:A:532:TYR:CE2	1:A:557:PRO:HD3	2.49	0.48
2:L:74:LEU:HD12	2:L:75:ALA:H	1.78	0.48
3:H:87:ARG:HG3	3:H:89:ASP:H	1.77	0.48
1:A:149:ASP:CG	1:A:195:ARG:H	2.16	0.48
1:A:284:THR:HG22	1:A:285:ASP:N	2.29	0.48
2:L:34:VAL:HA	2:L:90:THR:O	2.13	0.48
1:A:50:SER:O	1:A:53:GLN:HG2	2.14	0.48
3:H:101:GLY:HA3	3:H:102:TYR:CD1	2.45	0.48
1:A:143:ASP:OD1	1:A:143:ASP:N	2.46	0.48
1:A:439:LEU:HD12	1:A:464:PHE:HE1	1.78	0.48
2:L:62:ARG:HH21	2:L:83:ASP:CG	2.17	0.47
3:H:143:LEU:HB2	3:H:216:VAL:HG11	1.95	0.47
3:H:51:VAL:CG1	3:H:51:VAL:O	2.61	0.47
1:A:466:ASN:ND2	1:A:469:GLN:HG3	2.29	0.47
1:A:39:GLU:OE2	1:A:61:TYR:OH	2.13	0.47
1:A:348:ILE:HD12	1:A:352:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:96:PRO:O	2:L:96:PRO:CD	2.63	0.47
1:A:143:ASP:C	1:A:145:ILE:H	2.18	0.47
1:A:454:PHE:CZ	1:A:487:LEU:HB3	2.50	0.47
2:L:33:PRO:HG2	2:L:34:VAL:HG23	1.97	0.47
1:A:217:GLN:HB3	1:A:242:CYS:O	2.15	0.47
1:A:422:THR:HG23	1:A:445:LEU:HD23	1.96	0.47
2:L:20:LEU:HD22	2:L:103:SER:OG	2.15	0.47
2:L:28:ASN:HB2	2:L:31:ARG:NH1	2.30	0.47
1:A:121:ARG:HA	1:A:183:TRP:CD1	2.50	0.47
1:A:348:ILE:HG13	1:A:381:LEU:HD13	1.97	0.47
1:A:40:LEU:HD21	1:A:52:LEU:HD21	1.96	0.46
3:H:38:ARG:HA	3:H:93:VAL:O	2.15	0.46
1:A:52:LEU:C	1:A:54:ASP:H	2.18	0.46
1:A:511:GLN:O	1:A:536:ARG:HD2	2.16	0.46
2:L:59:VAL:HA	2:L:60:PRO:HD3	1.60	0.46
1:A:147:TRP:CH2	1:A:183:TRP:HH2	2.33	0.46
1:A:186:SER:OG	1:A:188:GLU:HG2	2.16	0.46
1:A:466:ASN:O	1:A:469:GLN:HB2	2.16	0.46
1:A:371:GLN:O	1:A:374:GLN:HB2	2.16	0.46
1:A:437:ARG:O	1:A:463:LEU:HA	2.16	0.46
3:H:206:LYS:HE2	3:H:206:LYS:O	2.16	0.46
3:H:205:HIS:CD2	3:H:207:PRO:HD2	2.51	0.46
1:A:17:PRO:HD2	1:A:18:GLU:OE1	2.15	0.46
2:L:93:ASP:HB3	2:L:94:SER:H	1.56	0.46
3:H:25:SER:C	3:H:26:SER:HG	2.16	0.45
1:A:542:HIS:HA	1:A:543:PRO:HD3	1.87	0.45
2:L:116:VAL:O	2:L:208:LYS:NZ	2.48	0.45
1:A:13:LEU:HA	1:A:14:PRO:HD3	1.78	0.45
3:H:50:ASP:O	3:H:70:MET:HE3	2.07	0.45
1:A:342:PHE:HA	1:A:345:CYS:SG	2.56	0.45
1:A:291:LEU:O	1:A:292:VAL:HG23	2.16	0.45
1:A:236:PHE:O	1:A:238:HIS:N	2.49	0.45
2:L:35:SER:HB2	2:L:47:LEU:HD11	1.98	0.45
3:H:83:LEU:HD13	3:H:86:LEU:HD21	1.97	0.45
1:A:321:TYR:HD1	1:A:349:PHE:HB2	1.82	0.45
1:A:439:LEU:HB2	1:A:463:LEU:HB3	1.98	0.45
1:A:227:HIS:CE1	1:A:241:ILE:HG23	2.52	0.45
1:A:35:GLN:HG2	1:A:35:GLN:H	1.46	0.45
3:H:24:ALA:HB3	3:H:29:PHE:CD2	2.51	0.45
2:L:120:PRO:HB3	2:L:210:PHE:CE1	2.52	0.45
3:H:6:GLN:N	3:H:110:GLN:OE1	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LEU:HD11	1:A:287:GLY:HA2	1.98	0.45
1:A:124:THR:O	1:A:150:ILE:HA	2.17	0.45
1:A:514:ARG:NH1	1:A:531:GLU:OE2	2.50	0.45
2:L:124:GLU:HG3	3:H:127:PHE:CE1	2.52	0.45
3:H:53:THR:HA	3:H:72:THR:HG21	1.99	0.44
1:A:140:CYS:HB3	1:A:141:TYR:CD1	2.52	0.44
1:A:300:VAL:HG11	1:A:310:GLU:CD	2.38	0.44
3:H:100:ARG:HB3	3:H:106:ASP:OD2	2.17	0.44
1:A:356:PRO:HG2	3:H:32:TYR:CE1	2.51	0.44
3:H:173:ALA:HB1	3:H:181:TYR:HB3	1.98	0.44
1:A:530:ARG:HA	1:A:530:ARG:HD3	1.82	0.44
1:A:453:CYS:SG	1:A:477:ARG:HD3	2.57	0.44
2:L:31:ARG:O	2:L:32:ASP:CB	2.65	0.44
1:A:450:THR:HB	1:A:451:HIS:CE1	2.52	0.44
1:A:490:HIS:HE1	1:A:492:LEU:HD22	1.82	0.44
2:L:30:GLY:N	2:L:31:ARG:CA	2.76	0.44
1:A:522:CYS:O	1:A:524:VAL:N	2.51	0.44
1:A:532:TYR:CZ	1:A:557:PRO:HD3	2.52	0.44
3:H:132:SER:OG	3:H:133:SER:N	2.50	0.44
3:H:11:LEU:HD21	3:H:115:THR:HG21	1.99	0.44
3:H:90:ASP:O	3:H:94:TYR:OH	2.33	0.44
3:H:214:LYS:HD2	3:H:214:LYS:HA	1.85	0.44
3:H:32:TYR:CD2	3:H:98:ARG:HD2	2.53	0.43
1:A:291:LEU:HB3	1:A:412:ARG:HB3	2.01	0.43
3:H:106:ASP:N	3:H:106:ASP:OD1	2.42	0.43
1:A:391:SER:HA	1:A:424:GLN:O	2.18	0.43
1:A:328:LEU:HD23	1:A:331:VAL:HG21	1.99	0.43
1:A:262:ASN:HA	1:A:263:PRO:HD2	1.81	0.43
1:A:355:LEU:O	1:A:358:SER:HB2	2.18	0.43
1:A:277:CYS:HA	1:A:278:PRO:HD3	1.67	0.43
1:A:295:LEU:HD12	1:A:295:LEU:HA	1.84	0.43
1:A:143:ASP:O	1:A:145:ILE:N	2.51	0.43
1:A:24:LEU:HD23	1:A:43:LEU:HD21	2.00	0.43
1:A:458:VAL:HG21	1:A:499:TRP:CE3	2.53	0.43
1:A:7:THR:OG1	1:A:39:GLU:HB2	2.18	0.43
3:H:126:VAL:HG21	3:H:203:VAL:HG21	1.99	0.43
1:A:383:GLU:HG2	1:A:383:GLU:O	2.18	0.43
1:A:23:MET:HG2	1:A:443:LEU:HD12	2.01	0.43
1:A:246:CYS:SG	1:A:268:THR:HG22	2.59	0.43
1:A:371:GLN:HA	1:A:372:PRO:HD3	1.76	0.42
2:L:90:THR:HB	2:L:92:TRP:HD1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:199:TYR:O	3:H:216:VAL:N	2.36	0.42
3:H:13:VAL:CG1	3:H:14:PRO:HD2	2.49	0.42
1:A:241:ILE:O	1:A:241:ILE:HG22	2.19	0.42
3:H:144:GLY:HA2	3:H:159:TRP:CZ2	2.54	0.42
1:A:546:GLN:HA	1:A:547:PRO:HD3	1.85	0.42
3:H:89:ASP:N	3:H:89:ASP:OD1	2.51	0.42
1:A:10:LYS:HB3	1:A:11:LEU:H	1.50	0.42
1:A:434:ARG:NE	1:A:516:GLN:HG3	2.34	0.42
3:H:12:LYS:HE2	3:H:18:VAL:HB	2.01	0.42
1:A:323:LEU:HD13	1:A:332:ARG:O	2.19	0.42
1:A:377:VAL:O	1:A:380:THR:HG22	2.19	0.42
3:H:106:ASP:O	3:H:108:TRP:HD1	2.02	0.42
1:A:153:LYS:C	1:A:155:ASN:H	2.22	0.42
1:A:19:THR:O	1:A:22:ASP:N	2.53	0.42
3:H:86:LEU:HD12	3:H:86:LEU:H	1.85	0.42
1:A:130:GLY:HA3	1:A:159:LEU:HD13	2.02	0.42
3:H:176:GLN:N	3:H:180:LEU:O	2.50	0.42
1:A:280:ASN:HD22	1:A:441:SER:HB3	1.85	0.42
1:A:426:LEU:HD23	1:A:426:LEU:HA	1.77	0.42
1:A:269:PHE:O	1:A:272:SER:N	2.30	0.42
3:H:87:ARG:HD2	3:H:89:ASP:OD2	2.20	0.42
1:A:149:ASP:OD1	1:A:196:THR:HG23	2.20	0.41
1:A:542:HIS:CB	1:A:559:ALA:HA	2.50	0.41
1:A:542:HIS:CG	1:A:559:ALA:HA	2.55	0.41
2:L:188:GLU:CD	2:L:212:ARG:HH21	2.23	0.41
3:H:70:MET:HE3	3:H:70:MET:HB2	1.92	0.41
3:H:175:LEU:HA	3:H:181:TYR:HA	2.02	0.41
1:A:399:ASP:HB2	1:A:431:LEU:O	2.20	0.41
2:L:177:SER:HB2	3:H:171:PHE:CE1	2.55	0.41
3:H:50:ASP:CG	3:H:51:VAL:N	2.72	0.41
1:A:375:LEU:C	1:A:377:VAL:N	2.71	0.41
1:A:63:LEU:HD12	1:A:64:ILE:N	2.35	0.41
2:L:52:ALA:HB3	2:L:53:PRO:HD3	2.02	0.41
3:H:24:ALA:HB3	3:H:29:PHE:HD2	1.85	0.41
2:L:114:PRO:HD3	2:L:199:HIS:ND1	2.35	0.41
2:L:26:ARG:O	2:L:28:ASN:N	2.53	0.41
2:L:6:GLN:HA	2:L:7:PRO:HA	1.77	0.41
1:A:492:LEU:HA	1:A:492:LEU:HD12	1.84	0.41
1:A:431:LEU:HD13	1:A:499:TRP:HZ3	1.85	0.41
1:A:454:PHE:HE1	1:A:487:LEU:HD23	1.85	0.41
2:L:90:THR:HB	2:L:92:TRP:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:HIS:HA	1:A:230:CYS:SG	2.60	0.41
2:L:111:VAL:HG13	2:L:141:TYR:O	2.21	0.41
1:A:149:ASP:OD2	1:A:194:THR:N	2.40	0.41
1:A:360:ASP:HA	1:A:369:PRO:HB3	2.02	0.41
1:A:132:LEU:CD1	1:A:161:LEU:HB3	2.50	0.41
1:A:66:HIS:HA	1:A:96:ASP:O	2.20	0.41
1:A:241:ILE:O	1:A:242:CYS:C	2.59	0.41
1:A:253:ASN:C	1:A:255:ASP:H	2.25	0.41
3:H:19:LYS:HG2	3:H:82:GLU:HG2	2.02	0.41
1:A:361:GLY:HA3	1:A:367:THR:O	2.21	0.41
2:L:122:SER:OG	3:H:127:PHE:HB3	2.21	0.41
3:H:32:TYR:O	3:H:53:THR:HG21	2.16	0.40
1:A:219:ALA:O	1:A:232:ALA:HB3	2.21	0.40
1:A:234:LEU:HD22	1:A:234:LEU:HA	1.90	0.40
1:A:345:CYS:O	1:A:380:THR:HG23	2.22	0.40
2:L:48:LEU:HA	2:L:59:VAL:HG11	2.02	0.40
1:A:113:GLY:O	1:A:138:GLN:HG3	2.21	0.40
1:A:98:GLY:HA3	1:A:137:PRO:HD2	2.03	0.40
1:A:166:ARG:HD3	1:A:168:ARG:O	2.20	0.40
1:A:145:ILE:HG13	1:A:183:TRP:CZ3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	551/564 (98%)	413 (75%)	88 (16%)	50 (9%)	1	11
2	L	213/215 (99%)	172 (81%)	30 (14%)	11 (5%)	2	25
3	H	216/218 (99%)	178 (82%)	31 (14%)	7 (3%)	5	40
All	All	980/997 (98%)	763 (78%)	149 (15%)	68 (7%)	1	18

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	37	ASN
1	A	53	GLN
1	A	96	ASP
1	A	121	ARG
1	A	178	LYS
1	A	220	ALA
1	A	257	PHE
1	A	270	GLY
1	A	302	ALA
1	A	396	SER
1	A	431	LEU
1	A	434	ARG
2	L	32	ASP
2	L	52	ALA
3	H	51	VAL
1	A	8	ASP
1	A	77	LEU
1	A	78	ARG
1	A	123	LEU
1	A	144	THR
1	A	202	CYS
1	A	237	ASN
1	A	279	TYR
1	A	376	GLN
1	A	416	ASN
1	A	426	LEU
1	A	440	GLY
1	A	523	ARG
1	A	529	PRO
1	A	549	ASN
2	L	27	THR
2	L	53	PRO
2	L	77	SER
3	H	9	GLY
3	H	120	SER
3	H	194	LEU
1	A	66	HIS
1	A	67	ASN
1	A	68	GLN
1	A	137	PRO
1	A	173	CYS

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Mol	Chain	Res	Type
1	A	238	HIS
1	A	242	CYS
1	A	256	THR
1	A	546	GLN
2	L	56	PRO
2	L	110	THR
2	L	205	PRO
3	H	132	SER
1	A	29	GLN
1	A	122	SER
1	A	153	LYS
1	A	154	ASN
1	A	211	THR
1	A	292	VAL
1	A	327	HIS
1	A	427	GLY
1	A	561	GLN
2	L	28	ASN
2	L	33	PRO
2	L	201	GLY
3	H	104	ALA
1	A	176	MET
3	H	28	THR
1	A	210	PRO
1	A	197	VAL
1	A	397	LEU

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	478/485 (99%)	383 (80%)	95 (20%)	1	9
2	L	182/183 (100%)	164 (90%)	18 (10%)	10	41
3	H	179/180 (99%)	158 (88%)	21 (12%)	7	32
All	All	839/848 (99%)	705 (84%)	134 (16%)	3	18

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	5	THR
1	A	9	MET
1	A	10	LYS
1	A	13	LEU
1	A	21	LEU
1	A	24	LEU
1	A	27	LEU
1	A	28	TYR
1	A	35	GLN
1	A	38	LEU
1	A	45	THR
1	A	53	GLN
1	A	57	GLU
1	A	68	GLN
1	A	70	ARG
1	A	71	GLN
1	A	75	GLN
1	A	76	ARG
1	A	77	LEU
1	A	78	ARG
1	A	80	VAL
1	A	84	GLN
1	A	92	LEU
1	A	96	ASP
1	A	101	LEU
1	A	122	SER
1	A	134	GLN
1	A	136	ASN
1	A	141	TYR
1	A	143	ASP
1	A	146	LEU
1	A	150	ILE
1	A	159	LEU
1	A	165	ASN
1	A	166	ARG
1	A	168	ARG
1	A	171	HIS
1	A	176	MET
1	A	186	SER
1	A	189	ASP
1	A	202	CYS

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Mol	Chain	Res	Type
1	A	205	CYS
1	A	216	GLU
1	A	222	CYS
1	A	227	HIS
1	A	231	LEU
1	A	234	LEU
1	A	250	VAL
1	A	255	ASP
1	A	257	PHE
1	A	273	CYS
1	A	275	THR
1	A	290	THR
1	A	291	LEU
1	A	293	CYS
1	A	300	VAL
1	A	301	THR
1	A	306	THR
1	A	311	LYS
1	A	312	CYS
1	A	316	CYS
1	A	318	ARG
1	A	325	MET
1	A	339	ILE
1	A	346	LYS
1	A	357	GLU
1	A	367	THR
1	A	374	GLN
1	A	377	VAL
1	A	395	ASP
1	A	397	LEU
1	A	404	GLN
1	A	408	VAL
1	A	437	ARG
1	A	439	LEU
1	A	450	THR
1	A	465	ARG
1	A	471	LEU
1	A	472	LEU
1	A	479	GLU
1	A	482	CYS
1	A	492	LEU
1	A	495	ARG

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Mol	Chain	Res	Type
1	A	504	THR
1	A	513	LEU
1	A	516	GLN
1	A	519	VAL
1	A	530	ARG
1	A	536	ARG
1	A	539	LEU
1	A	546	GLN
1	A	554	CYS
1	A	560	ASP
1	A	563	VAL
2	L	3	VAL
2	L	5	THR
2	L	11	SER
2	L	16	GLN
2	L	35	SER
2	L	50	SER
2	L	81	SER
2	L	90	THR
2	L	93	ASP
2	L	100	VAL
2	L	108	THR
2	L	118	ILE
2	L	130	THR
2	L	144	GLU
2	L	164	VAL
2	L	171	ASP
2	L	176	LEU
2	L	192	VAL
3	H	5	VAL
3	H	18	VAL
3	H	28	THR
3	H	30	THR
3	H	31	SER
3	H	34	ILE
3	H	57	ASN
3	H	67	ARG
3	H	76	THR
3	H	81	MET
3	H	83	LEU
3	H	89	ASP
3	H	102	TYR

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Mol	Chain	Res	Type
3	H	103	TYR
3	H	110	GLN
3	H	112	THR
3	H	115	THR
3	H	188	THR
3	H	198	THR
3	H	202	ASN
3	H	206	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates 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	A	555/564 (98%)	-0.42	11 (1%) 68 59	23, 40, 101, 132	0
2	L	215/215 (100%)	0.79	29 (13%) 4 5	53, 146, 253, 292	0
3	H	218/218 (100%)	0.45	24 (11%) 7 7	35, 123, 257, 278	0
All	All	988/997 (99%)	0.04	64 (6%) 22 17	23, 67, 232, 292	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	547	PRO	7.6
3	H	184	SER	6.2
3	H	185	SER	5.5
2	L	182	LEU	5.0
2	L	53	PRO	4.8
3	H	157	VAL	4.8
2	L	2	SER	4.6
3	H	134	LYS	4.6
3	H	186	VAL	4.5
2	L	148	GLN	4.4
3	H	188	THR	4.3
1	A	254	THR	3.8
2	L	6	GLN	3.8
2	L	123	ASP	3.7
2	L	153	ASN	3.7
1	A	99	ASP	3.6
3	H	8	GLY	3.6
2	L	211	ASN	3.6
2	L	209	SER	3.5
3	H	135	SER	3.5
3	H	187	VAL	3.4
2	L	183	SER	3.4
3	H	203	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
3	H	138	GLY	3.3
1	A	156	GLN	3.2
1	A	256	THR	3.2
1	A	100	PRO	3.2
1	A	255	ASP	3.2
1	A	546	GLN	3.1
3	H	167	GLY	3.0
1	A	157	LEU	2.9
1	A	101	LEU	2.9
2	L	195	CYS	2.8
2	L	105	THR	2.8
3	H	156	THR	2.8
3	H	102	TYR	2.7
2	L	94	SER	2.7
2	L	31	ARG	2.7
3	H	169	HIS	2.6
2	L	207	THR	2.6
2	L	30	GLY	2.6
2	L	117	PHE	2.6
2	L	197	VAL	2.5
3	H	133	SER	2.5
2	L	127	LYS	2.5
2	L	200	GLN	2.5
2	L	181	THR	2.4
3	H	182	SER	2.4
3	H	148	LYS	2.3
2	L	9	SER	2.3
3	H	166	SER	2.3
3	H	162	GLY	2.3
2	L	178	SER	2.3
2	L	196	GLU	2.3
2	L	11	SER	2.3
2	L	32	ASP	2.2
2	L	116	VAL	2.2
3	H	191	SER	2.2
3	H	139	GLY	2.1
1	A	252	TYR	2.1
2	L	109	VAL	2.1
2	L	1	GLN	2.1
3	H	210	THR	2.1
3	H	218	PRO	2.1

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 carbohydrates 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.