



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:33 AM UTC

PDB ID : 3VA6 / pdb_00003va6
Title : Crystal Structure of the extracellular domain of the putative hybrid two component system BT4673 from *B. thetaiotaomicron*
Authors : Zhang, Z.; Liu, Q.; Hendrickson, W.A.
Deposited on : 2011-12-28
Resolution : 2.80 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

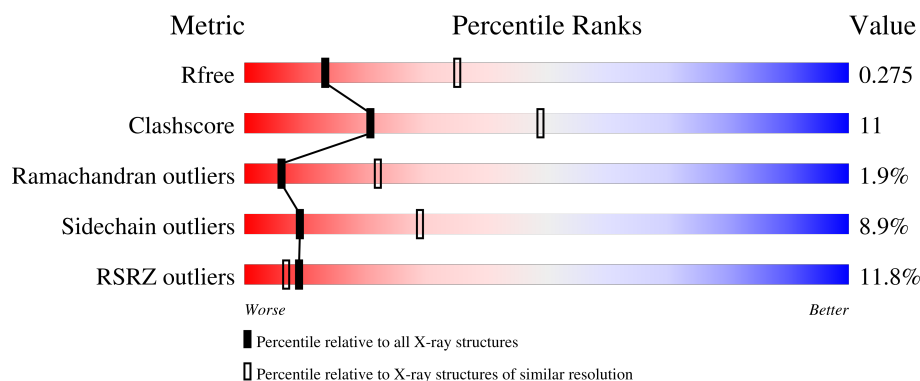
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	758	15% 75% 19% ..
1	B	758	8% 72% 20% 5% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12203 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 Two-component system sensor histidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	747	Total	C	N	O	S	0	0	0
			6077	3855	1043	1162	17			
1	B	743	Total	C	N	O	S	0	0	0
			6032	3828	1028	1158	18			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	LEU	-	expression tag	UNP Q89YQ8
A	29	GLU	-	expression tag	UNP Q89YQ8
A	778	LEU	-	expression tag	UNP Q89YQ8
A	779	GLU	-	expression tag	UNP Q89YQ8
A	780	HIS	-	expression tag	UNP Q89YQ8
A	781	HIS	-	expression tag	UNP Q89YQ8
A	782	HIS	-	expression tag	UNP Q89YQ8
A	783	HIS	-	expression tag	UNP Q89YQ8
A	784	HIS	-	expression tag	UNP Q89YQ8
A	785	HIS	-	expression tag	UNP Q89YQ8
B	28	LEU	-	expression tag	UNP Q89YQ8
B	29	GLU	-	expression tag	UNP Q89YQ8
B	778	LEU	-	expression tag	UNP Q89YQ8
B	779	GLU	-	expression tag	UNP Q89YQ8
B	780	HIS	-	expression tag	UNP Q89YQ8
B	781	HIS	-	expression tag	UNP Q89YQ8
B	782	HIS	-	expression tag	UNP Q89YQ8
B	783	HIS	-	expression tag	UNP Q89YQ8
B	784	HIS	-	expression tag	UNP Q89YQ8
B	785	HIS	-	expression tag	UNP Q89YQ8

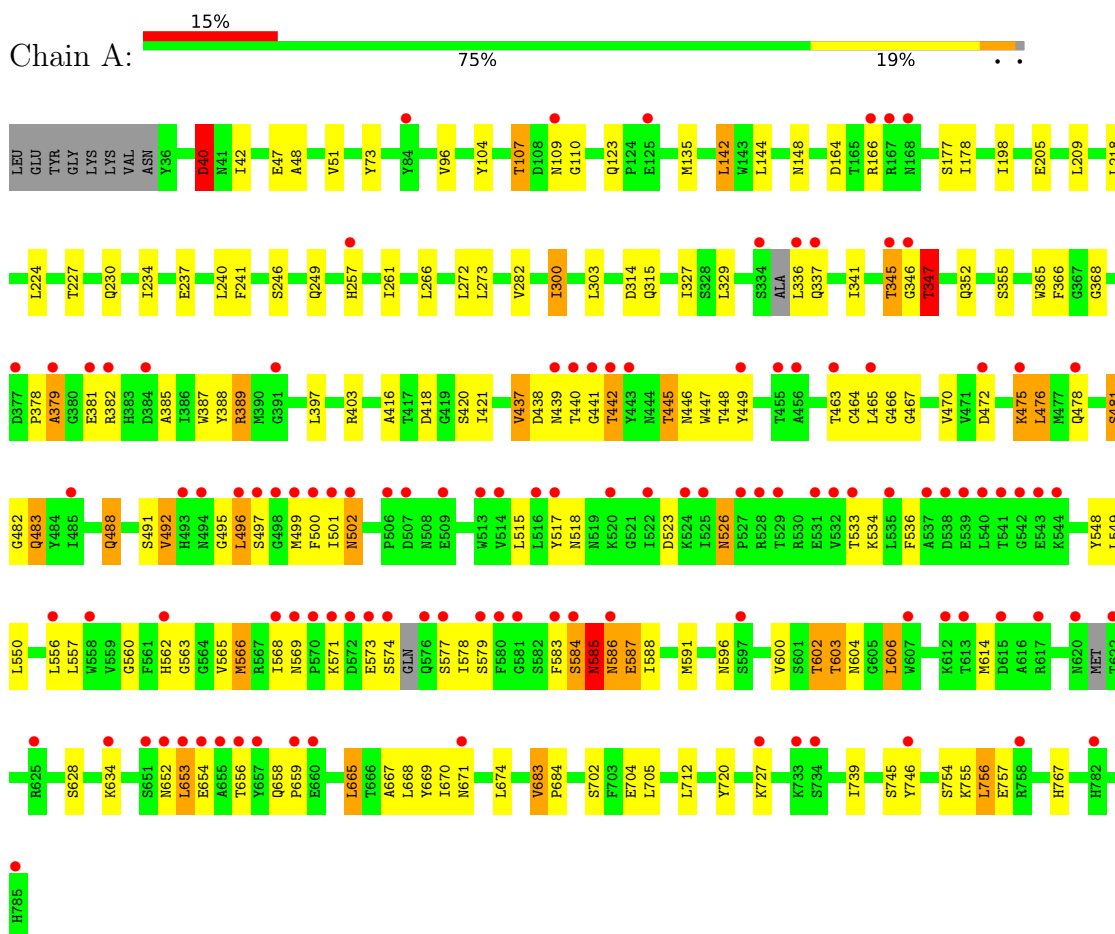
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	48	Total 48	O 48	0	0
2	B	46	Total 46	O 46	0	0

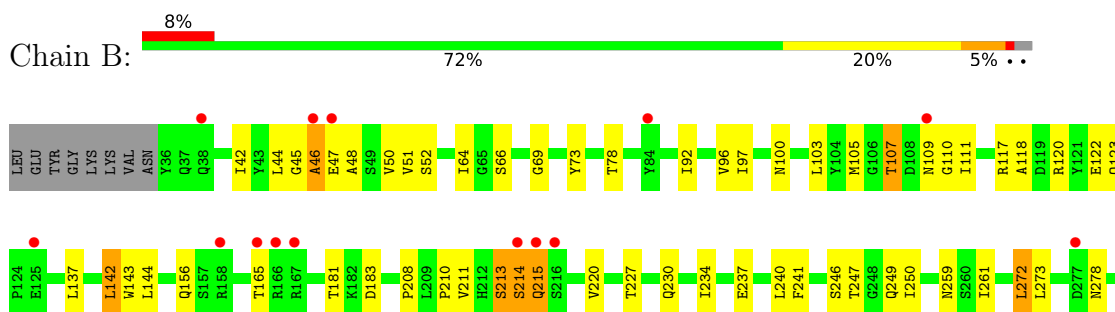
3 Residue-property plots

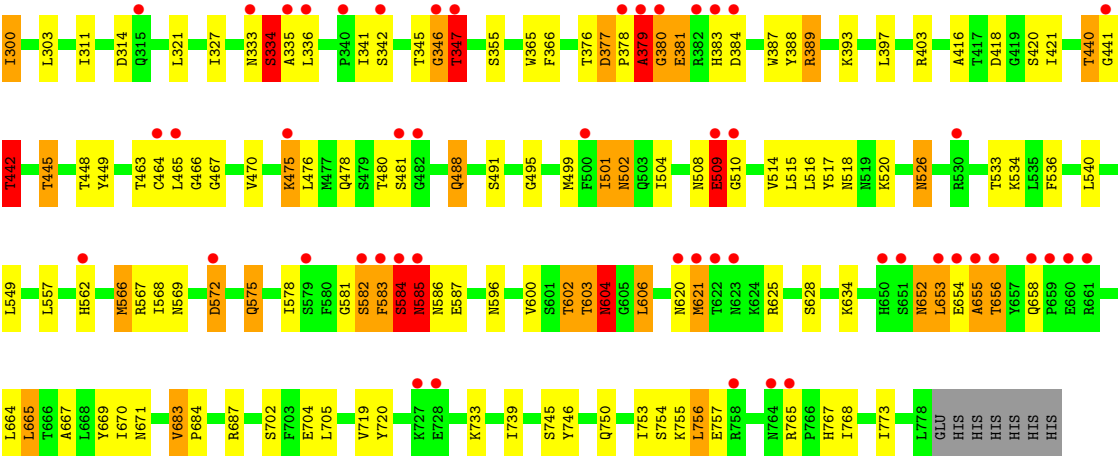
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Two-component system sensor histidine kinase



- Molecule 1: Two-component system sensor histidine kinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	87.88Å 87.88Å 430.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.86 – 2.80 45.86 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.2 (45.86-2.80) 92.4 (45.86-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.216 , 0.274 0.218 , 0.275	Depositor DCC
R_{free} test set	2024 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	1.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.6	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	0.91	EDS
Total number of atoms	12203	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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	0.85	3/6232 (0.0%)	0.87	6/8466 (0.1%)
1	B	0.88	1/6184 (0.0%)	0.95	16/8405 (0.2%)
All	All	0.87	4/12416 (0.0%)	0.91	22/16871 (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
1	B	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	HIS	CG-CD2	6.28	1.42	1.35
1	A	562	HIS	CG-CD2	5.32	1.41	1.35
1	A	257	HIS	CE1-NE2	5.30	1.37	1.32
1	B	562	HIS	CG-CD2	5.16	1.41	1.35

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	380	GLY	N-CA-C	11.39	126.39	112.73
1	B	440	THR	N-CA-C	-7.64	100.24	110.55
1	B	475	LYS	N-CA-C	-7.57	100.54	110.53
1	B	572	ASP	N-CA-C	-7.10	98.73	110.17
1	A	345	THR	CB-CA-C	-6.56	100.66	110.24
1	B	509	GLU	N-CA-C	-6.50	96.96	110.80
1	B	379	ALA	CA-C-N	6.18	126.84	119.98
1	B	379	ALA	C-N-CA	6.18	126.84	119.98
1	A	577	SER	N-CA-C	5.93	118.30	108.99
1	A	40	ASP	CB-CA-C	5.92	120.44	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	481	SER	N-CA-C	5.89	119.57	112.38
1	B	495	GLY	N-CA-C	5.63	121.47	114.37
1	B	50	VAL	N-CA-C	5.58	115.90	107.80
1	B	69	GLY	N-CA-C	5.40	117.72	110.43
1	B	584	SER	CA-C-N	5.34	131.31	121.70
1	B	584	SER	C-N-CA	5.34	131.31	121.70
1	A	164	ASP	N-CA-C	5.18	115.12	108.34
1	A	476	LEU	N-CA-C	-5.15	107.12	113.41
1	B	215	GLN	N-CA-C	5.13	117.95	109.85
1	B	658	GLN	N-CA-C	5.10	116.09	109.72
1	B	442	THR	N-CA-C	5.06	119.45	113.12
1	A	178	ILE	CB-CA-C	-5.06	102.95	110.33

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	213	SER	Peptide
1	B	441	GLY	Peptide
1	B	508	ASN	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	6077	0	5785	120	0
1	B	6032	0	5767	148	0
2	A	48	0	0	1	0
2	B	46	0	0	4	0
All	All	12203	0	11552	263	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 11.

All (263) 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:A:492:VAL:HG11	1:A:499:MET:HE2	1.28	1.07
1:A:586:ASN:HB3	1:A:587:GLU:HA	1.26	1.06
1:A:578:ILE:HG23	1:A:614:MET:HE2	1.43	0.97
1:B:46:ALA:H	1:B:47:GLU:HA	1.32	0.92
1:A:578:ILE:HG23	1:A:614:MET:CE	2.00	0.90
1:A:586:ASN:HB3	1:A:587:GLU:CA	2.02	0.89
1:A:586:ASN:CB	1:A:587:GLU:HA	2.02	0.89
1:B:420:SER:OG	1:B:445:THR:HG22	1.74	0.88
1:A:585:ASN:O	1:A:586:ASN:HB2	1.74	0.88
1:B:584:SER:OG	1:B:585:ASN:HB3	1.75	0.86
1:B:584:SER:CB	1:B:585:ASN:HB3	2.06	0.86
1:A:658:GLN:NE2	1:A:712:LEU:HD21	1.92	0.83
1:A:345:THR:HG23	1:A:385:ALA:HB3	1.62	0.81
1:A:420:SER:OG	1:A:445:THR:HG22	1.80	0.80
1:A:96:VAL:HG12	1:A:135:MET:CE	2.12	0.80
1:B:45:GLY:O	1:B:46:ALA:HB2	1.82	0.79
1:B:517:TYR:CE2	1:B:518:ASN:ND2	2.52	0.78
1:B:120:ARG:NE	1:B:122:GLU:OE2	2.17	0.77
1:B:540:LEU:HD11	1:B:566:MET:HE2	1.64	0.77
1:B:463:THR:HG22	1:B:466:GLY:H	1.50	0.77
1:A:230:GLN:HE21	1:B:230:GLN:NE2	1.82	0.77
1:A:96:VAL:HG12	1:A:135:MET:HE3	1.66	0.76
1:A:584:SER:N	1:A:585:ASN:O	2.18	0.76
1:B:45:GLY:O	1:B:46:ALA:CB	2.34	0.76
1:B:569:ASN:O	1:B:572:ASP:O	2.04	0.75
1:B:475:LYS:HE2	2:B:820:HOH:O	1.85	0.75
1:B:333:ASN:O	1:B:334:SER:HB2	1.87	0.74
1:A:230:GLN:HE21	1:B:230:GLN:HE21	1.32	0.73
1:A:378:PRO:O	1:A:379:ALA:HB2	1.87	0.73
1:B:380:GLY:O	1:B:381:GLU:HB2	1.88	0.73
1:A:578:ILE:CG2	1:A:614:MET:HE2	2.19	0.72
1:B:750:GLN:HE21	1:B:768:ILE:HG21	1.54	0.72
1:A:584:SER:HA	1:A:585:ASN:O	1.89	0.72
1:B:667:ALA:HB3	1:B:704:GLU:HB2	1.71	0.72
1:B:526:ASN:C	1:B:526:ASN:HD22	1.98	0.72
1:B:247:THR:OG1	1:B:249:GLN:HG3	1.90	0.71
1:B:750:GLN:HE21	1:B:768:ILE:CG2	2.05	0.70
1:B:583:PHE:O	1:B:586:ASN:ND2	2.25	0.70
1:B:379:ALA:C	1:B:383:HIS:HE1	2.00	0.70
1:A:346:GLY:HA2	1:A:347:THR:O	1.93	0.69
1:A:658:GLN:HE21	1:A:712:LEU:HD21	1.57	0.69
1:A:96:VAL:CG1	1:A:135:MET:HE3	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:SER:CA	1:A:585:ASN:O	2.41	0.69
1:A:403:ARG:NH2	1:B:156:GLN:O	2.26	0.69
1:B:377:ASP:O	1:B:383:HIS:ND1	2.26	0.69
1:A:40:ASP:OD2	1:A:329:LEU:HD23	1.93	0.68
1:B:142:LEU:HD13	1:B:144:LEU:HD21	1.74	0.68
1:B:118:ALA:HB1	1:B:120:ARG:HD3	1.75	0.68
1:A:563:GLY:HA2	1:A:586:ASN:ND2	2.08	0.68
1:B:536:PHE:HB3	1:B:566:MET:HE1	1.77	0.67
1:B:208:PRO:O	1:B:250:ILE:HD13	1.94	0.67
1:A:378:PRO:O	1:A:379:ALA:CB	2.40	0.66
1:B:440:THR:OG1	1:B:442:THR:HG23	1.95	0.66
1:B:416:ALA:HB1	1:B:448:THR:HG22	1.77	0.66
1:B:520:LYS:HE3	2:B:816:HOH:O	1.94	0.66
1:A:526:ASN:HD22	1:A:526:ASN:C	2.02	0.66
1:A:492:VAL:CG1	1:A:499:MET:HE2	2.16	0.66
1:A:585:ASN:O	1:A:586:ASN:CB	2.44	0.66
1:A:416:ALA:HB1	1:A:448:THR:HG22	1.77	0.65
1:B:346:GLY:HA2	1:B:347:THR:O	1.98	0.64
1:A:475:LYS:HD3	1:A:475:LYS:N	2.13	0.64
1:B:421:ILE:CG2	1:B:448:THR:HG21	2.28	0.64
1:B:214:SER:OG	1:B:215:GLN:HG2	1.98	0.64
1:B:655:ALA:HA	1:B:656:THR:C	2.21	0.64
1:B:584:SER:CA	1:B:585:ASN:HB3	2.27	0.63
1:A:421:ILE:CG2	1:A:448:THR:HG21	2.29	0.63
1:A:463:THR:HG22	1:A:466:GLY:H	1.62	0.63
1:B:143:TRP:O	1:B:144:LEU:HD23	2.00	0.62
1:B:582:SER:O	1:B:583:PHE:HB2	2.00	0.61
1:A:104:TYR:O	1:A:135:MET:HE1	1.99	0.61
1:A:502:ASN:HB3	1:A:515:LEU:HD12	1.80	0.61
1:A:602:THR:HG22	1:A:604:ASN:N	2.15	0.61
1:B:566:MET:SD	1:B:575:GLN:HG3	2.40	0.60
1:B:578:ILE:C	1:B:578:ILE:HD12	2.27	0.60
1:A:445:THR:O	1:A:445:THR:CG2	2.50	0.60
1:A:674:LEU:HD23	1:A:674:LEU:C	2.26	0.60
1:B:501:ILE:HG22	1:B:516:LEU:HG	1.83	0.59
1:A:602:THR:HG22	1:A:604:ASN:H	1.66	0.59
1:B:379:ALA:C	1:B:383:HIS:CE1	2.80	0.59
1:B:421:ILE:HG22	1:B:448:THR:HG21	1.85	0.58
1:B:272:LEU:HD13	1:B:272:LEU:C	2.28	0.58
1:B:502:ASN:HB2	1:B:515:LEU:HD12	1.84	0.58
1:B:566:MET:HE3	1:B:568:ILE:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:LYS:CE	2:B:820:HOH:O	2.46	0.57
1:A:96:VAL:HG12	1:A:135:MET:HE1	1.84	0.57
1:B:46:ALA:N	1:B:47:GLU:HA	2.06	0.57
1:A:437:VAL:HG23	1:A:438:ASP:O	2.04	0.57
1:A:492:VAL:HG11	1:A:499:MET:CE	2.19	0.57
1:A:464:CYS:O	1:A:465:LEU:HB2	2.04	0.57
1:A:583:PHE:HA	1:A:584:SER:C	2.29	0.57
1:B:311:ILE:HG23	1:B:321:LEU:HD23	1.86	0.57
1:B:334:SER:CB	1:B:335:ALA:HA	2.35	0.57
1:B:378:PRO:O	1:B:379:ALA:HB2	2.04	0.57
1:A:665:LEU:HD22	1:A:767:HIS:NE2	2.19	0.56
1:A:142:LEU:HD13	1:A:144:LEU:HD21	1.87	0.56
1:A:272:LEU:C	1:A:272:LEU:HD13	2.29	0.56
1:B:51:VAL:HG13	1:B:64:ILE:HG23	1.86	0.56
1:B:272:LEU:HD13	1:B:273:LEU:N	2.20	0.56
1:B:566:MET:CE	1:B:568:ILE:HD11	2.35	0.56
1:B:602:THR:HG22	1:B:604:ASN:CB	2.36	0.56
1:A:345:THR:HG23	1:A:385:ALA:CB	2.34	0.56
1:B:463:THR:HB	1:B:467:GLY:O	2.06	0.56
1:A:345:THR:CG2	1:A:385:ALA:HB3	2.35	0.56
1:A:587:GLU:N	1:A:603:THR:OG1	2.38	0.56
1:B:107:THR:HG22	1:B:109:ASN:N	2.21	0.55
1:A:42:ILE:HD13	1:A:73:TYR:CE2	2.41	0.55
1:A:237:GLU:HG3	2:A:838:HOH:O	2.06	0.55
1:B:420:SER:OG	1:B:445:THR:CG2	2.51	0.55
1:B:602:THR:HG22	1:B:604:ASN:HB2	1.88	0.55
1:B:475:LYS:O	1:B:476:LEU:HB3	2.07	0.54
1:A:51:VAL:HG21	1:A:327:ILE:HG13	1.90	0.54
1:A:463:THR:HB	1:A:467:GLY:O	2.07	0.54
1:A:421:ILE:HG22	1:A:448:THR:HG21	1.90	0.54
1:B:381:GLU:H	1:B:383:HIS:CE1	2.25	0.54
1:B:584:SER:CB	1:B:585:ASN:CB	2.82	0.54
1:B:664:LEU:HD23	1:B:687:ARG:HG3	1.90	0.54
1:B:509:GLU:HG3	1:B:510:GLY:H	1.72	0.53
1:A:683:VAL:HG12	1:A:684:PRO:HD2	1.90	0.53
1:A:475:LYS:N	1:A:475:LYS:CD	2.72	0.53
1:B:504:ILE:HG22	1:B:514:VAL:HG13	1.90	0.53
1:A:652:ASN:C	1:A:654:GLU:H	2.16	0.53
1:B:654:GLU:O	1:B:655:ALA:C	2.52	0.52
1:A:107:THR:HG22	1:A:109:ASN:N	2.25	0.52
1:A:517:TYR:CE2	1:A:518:ASN:ND2	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:602:THR:CG2	1:B:604:ASN:HB2	2.40	0.52
1:B:620:ASN:O	1:B:621:MET:C	2.53	0.52
1:B:445:THR:CG2	1:B:445:THR:O	2.58	0.52
1:B:750:GLN:NE2	1:B:768:ILE:HG21	2.23	0.52
1:A:492:VAL:N	1:A:495:GLY:O	2.44	0.51
1:B:509:GLU:CG	1:B:510:GLY:H	2.23	0.51
1:B:583:PHE:HA	1:B:584:SER:CB	2.41	0.51
1:B:381:GLU:HA	1:B:383:HIS:CD2	2.46	0.51
1:B:683:VAL:HG12	1:B:684:PRO:HD2	1.92	0.51
1:B:665:LEU:HD22	1:B:767:HIS:NE2	2.26	0.51
1:A:381:GLU:HB3	1:B:393:LYS:NZ	2.26	0.51
1:B:449:TYR:CE1	1:B:464:CYS:HB2	2.47	0.50
1:B:584:SER:OG	1:B:585:ASN:CB	2.53	0.50
1:B:107:THR:CG2	1:B:109:ASN:H	2.25	0.50
1:A:578:ILE:C	1:A:578:ILE:HD12	2.36	0.50
1:A:497:SER:HG	1:A:523:ASP:CG	2.20	0.50
1:B:118:ALA:CB	1:B:120:ARG:HD3	2.41	0.49
1:B:470:VAL:HB	1:B:488:GLN:HG3	1.94	0.49
1:A:550:LEU:HD12	1:A:550:LEU:C	2.37	0.49
1:A:658:GLN:NE2	1:A:712:LEU:CD2	2.70	0.49
1:B:142:LEU:HD22	1:B:143:TRP:O	2.13	0.49
1:B:719:VAL:HG13	1:B:756:LEU:HD13	1.95	0.49
1:B:705:LEU:HD22	1:B:753:ILE:HD13	1.94	0.49
1:B:379:ALA:O	1:B:383:HIS:CE1	2.65	0.49
1:B:652:ASN:CG	1:B:653:LEU:H	2.20	0.49
1:A:224:LEU:HD21	1:A:266:LEU:HG	1.93	0.49
1:A:107:THR:HG22	1:A:110:GLY:H	1.78	0.49
1:A:667:ALA:HB3	1:A:704:GLU:HB2	1.93	0.49
1:B:572:ASP:O	1:B:572:ASP:OD1	2.31	0.48
1:A:560:GLY:HA2	1:A:565:VAL:HG12	1.95	0.48
1:B:765:ARG:NH1	2:B:830:HOH:O	2.45	0.48
1:A:107:THR:HG22	1:A:110:GLY:N	2.28	0.48
1:A:720:TYR:CE2	1:A:739:ILE:HG23	2.48	0.48
1:A:314:ASP:OD2	1:A:314:ASP:C	2.57	0.48
1:A:439:ASN:OD1	1:A:440:THR:HG23	2.14	0.48
1:A:47:GLU:HG3	1:A:48:ALA:N	2.29	0.47
1:B:208:PRO:O	1:B:250:ILE:CD1	2.62	0.47
1:B:314:ASP:OD2	1:B:314:ASP:C	2.57	0.47
1:A:556:LEU:HD23	1:A:569:ASN:HA	1.94	0.47
1:A:600:VAL:O	1:A:606:LEU:HD23	2.15	0.47
1:B:107:THR:HG22	1:B:110:GLY:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:THR:OG1	1:B:346:GLY:N	2.47	0.47
1:A:569:ASN:HB3	1:A:573:GLU:CB	2.45	0.47
1:B:240:LEU:HB2	1:B:261:ILE:CD1	2.45	0.47
1:A:563:GLY:HA2	1:A:586:ASN:HD22	1.78	0.47
1:B:516:LEU:HD12	1:B:516:LEU:N	2.30	0.46
1:B:584:SER:N	1:B:585:ASN:HB3	2.29	0.46
1:A:470:VAL:HB	1:A:488:GLN:HG3	1.97	0.46
1:B:42:ILE:HD13	1:B:73:TYR:CE2	2.50	0.46
1:B:48:ALA:HB1	1:B:66:SER:HB2	1.97	0.46
1:B:97:ILE:HG12	1:B:103:LEU:CD2	2.44	0.46
1:B:381:GLU:N	1:B:383:HIS:CE1	2.82	0.46
1:B:585:ASN:CG	1:B:586:ASN:N	2.73	0.46
1:B:720:TYR:CE2	1:B:739:ILE:HG23	2.51	0.46
1:A:387:TRP:CD1	1:A:389:ARG:HD2	2.50	0.46
1:A:107:THR:CG2	1:A:109:ASN:H	2.29	0.46
1:B:475:LYS:O	1:B:476:LEU:CB	2.61	0.46
1:A:495:GLY:O	1:A:496:LEU:HB2	2.15	0.46
1:A:566:MET:HG2	1:A:568:ILE:HD11	1.97	0.46
1:B:44:LEU:HD23	1:B:78:THR:HG21	1.97	0.46
1:B:445:THR:O	1:B:445:THR:HG23	2.15	0.46
1:A:272:LEU:HD13	1:A:273:LEU:N	2.31	0.46
1:A:669:TYR:HB2	1:A:702:SER:HB2	1.98	0.46
1:B:259:ASN:HD21	1:B:278:ASN:HB2	1.81	0.46
1:B:491:SER:HB2	1:B:499:MET:SD	2.56	0.46
1:A:569:ASN:HB3	1:A:573:GLU:HB3	1.96	0.46
1:B:220:VAL:HG13	1:B:234:ILE:HG23	1.98	0.46
1:B:272:LEU:C	1:B:272:LEU:CD1	2.89	0.45
1:B:463:THR:CG2	1:B:466:GLY:H	2.23	0.45
1:A:441:GLY:HA2	1:A:442:THR:O	2.15	0.45
1:A:445:THR:O	1:A:445:THR:HG23	2.15	0.45
1:A:705:LEU:HD12	1:A:705:LEU:C	2.41	0.45
1:B:51:VAL:HG21	1:B:327:ILE:HG13	1.98	0.45
1:A:586:ASN:C	1:A:603:THR:OG1	2.59	0.45
1:B:92:ILE:HG23	1:B:105:MET:HB3	1.99	0.45
1:A:209:LEU:HD21	1:A:234:ILE:HD13	1.98	0.44
1:B:300:ILE:HG23	1:B:300:ILE:O	2.15	0.44
1:B:52:SER:OG	1:B:92:ILE:O	2.30	0.44
1:B:387:TRP:CD1	1:B:389:ARG:HD2	2.53	0.44
1:A:240:LEU:HB2	1:A:261:ILE:CD1	2.47	0.44
1:A:756:LEU:HD12	1:A:756:LEU:HA	1.91	0.44
1:A:482:GLY:N	1:A:483:GLN:O	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ALA:H	1:B:47:GLU:CA	2.18	0.44
1:B:388:TYR:HB3	1:B:397:LEU:HG	2.00	0.44
1:A:482:GLY:HA3	1:A:483:GLN:CB	2.47	0.44
1:A:536:PHE:HE1	1:A:574:SER:HB3	1.83	0.44
1:B:240:LEU:HB2	1:B:261:ILE:HD12	1.99	0.44
1:B:311:ILE:HG23	1:B:321:LEU:CD2	2.47	0.43
1:B:665:LEU:HD22	1:B:767:HIS:CD2	2.54	0.43
1:B:365:TRP:C	1:B:366:PHE:HD1	2.27	0.43
1:B:600:VAL:O	1:B:606:LEU:HD23	2.18	0.43
1:A:665:LEU:HD22	1:A:767:HIS:HE2	1.82	0.43
1:B:107:THR:HG22	1:B:110:GLY:H	1.82	0.43
1:B:143:TRP:C	1:B:144:LEU:HD23	2.44	0.43
1:B:669:TYR:HB2	1:B:702:SER:HB2	1.99	0.43
1:A:591:MET:HG2	1:A:600:VAL:HG13	2.00	0.43
1:B:719:VAL:HG13	1:B:756:LEU:CD1	2.49	0.43
1:B:234:ILE:HB	1:B:241:PHE:HB2	2.01	0.43
1:B:509:GLU:HG3	1:B:510:GLY:N	2.33	0.43
1:B:670:ILE:O	1:B:671:ASN:C	2.62	0.43
1:B:567:ARG:O	1:B:575:GLN:HA	2.19	0.42
1:A:300:ILE:O	1:A:300:ILE:HG23	2.18	0.42
1:B:536:PHE:CB	1:B:566:MET:HE1	2.48	0.42
1:A:365:TRP:C	1:A:366:PHE:HD1	2.27	0.42
1:B:47:GLU:HA	1:B:47:GLU:OE1	2.19	0.42
1:B:746:TYR:HA	1:B:773:ILE:HB	2.01	0.42
1:B:181:THR:OG1	1:B:183:ASP:OD1	2.35	0.42
1:A:670:ILE:O	1:A:671:ASN:C	2.62	0.42
1:A:548:TYR:HD1	1:A:591:MET:HE2	1.85	0.42
1:A:665:LEU:HD22	1:A:767:HIS:CD2	2.54	0.42
1:B:100:ASN:O	1:B:117:ARG:NH1	2.50	0.41
1:B:335:ALA:O	1:B:655:ALA:HB1	2.21	0.41
1:B:378:PRO:O	1:B:379:ALA:CB	2.67	0.41
1:A:652:ASN:O	1:A:654:GLU:N	2.47	0.41
1:B:377:ASP:O	1:B:383:HIS:CE1	2.73	0.41
1:B:111:ILE:O	1:B:123:GLN:NE2	2.54	0.41
1:B:581:GLY:O	1:B:582:SER:C	2.63	0.41
1:B:111:ILE:HD11	1:B:144:LEU:HD13	2.02	0.41
1:B:210:PRO:CD	1:B:250:ILE:HG21	2.51	0.41
1:B:403:ARG:NH1	1:B:418:ASP:OD2	2.54	0.41
1:A:198:ILE:HD11	1:A:205:GLU:HB2	2.03	0.41
1:A:337:GLN:OE1	1:A:659:PRO:HB3	2.20	0.41
1:B:333:ASN:O	1:B:334:SER:CB	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:C	1:A:272:LEU:CD1	2.94	0.41
1:A:403:ARG:NH1	1:A:418:ASP:OD2	2.54	0.41
1:A:449:TYR:CE1	1:A:464:CYS:HB2	2.56	0.41
1:B:107:THR:CG2	1:B:109:ASN:N	2.84	0.41
1:B:540:LEU:HD11	1:B:566:MET:CE	2.43	0.41
1:A:234:ILE:HB	1:A:241:PHE:HB2	2.03	0.40
1:A:746:TYR:CD1	1:A:746:TYR:C	2.98	0.40
1:B:526:ASN:C	1:B:526:ASN:ND2	2.67	0.40
1:A:560:GLY:CA	1:A:588:ILE:HD12	2.51	0.40
1:A:388:TYR:HB3	1:A:397:LEU:HG	2.03	0.40
1:A:446:ASN:HD22	1:A:446:ASN:HA	1.73	0.40
1:A:447:TRP:CZ3	1:A:465:LEU:HD12	2.56	0.40
1:A:668:LEU:HD23	1:A:683:VAL:HG11	2.03	0.40
1:A:352:GLN:O	1:A:368:GLY:HA3	2.22	0.40
1:A:107:THR:CG2	1:A:109:ASN:N	2.85	0.40
1:A:381:GLU:HB3	1:B:393:LYS:HZ2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/758 (98%)	682 (92%)	46 (6%)	11 (2%)	8	28
1	B	741/758 (98%)	685 (92%)	39 (5%)	17 (2%)	5	18
All	All	1480/1516 (98%)	1367 (92%)	85 (6%)	28 (2%)	6	22

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	ALA
1	A	492	VAL

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Mol	Chain	Res	Type
1	A	585	ASN
1	A	586	ASN
1	B	46	ALA
1	B	334	SER
1	B	379	ALA
1	B	582	SER
1	B	583	PHE
1	B	585	ASN
1	B	604	ASN
1	A	347	THR
1	A	442	THR
1	A	496	LEU
1	B	346	GLY
1	B	347	THR
1	B	381	GLU
1	B	603	THR
1	B	621	MET
1	B	655	ALA
1	A	481	SER
1	A	502	ASN
1	A	653	LEU
1	B	502	ASN
1	B	652	ASN
1	B	214	SER
1	B	584	SER
1	A	483	GLN

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	666/676 (98%)	607 (91%)	59 (9%)	9	29
1	B	662/676 (98%)	603 (91%)	59 (9%)	9	29
All	All	1328/1352 (98%)	1210 (91%)	118 (9%)	9	29

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	107	THR
1	A	123	GLN
1	A	142	LEU
1	A	148	ASN
1	A	166	ARG
1	A	177	SER
1	A	218	LEU
1	A	227	THR
1	A	246	SER
1	A	249	GLN
1	A	282	VAL
1	A	300	ILE
1	A	303	LEU
1	A	315	GLN
1	A	336	LEU
1	A	341	ILE
1	A	347	THR
1	A	355	SER
1	A	382	ARG
1	A	389	ARG
1	A	437	VAL
1	A	445	THR
1	A	472	ASP
1	A	475	LYS
1	A	476	LEU
1	A	478	GLN
1	A	481	SER
1	A	488	GLN
1	A	491	SER
1	A	500	PHE
1	A	501	ILE
1	A	526	ASN
1	A	533	THR
1	A	534	LYS
1	A	549	LEU
1	A	557	LEU
1	A	566	MET
1	A	571	LYS
1	A	579	SER
1	A	584	SER
1	A	585	ASN
1	A	587	GLU

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Mol	Chain	Res	Type
1	A	596	ASN
1	A	602	THR
1	A	603	THR
1	A	606	LEU
1	A	628	SER
1	A	634	LYS
1	A	653	LEU
1	A	656	THR
1	A	665	LEU
1	A	683	VAL
1	A	727	LYS
1	A	745	SER
1	A	754	SER
1	A	755	LYS
1	A	756	LEU
1	A	757	GLU
1	B	96	VAL
1	B	107	THR
1	B	137	LEU
1	B	142	LEU
1	B	165	THR
1	B	211	VAL
1	B	213	SER
1	B	227	THR
1	B	237	GLU
1	B	246	SER
1	B	272	LEU
1	B	300	ILE
1	B	303	LEU
1	B	334	SER
1	B	336	LEU
1	B	341	ILE
1	B	342	SER
1	B	347	THR
1	B	355	SER
1	B	376	THR
1	B	377	ASP
1	B	384	ASP
1	B	389	ARG
1	B	442	THR
1	B	445	THR
1	B	465	LEU

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Mol	Chain	Res	Type
1	B	478	GLN
1	B	480	THR
1	B	488	GLN
1	B	501	ILE
1	B	509	GLU
1	B	526	ASN
1	B	533	THR
1	B	534	LYS
1	B	549	LEU
1	B	557	LEU
1	B	566	MET
1	B	575	GLN
1	B	584	SER
1	B	585	ASN
1	B	587	GLU
1	B	596	ASN
1	B	602	THR
1	B	603	THR
1	B	604	ASN
1	B	606	LEU
1	B	625	ARG
1	B	628	SER
1	B	634	LYS
1	B	653	LEU
1	B	656	THR
1	B	665	LEU
1	B	683	VAL
1	B	733	LYS
1	B	745	SER
1	B	754	SER
1	B	755	LYS
1	B	756	LEU
1	B	757	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
1	A	173	ASN
1	A	242	GLN
1	A	249	GLN
1	A	259	ASN

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Mol	Chain	Res	Type
1	A	305	ASN
1	A	310	ASN
1	A	343	GLN
1	A	422	ASN
1	A	446	ASN
1	A	478	GLN
1	A	511	ASN
1	A	526	ASN
1	A	596	ASN
1	A	658	GLN
1	A	673	GLN
1	A	730	ASN
1	A	748	ASN
1	A	750	GLN
1	A	783	HIS
1	A	784	HIS
1	B	79	GLN
1	B	173	ASN
1	B	215	GLN
1	B	230	GLN
1	B	242	GLN
1	B	259	ASN
1	B	383	HIS
1	B	439	ASN
1	B	446	ASN
1	B	478	GLN
1	B	483	GLN
1	B	502	ASN
1	B	508	ASN
1	B	526	ASN
1	B	586	ASN
1	B	730	ASN
1	B	748	ASN
1	B	750	GLN
1	B	770	ASN

5.3.3 RNA ⓘ

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	A	747/758 (98%)	0.91	112 (14%) 5 4	52, 70, 123, 152	6 (0%)
1	B	743/758 (98%)	0.69	64 (8%) 16 12	36, 65, 88, 112	7 (0%)
All	All	1490/1516 (98%)	0.80	176 (11%) 9 7	36, 67, 112, 152	13 (0%)

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	215	GLN	6.6
1	B	216	SER	6.3
1	A	785	HIS	5.6
1	A	538	ASP	5.3
1	B	382	ARG	5.0
1	B	655	ALA	4.7
1	A	499	MET	4.3
1	A	494	ASN	4.0
1	B	166	ARG	3.9
1	A	84	TYR	3.8
1	B	335	ALA	3.8
1	A	572	ASP	3.7
1	A	465	LEU	3.7
1	A	574	SER	3.7
1	A	576	GLN	3.7
1	B	475	LYS	3.7
1	A	734	SER	3.6
1	B	333	ASN	3.6
1	A	613	THR	3.5
1	A	500	PHE	3.5
1	B	764	ASN	3.5
1	B	500	PHE	3.4
1	A	441	GLY	3.4
1	B	659	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	379	ALA	3.4
1	A	345	THR	3.4
1	B	621	MET	3.3
1	A	579	SER	3.3
1	A	527	PRO	3.2
1	A	571	LYS	3.2
1	B	622	THR	3.2
1	B	383	HIS	3.2
1	A	533	THR	3.2
1	A	568	ILE	3.2
1	B	653	LEU	3.1
1	A	653	LEU	3.1
1	A	443	TYR	3.1
1	A	583	PHE	3.1
1	A	125	GLU	3.1
1	A	167	ARG	3.1
1	A	382	ARG	3.1
1	B	46	ALA	3.0
1	A	569	ASN	3.0
1	B	125	GLU	3.0
1	B	336	LEU	3.0
1	B	585	ASN	3.0
1	A	612	LYS	2.9
1	A	542	GLY	2.9
1	A	166	ARG	2.9
1	B	583	PHE	2.9
1	B	562	HIS	2.9
1	B	482	GLY	2.8
1	B	765	ARG	2.8
1	B	582	SER	2.8
1	A	506	PRO	2.8
1	A	617	ARG	2.8
1	B	84	TYR	2.8
1	B	656	THR	2.8
1	A	528	ARG	2.8
1	A	493	HIS	2.8
1	A	517	TYR	2.7
1	B	167	ARG	2.7
1	A	746	TYR	2.7
1	A	455	THR	2.7
1	A	532	VAL	2.7
1	A	539	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	109	ASN	2.6
1	B	464	CYS	2.6
1	A	391	GLY	2.6
1	A	442	THR	2.6
1	A	485	ILE	2.6
1	A	531	GLU	2.6
1	A	573	GLU	2.6
1	A	456	ALA	2.6
1	B	315	GLN	2.6
1	A	727	LYS	2.6
1	A	543	GLU	2.6
1	A	168	ASN	2.6
1	A	671	ASN	2.6
1	B	384	ASP	2.6
1	B	651	SER	2.5
1	A	634	LYS	2.5
1	A	496	LEU	2.5
1	A	522	ILE	2.5
1	B	579	SER	2.5
1	A	440	THR	2.5
1	A	513	TRP	2.4
1	A	337	GLN	2.4
1	A	620	ASN	2.4
1	A	524	LYS	2.4
1	B	165	THR	2.4
1	A	562	HIS	2.4
1	B	346	GLY	2.4
1	B	530	ARG	2.4
1	A	558	TRP	2.4
1	A	655	ALA	2.4
1	A	502	ASN	2.4
1	A	544	LYS	2.4
1	A	334	SER	2.4
1	B	658	GLN	2.4
1	A	525	ILE	2.4
1	A	475	LYS	2.3
1	A	625	ARG	2.3
1	B	572	ASP	2.3
1	B	38	GLN	2.3
1	A	336	LEU	2.3
1	B	214	SER	2.3
1	B	441	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	586	ASN	2.3
1	B	620	ASN	2.3
1	A	556	LEU	2.3
1	A	257	HIS	2.3
1	A	497	SER	2.3
1	A	733	LYS	2.3
1	A	449	TYR	2.3
1	A	346	GLY	2.3
1	B	728	GLU	2.3
1	A	472	ASP	2.3
1	A	507	ASP	2.3
1	A	597	SER	2.3
1	B	584	SER	2.3
1	A	657	TYR	2.3
1	A	109	ASN	2.2
1	A	540	LEU	2.2
1	B	347	THR	2.2
1	A	580	PHE	2.2
1	B	623	ASN	2.2
1	B	158	ARG	2.2
1	A	584	SER	2.2
1	A	498	GLY	2.2
1	B	380	GLY	2.2
1	A	654	GLU	2.2
1	A	384	ASP	2.2
1	A	570	PRO	2.2
1	A	577	SER	2.2
1	B	481	SER	2.2
1	A	535	LEU	2.2
1	B	654	GLU	2.2
1	B	661	ARG	2.2
1	A	656	THR	2.2
1	A	509	GLU	2.2
1	A	501	ILE	2.1
1	A	377	ASP	2.1
1	B	277	ASP	2.1
1	B	727	LYS	2.1
1	A	581	GLY	2.1
1	B	510	GLY	2.1
1	A	516	LEU	2.1
1	A	379	ALA	2.1
1	A	651	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	660	GLU	2.1
1	A	782	HIS	2.1
1	B	650	HIS	2.1
1	A	514	VAL	2.1
1	A	659	PRO	2.1
1	A	520	LYS	2.1
1	B	465	LEU	2.1
1	A	758	ARG	2.1
1	B	758	ARG	2.1
1	A	652	ASN	2.1
1	A	463	THR	2.1
1	A	541	THR	2.1
1	A	622	THR	2.1
1	A	660	GLU	2.1
1	A	607	TRP	2.1
1	B	509	GLU	2.1
1	A	439	ASN	2.0
1	A	529	THR	2.0
1	A	615	ASP	2.0
1	B	47	GLU	2.0
1	A	478	GLN	2.0
1	B	342	SER	2.0
1	B	340	PRO	2.0
1	B	378	PRO	2.0
1	A	537	ALA	2.0
1	A	381	GLU	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 [i](#)

There are no such residues in this entry.