Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2023 – 06:28 AM EDT

PDB ID	:	4DDV
Title	:	Thermotoga maritima reverse gyrase, triclinic form
Authors	:	Rudolph, M.G.; Klostermeier, D.
Deposited on	:	2012-01-19
Resolution	:	3.46 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.46 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.
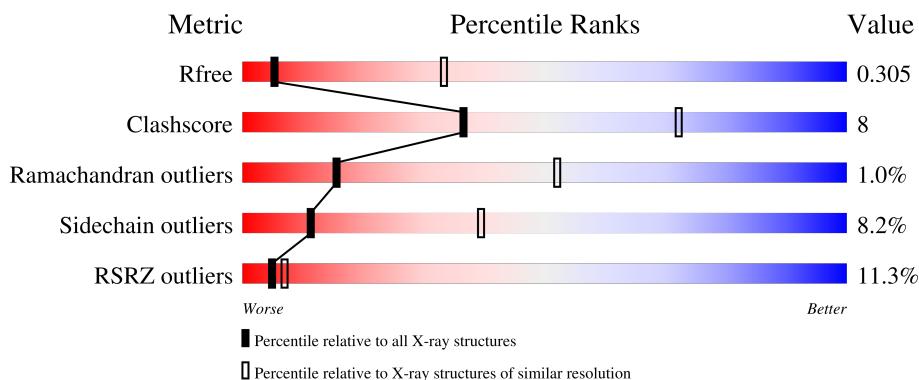
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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 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 <=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	1104	
1	B	1104	
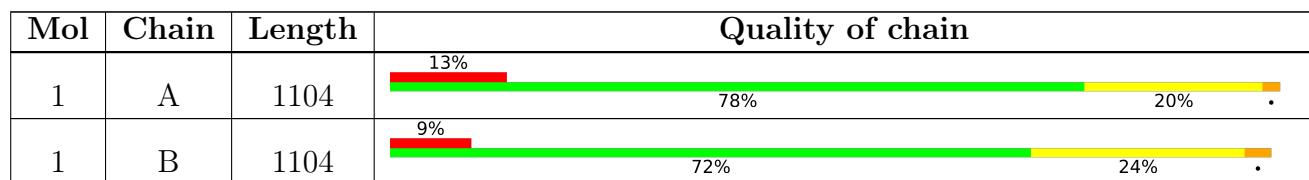
2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 18064 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 Reverse gyrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1102	Total 9030	C 5759	N 1563	O 1682	S 26	0	0	0
1	B	1102	Total 9030	C 5759	N 1563	O 1682	S 26	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	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: Reverse gyrase

• Molecule 1: Reverse gyrase

Chain B:
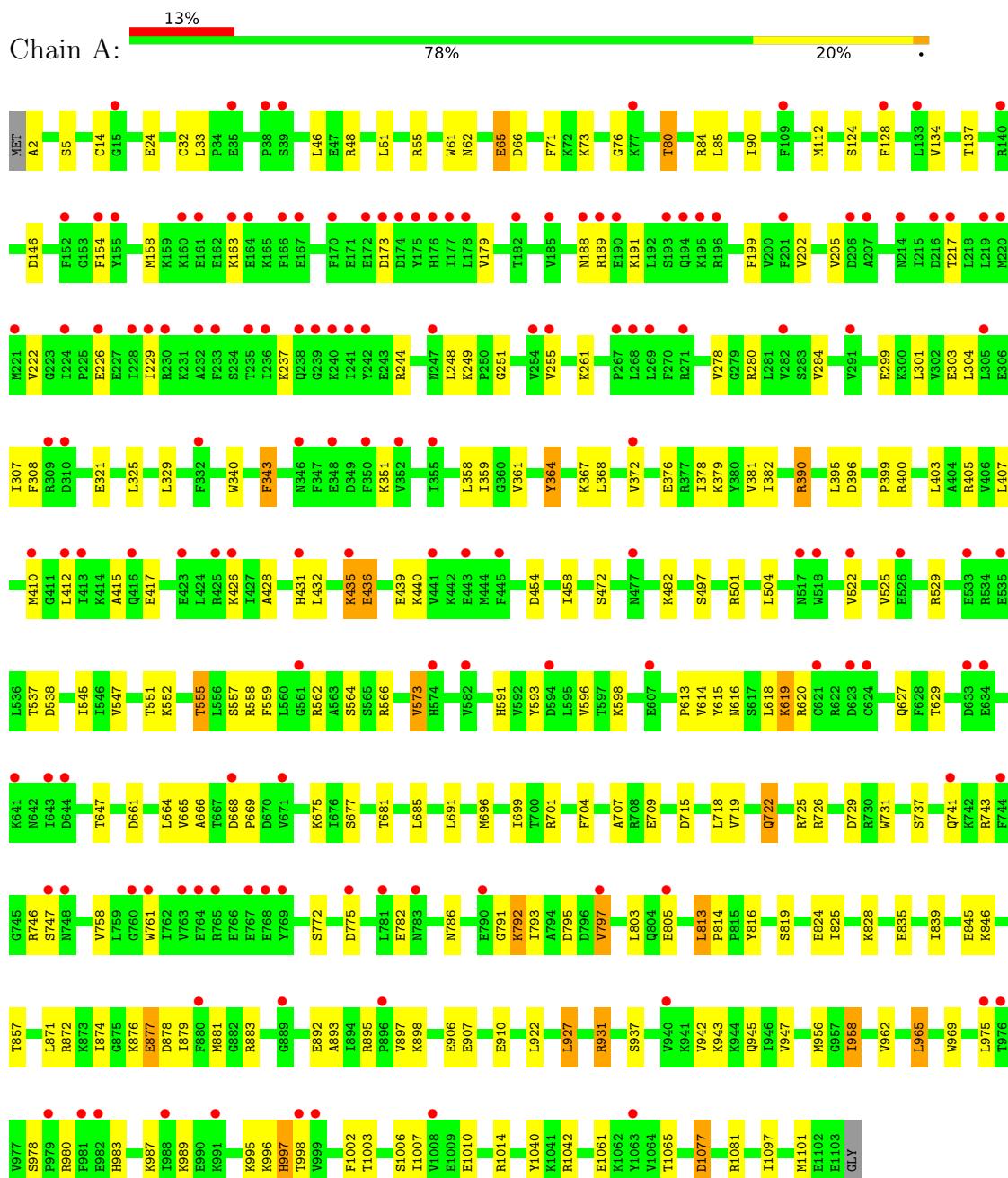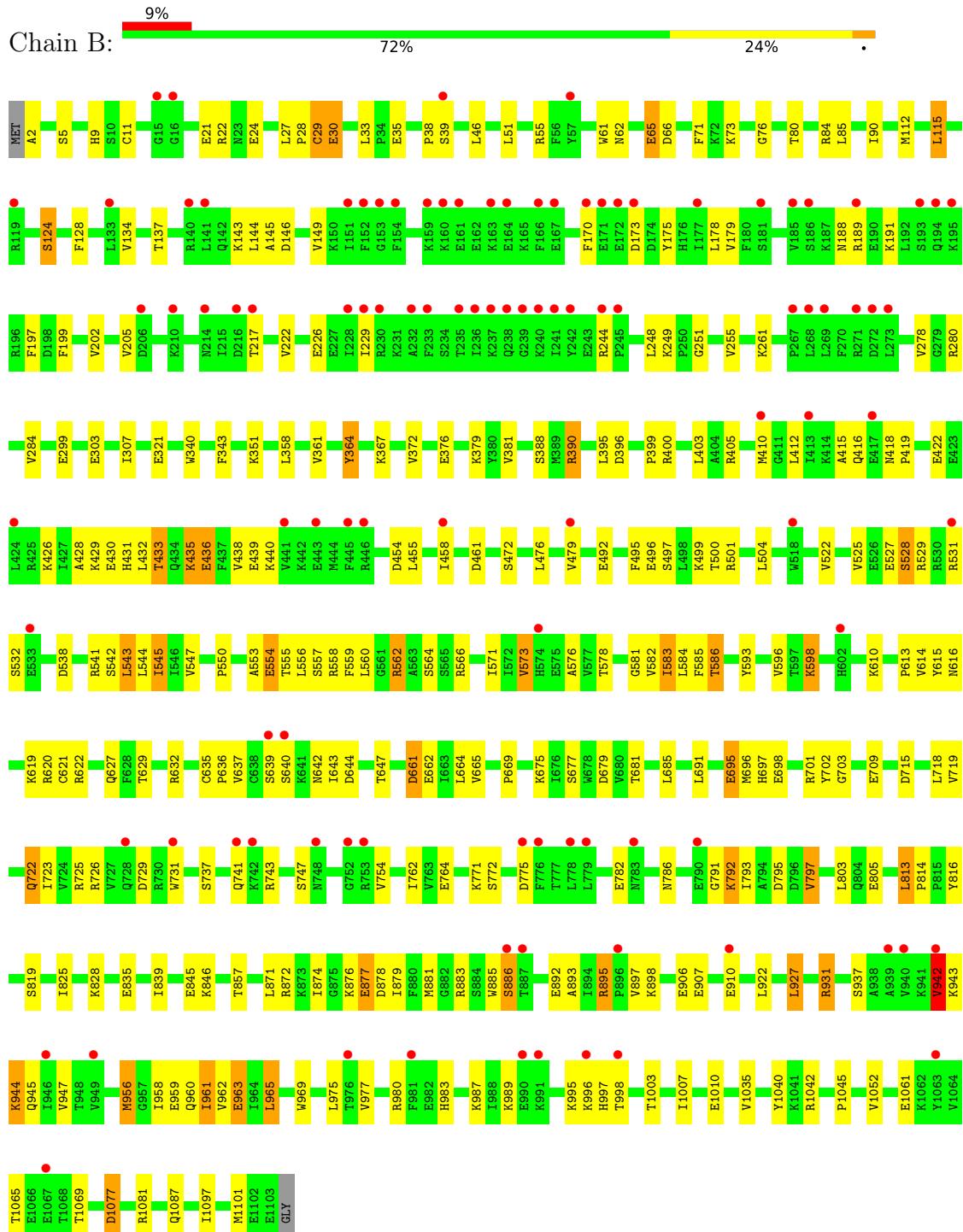
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	95.71Å 101.25Å 104.43Å 113.61° 97.50° 110.42°	Depositor
Resolution (Å)	49.11 – 3.46 49.11 – 3.46	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.11-3.46) 98.3 (49.11-3.46)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.235 , 0.278 0.260 , 0.305	Depositor DCC
R_{free} test set	2069 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	82.1	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 89.2	EDS
L-test for twinning[2]	$< |L| > = 0.40, < L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	18064	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6894e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.47	0/9191	0.64	0/12356
1	B	0.58	0/9191	0.74	1/12356 (0.0%)
All	All	0.53	0/18382	0.69	1/24712 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	942	VAL	N-CA-CB	-5.18	100.11	111.50

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	9030	0	9187	130	0
1	B	9030	0	9187	162	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
All	All	18064	0	18374	289	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 8.

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All (289) 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:958:ILE:CD1	1:A:958:ILE:CG1	1.77	1.57
1:B:961:ILE:CD1	1:B:961:ILE:CG1	1.74	1.56
1:B:544:LEU:HD12	1:B:584:LEU:O	1.67	0.95
1:A:14:CYS:HB3	1:A:32:CYS:SG	2.10	0.91
1:A:722:GLN:HE22	1:A:726:ARG:HB2	1.37	0.89
1:B:543:LEU:HD21	1:B:664:LEU:HD12	1.55	0.88
1:B:722:GLN:HE22	1:B:726:ARG:HB2	1.37	0.85
1:A:746:ARG:HE	1:B:426:LYS:HE2	1.40	0.85
1:B:741:GLN:HG2	1:B:747:SER:HA	1.60	0.84
1:B:555:THR:HG21	1:B:846:LYS:HA	1.61	0.83
1:B:681:THR:HG22	1:B:691:LEU:HD22	1.61	0.82
1:A:681:THR:HG22	1:A:691:LEU:HD22	1.64	0.80
1:A:412:LEU:HD21	1:A:426:LYS:HB3	1.66	0.77
1:B:555:THR:HG22	1:B:558:ARG:NH2	2.00	0.77
1:A:555:THR:HG21	1:A:846:LYS:HA	1.67	0.77
1:A:399:PRO:O	1:A:403:LEU:HD12	1.87	0.74
1:B:669:PRO:HG2	1:B:697:HIS:CD2	2.22	0.74
1:B:399:PRO:O	1:B:403:LEU:HD12	1.88	0.74
1:A:962:VAL:HG11	1:A:980:ARG:HG3	1.70	0.74
1:B:61:TRP:O	1:B:65:GLU:HG3	1.90	0.72
1:A:958:ILE:CD1	1:A:958:ILE:HA	2.18	0.72
1:A:202:VAL:HB	1:A:255:VAL:HG12	1.72	0.72
1:A:61:TRP:O	1:A:65:GLU:HG3	1.91	0.70
1:B:202:VAL:HB	1:B:255:VAL:HG12	1.72	0.70
1:B:698:GLU:O	1:B:703:GLY:HA3	1.93	0.69
1:B:722:GLN:NE2	1:B:726:ARG:HB2	2.08	0.69
1:A:80:THR:OG1	1:A:538:ASP:OD2	2.08	0.68
1:B:556:LEU:HD23	1:B:559:PHE:CZ	2.28	0.68
1:B:556:LEU:HB3	1:B:560:LEU:HD12	1.76	0.67
1:A:741:GLN:HG2	1:A:747:SER:HA	1.78	0.66
1:B:621:CYS:HA	1:B:643:ILE:HG22	1.76	0.65
1:A:722:GLN:NE2	1:A:726:ARG:HB2	2.09	0.65
1:B:573:VAL:HA	1:B:586:THR:HB	1.78	0.65
1:A:555:THR:HG22	1:A:558:ARG:NH2	2.12	0.65
1:A:620:ARG:HG3	1:A:627:GLN:HG2	1.79	0.65
1:B:178:LEU:HD12	1:B:197:PHE:HZ	1.62	0.64
1:B:556:LEU:HB3	1:B:560:LEU:CD1	2.28	0.64
1:A:772:SER:HB3	1:A:998:THR:HB	1.79	0.64
1:B:772:SER:HB3	1:B:998:THR:HB	1.79	0.64
1:B:944:LYS:HB3	1:B:961:ILE:HG23	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ARG:NH1	1:B:661:ASP:OD2	2.32	0.62
1:B:340:TRP:HB3	1:B:364:TYR:HE1	1.65	0.62
1:B:495:PHE:CZ	1:B:499:LYS:HD3	2.35	0.61
1:B:675:LYS:HG2	1:B:722:GLN:HG3	1.82	0.61
1:A:244:ARG:HD2	1:A:248:LEU:HD23	1.82	0.61
1:A:340:TRP:HB3	1:A:364:TYR:HE1	1.64	0.61
1:A:405:ARG:NH1	1:A:907:GLU:OE1	2.34	0.61
1:B:405:ARG:NH1	1:B:907:GLU:OE1	2.35	0.60
1:B:593:TYR:HB3	1:B:615:TYR:HB3	1.84	0.60
1:B:857:THR:HA	1:B:893:ALA:HB2	1.83	0.59
1:B:883:ARG:NH2	1:B:937:SER:O	2.31	0.59
1:A:857:THR:HA	1:A:893:ALA:HB2	1.85	0.59
1:B:244:ARG:HD2	1:B:248:LEU:HD23	1.84	0.59
1:B:431:HIS:HB3	1:B:436:GLU:HB3	1.84	0.59
1:A:482:LYS:O	1:A:529:ARG:NH1	2.37	0.58
1:A:675:LYS:HG2	1:A:722:GLN:HG3	1.85	0.58
1:B:762:ILE:HD13	1:B:1035:VAL:HG21	1.86	0.58
1:A:62:ASN:HA	1:A:65:GLU:CD	2.23	0.58
1:A:124:SER:HB3	1:A:199:PHE:HB3	1.85	0.58
1:B:576:ALA:HB3	1:B:583:ILE:HG22	1.85	0.58
1:B:665:VAL:HG11	1:B:677:SER:HA	1.86	0.58
1:A:746:ARG:NE	1:B:426:LYS:HE2	2.15	0.58
1:B:805:GLU:HG3	1:B:945:GLN:HG3	1.86	0.58
1:B:62:ASN:HA	1:B:65:GLU:CD	2.25	0.57
1:B:943:LYS:HB2	1:B:965:LEU:HD11	1.84	0.57
1:B:635:CYS:O	1:B:639:SER:HA	2.05	0.57
1:A:969:TRP:CH2	1:A:975:LEU:HD13	2.40	0.57
1:A:1010:GLU:OE1	1:A:1014:ARG:NH1	2.37	0.57
1:A:504:LEU:HD12	1:A:898:LYS:HE3	1.87	0.57
1:A:593:TYR:HB3	1:A:615:TYR:HB3	1.85	0.56
1:B:554:GLU:O	1:B:557:SER:OG	2.16	0.56
1:B:669:PRO:HG3	1:B:695:GLU:HB2	1.86	0.56
1:A:997:HIS:CD2	1:A:997:HIS:H	2.22	0.56
1:B:782:GLU:HA	1:B:989:LYS:HE3	1.87	0.55
1:B:632:ARG:NH2	1:B:636:PRO:HB3	2.21	0.55
1:B:872:ARG:HA	1:B:877:GLU:HB3	1.87	0.55
1:B:545:ILE:HD11	1:B:583:ILE:HG13	1.87	0.55
1:A:381:VAL:HG23	1:A:472:SER:HB3	1.89	0.55
1:B:550:PRO:O	1:B:553:ALA:HB3	2.06	0.55
1:A:497:SER:O	1:A:501:ARG:HG2	2.07	0.55
1:A:699:ILE:HD12	1:A:845:GLU:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:GLU:O	1:B:307:ILE:HG12	2.07	0.54
1:B:962:VAL:HG11	1:B:980:ARG:CZ	2.37	0.54
1:A:883:ARG:NH2	1:A:937:SER:O	2.29	0.54
1:A:816:TYR:CZ	1:A:931:ARG:HG3	2.42	0.54
1:A:872:ARG:HA	1:A:877:GLU:HB3	1.89	0.54
1:A:557:SER:HB2	1:A:562:ARG:HB2	1.88	0.54
1:B:497:SER:O	1:B:501:ARG:HG2	2.08	0.54
1:A:782:GLU:HA	1:A:989:LYS:HE3	1.89	0.54
1:B:557:SER:HB2	1:B:562:ARG:HB2	1.90	0.54
1:A:84:ARG:NH1	1:A:661:ASP:OD2	2.41	0.53
1:B:381:VAL:HG23	1:B:472:SER:HB3	1.89	0.53
1:B:816:TYR:CZ	1:B:931:ARG:HG3	2.44	0.53
1:A:696:MET:SD	1:A:704:PHE:HD1	2.31	0.53
1:A:825:ILE:HG12	1:A:927:LEU:HD23	1.91	0.53
1:B:669:PRO:HG2	1:B:697:HIS:HD2	1.71	0.53
1:A:665:VAL:HG11	1:A:677:SER:HA	1.90	0.52
1:B:969:TRP:CH2	1:B:975:LEU:HD13	2.44	0.52
1:A:619:LYS:NZ	1:A:629:THR:O	2.40	0.52
1:B:222:VAL:HB	1:B:251:GLY:H	1.75	0.52
1:A:906:GLU:HG2	1:A:922:LEU:HD13	1.91	0.52
1:A:222:VAL:HB	1:A:251:GLY:H	1.74	0.52
1:A:892:GLU:OE2	1:A:895:ARG:NH1	2.43	0.52
1:B:340:TRP:HB3	1:B:364:TYR:CE1	2.45	0.52
1:B:675:LYS:CG	1:B:722:GLN:HG3	2.40	0.52
1:B:504:LEU:HD12	1:B:898:LYS:HE3	1.92	0.52
1:B:582:VAL:HG12	1:B:583:ILE:H	1.73	0.52
1:B:582:VAL:HG12	1:B:583:ILE:N	2.25	0.51
1:B:351:LYS:NZ	1:B:372:VAL:HG11	2.26	0.51
1:B:906:GLU:HG2	1:B:922:LEU:HD13	1.92	0.51
1:B:361:VAL:HB	1:B:364:TYR:HB2	1.91	0.51
1:A:552:LYS:HG2	1:A:699:ILE:HD13	1.92	0.51
1:A:558:ARG:HG3	1:A:558:ARG:HH11	1.75	0.51
1:A:813:LEU:HD23	1:A:814:PRO:HD2	1.93	0.51
1:A:303:GLU:O	1:A:307:ILE:HG12	2.10	0.50
1:B:675:LYS:CB	1:B:722:GLN:HG3	2.41	0.50
1:A:731:TRP:HB3	1:A:1097:ILE:HG13	1.93	0.50
1:B:944:LYS:HE3	1:B:959:GLU:OE1	2.11	0.50
1:B:825:ILE:HG12	1:B:927:LEU:HD23	1.92	0.50
1:B:33:LEU:HD21	1:B:38:PRO:HG2	1.93	0.50
1:B:556:LEU:HD23	1:B:559:PHE:HZ	1.72	0.50
1:B:559:PHE:HB2	1:B:701:ARG:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:LYS:CB	1:A:722:GLN:HG3	2.42	0.50
1:A:876:LYS:O	1:A:879:ILE:HG12	2.11	0.50
1:B:395:LEU:HD11	1:B:428:ALA:HA	1.94	0.50
1:B:431:HIS:CD2	1:B:440:LYS:HE2	2.47	0.49
1:A:361:VAL:HB	1:A:364:TYR:HB2	1.94	0.49
1:B:307:ILE:HG22	1:B:522:VAL:HG21	1.94	0.49
1:A:1061:GLU:O	1:A:1065:THR:OG1	2.30	0.49
1:B:145:ALA:HB1	1:B:149:VAL:HG21	1.93	0.49
1:B:892:GLU:OE2	1:B:895:ARG:NH1	2.45	0.49
1:A:814:PRO:O	1:A:931:ARG:NH1	2.45	0.49
1:B:543:LEU:HD21	1:B:664:LEU:CD1	2.37	0.49
1:A:340:TRP:HB3	1:A:364:TYR:CE1	2.44	0.49
1:B:188:ASN:HB3	1:B:191:LYS:HD2	1.94	0.49
1:A:897:VAL:HG23	1:A:898:LYS:HG3	1.93	0.49
1:B:876:LYS:O	1:B:879:ILE:HG12	2.12	0.49
1:A:545:ILE:HD13	1:A:664:LEU:HB2	1.95	0.49
1:B:390:ARG:HG3	1:B:458:ILE:HG13	1.94	0.49
1:A:871:LEU:HA	1:A:874:ILE:HG22	1.95	0.49
1:A:596:VAL:HG12	1:A:598:LYS:H	1.78	0.48
1:B:943:LYS:HB2	1:B:965:LEU:CD1	2.42	0.48
1:B:620:ARG:HG3	1:B:627:GLN:HG2	1.95	0.48
1:B:731:TRP:HB3	1:B:1097:ILE:HG13	1.95	0.48
1:B:71:PHE:CD2	1:B:112:MET:HG2	2.48	0.48
1:B:479:VAL:HB	1:B:532:SER:HB3	1.94	0.48
1:B:871:LEU:HA	1:B:874:ILE:HG22	1.94	0.48
1:A:2:ALA:HB2	1:A:24:GLU:OE1	2.14	0.48
1:B:24:GLU:HA	1:B:685:LEU:HD23	1.96	0.48
1:B:543:LEU:O	1:B:583:ILE:HA	2.14	0.48
1:B:719:VAL:O	1:B:722:GLN:HB3	2.14	0.48
1:B:813:LEU:HD23	1:B:814:PRO:HD2	1.96	0.48
1:A:62:ASN:HA	1:A:65:GLU:OE2	2.13	0.47
1:A:675:LYS:CG	1:A:722:GLN:HG3	2.43	0.47
1:B:62:ASN:HA	1:B:65:GLU:OE2	2.14	0.47
1:B:897:VAL:HG23	1:B:898:LYS:HG3	1.96	0.47
1:B:1061:GLU:O	1:B:1065:THR:OG1	2.32	0.47
1:A:205:VAL:HG21	1:A:278:VAL:HG11	1.97	0.47
1:A:351:LYS:NZ	1:A:372:VAL:HG11	2.29	0.47
1:A:390:ARG:HG3	1:A:458:ILE:HG13	1.96	0.47
1:A:675:LYS:HB2	1:A:722:GLN:HG3	1.97	0.47
1:B:128:PHE:CZ	1:B:137:THR:HG21	2.50	0.47
1:B:226:GLU:HA	1:B:229:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:803:LEU:HD11	1:B:945:GLN:NE2	2.29	0.47
1:A:188:ASN:HB3	1:A:191:LYS:HD2	1.95	0.47
1:A:226:GLU:HA	1:A:229:ILE:HD12	1.97	0.47
1:A:307:ILE:HG22	1:A:522:VAL:HG21	1.96	0.47
1:B:620:ARG:NH2	1:B:622:ARG:HA	2.30	0.47
1:B:803:LEU:HD13	1:B:947:VAL:HG13	1.97	0.47
1:B:22:ARG:HG2	1:B:27:LEU:HB2	1.96	0.47
1:B:566:ARG:HB2	1:B:573:VAL:HG13	1.96	0.47
1:B:571:ILE:HD12	1:B:586:THR:HG21	1.97	0.47
1:A:547:VAL:HG12	1:A:666:ALA:HB3	1.96	0.46
1:A:596:VAL:HG23	1:A:614:VAL:O	2.15	0.46
1:B:205:VAL:HG21	1:B:278:VAL:HG11	1.96	0.46
1:B:528:SER:HB2	1:B:531:ARG:NH2	2.30	0.46
1:B:944:LYS:CB	1:B:961:ILE:HG23	2.45	0.46
1:A:71:PHE:CD2	1:A:112:MET:HG2	2.50	0.46
1:B:134:VAL:HG13	1:B:179:VAL:HG12	1.97	0.46
1:B:961:ILE:CD1	1:B:961:ILE:CB	2.83	0.46
1:A:395:LEU:HD11	1:A:428:ALA:HA	1.97	0.46
1:A:696:MET:HG2	1:A:707:ALA:HB2	1.98	0.46
1:B:754:VAL:HG22	1:B:1069:THR:CG2	2.45	0.46
1:A:24:GLU:HA	1:A:685:LEU:HD23	1.98	0.46
1:A:237:LYS:HE2	1:B:637:VAL:CG1	2.46	0.46
1:A:958:ILE:HA	1:A:958:ILE:HD13	1.95	0.46
1:A:329:LEU:HD12	1:A:359:ILE:HD11	1.98	0.46
1:B:578:THR:HG21	1:B:583:ILE:HD13	1.96	0.45
1:B:797:VAL:HG23	1:B:987:LYS:HA	1.98	0.45
1:A:1002:PHE:HE1	1:A:1010:GLU:HG3	1.81	0.45
1:A:559:PHE:HB2	1:A:701:ARG:CZ	2.46	0.45
1:A:435:LYS:H	1:A:435:LYS:HD2	1.82	0.45
1:A:803:LEU:CD1	1:A:947:VAL:HG22	2.46	0.45
1:A:1003:THR:O	1:A:1007:ILE:HG13	2.15	0.45
1:B:803:LEU:CD1	1:B:947:VAL:HG22	2.46	0.45
1:B:997:HIS:CD2	1:B:997:HIS:N	2.85	0.45
1:B:1003:THR:O	1:B:1007:ILE:HG13	2.17	0.45
1:B:46:LEU:HD13	1:B:51:LEU:HD23	1.99	0.45
1:B:596:VAL:HG12	1:B:598:LYS:H	1.82	0.45
1:B:2:ALA:HB2	1:B:24:GLU:OE1	2.17	0.45
1:B:675:LYS:HB2	1:B:722:GLN:HG3	1.98	0.45
1:B:11:CYS:SG	1:B:29:CYS:HB3	2.57	0.45
1:B:620:ARG:O	1:B:644:ASP:N	2.47	0.45
1:A:616:ASN:ND2	1:A:629:THR:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:665:VAL:HG21	1:B:681:THR:HG23	1.97	0.44
1:B:558:ARG:HG3	1:B:558:ARG:HH11	1.82	0.44
1:A:958:ILE:CD1	1:A:958:ILE:CB	2.81	0.44
1:A:308:PHE:HE2	1:A:382:ILE:HD11	1.82	0.44
1:B:885:TRP:O	1:B:886:SER:HB2	2.18	0.44
1:A:33:LEU:HD12	1:A:48:ARG:HD2	2.00	0.44
1:A:566:ARG:HB2	1:A:573:VAL:HG13	1.98	0.44
1:A:668:ASP:HA	1:A:669:PRO:HD3	1.85	0.44
1:A:591:HIS:HB2	1:A:618:LEU:HD12	2.00	0.44
1:B:816:TYR:O	1:B:893:ALA:HB1	2.18	0.44
1:A:134:VAL:HG13	1:A:179:VAL:HG12	1.99	0.43
1:A:943:LYS:HB2	1:A:965:LEU:HD21	2.00	0.43
1:B:615:TYR:OH	1:B:723:ILE:HG12	2.17	0.43
1:B:543:LEU:HD12	1:B:662:GLU:HB3	1.99	0.43
1:B:814:PRO:O	1:B:931:ARG:NH1	2.51	0.43
1:A:128:PHE:CZ	1:A:137:THR:HG21	2.53	0.43
1:A:343:PHE:HB3	1:A:368:LEU:HD11	1.99	0.43
1:A:835:GLU:O	1:A:839:ILE:HG12	2.19	0.43
1:B:419:PRO:O	1:B:422:GLU:HB3	2.19	0.43
1:B:835:GLU:O	1:B:839:ILE:HG12	2.19	0.43
1:B:115:LEU:HD11	1:B:145:ALA:HB2	2.00	0.43
1:B:596:VAL:HG22	1:B:616:ASN:HB2	2.00	0.43
1:A:378:ILE:O	1:A:529:ARG:NH2	2.51	0.43
1:B:496:GLU:O	1:B:500:THR:HG23	2.18	0.43
1:A:715:ASP:OD1	1:A:718:LEU:HD13	2.19	0.43
1:B:189:ARG:HG3	1:B:217:THR:OG1	2.18	0.43
1:A:719:VAL:O	1:A:722:GLN:HB3	2.19	0.43
1:A:407:LEU:HD13	1:A:412:LEU:HD23	2.00	0.43
1:A:805:GLU:HG2	1:A:945:GLN:HB3	2.01	0.43
1:B:1077:ASP:HB3	1:B:1081:ARG:HH12	1.84	0.43
1:B:22:ARG:NE	1:B:28:PRO:O	2.52	0.42
1:B:622:ARG:HB2	1:B:642:ASN:OD1	2.20	0.42
1:B:942:VAL:HG22	1:B:963:GLU:O	2.19	0.42
1:A:996:LYS:HD3	1:A:996:LYS:HA	1.73	0.42
1:A:1077:ASP:HB3	1:A:1081:ARG:HH12	1.85	0.42
1:B:143:LYS:HG3	1:B:144:LEU:HG	2.02	0.42
1:A:189:ARG:HG3	1:A:217:THR:OG1	2.18	0.42
1:B:943:LYS:HE3	1:B:965:LEU:HD11	2.02	0.42
1:A:46:LEU:HD13	1:A:51:LEU:HD23	2.00	0.42
1:A:797:VAL:HG23	1:A:987:LYS:HA	2.02	0.42
1:A:805:GLU:CG	1:A:945:GLN:HB3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LEU:HD23	1:A:304:LEU:HA	1.79	0.42
1:B:956:MET:HE3	1:B:956:MET:HB3	1.86	0.42
1:A:301:LEU:HD23	1:A:325:LEU:HD11	2.01	0.42
1:A:665:VAL:HG21	1:A:681:THR:HG23	2.01	0.42
1:B:405:ARG:HD2	1:B:910:GLU:OE1	2.19	0.42
1:A:803:LEU:HD13	1:A:947:VAL:HG13	2.01	0.42
1:B:1097:ILE:HD13	1:B:1097:ILE:HA	1.99	0.42
1:A:405:ARG:HD2	1:A:910:GLU:OE1	2.20	0.42
1:B:436:GLU:O	1:B:440:LYS:HG2	2.20	0.42
1:A:154:PHE:CE1	1:A:163:LYS:HG3	2.55	0.41
1:A:816:TYR:O	1:A:893:ALA:HB1	2.20	0.41
1:A:436:GLU:O	1:A:440:LYS:HG2	2.20	0.41
1:A:737:SER:O	1:A:741:GLN:HG3	2.20	0.41
1:A:795:ASP:N	1:A:795:ASP:OD1	2.49	0.41
1:B:762:ILE:HG22	1:B:1045:PRO:HD3	2.01	0.41
1:A:379:LYS:HB3	1:A:525:VAL:HG11	2.02	0.41
1:A:758:VAL:O	1:A:761:TRP:HB2	2.20	0.41
1:B:433:THR:C	1:B:435:LYS:H	2.24	0.41
1:B:610:LYS:HG2	1:B:1087:GLN:HG2	2.02	0.41
1:A:824:GLU:OE2	1:A:931:ARG:NH2	2.52	0.41
1:B:175:TYR:HB2	1:B:178:LEU:HD21	2.03	0.41
1:B:545:ILE:HD13	1:B:585:PHE:HB3	2.03	0.41
1:B:715:ASP:OD1	1:B:718:LEU:HD13	2.20	0.41
1:B:1040:TYR:HB2	1:B:1042:ARG:HD2	2.02	0.41
1:A:958:ILE:CD1	1:A:958:ILE:CA	2.95	0.41
1:A:5:SER:HB3	1:A:613:PRO:HD2	2.03	0.41
1:A:1002:PHE:HD1	1:A:1006:SER:OG	2.04	0.41
1:B:5:SER:HB3	1:B:613:PRO:HD2	2.02	0.41
1:B:351:LYS:HZ2	1:B:372:VAL:HG11	1.86	0.41
1:B:543:LEU:HD23	1:B:545:ILE:HG13	2.03	0.41
1:B:737:SER:O	1:B:741:GLN:HG3	2.20	0.41
1:B:795:ASP:OD1	1:B:795:ASP:N	2.51	0.41
1:B:388:SER:HA	1:B:461:ASP:H	1.86	0.41
1:B:545:ILE:O	1:B:585:PHE:HA	2.21	0.41
1:B:596:VAL:HG23	1:B:614:VAL:O	2.21	0.41
1:B:124:SER:HB3	1:B:199:PHE:HD2	1.86	0.40
1:A:696:MET:HG2	1:A:707:ALA:CB	2.51	0.40
1:A:1040:TYR:HB2	1:A:1042:ARG:HD2	2.03	0.40
1:B:379:LYS:HB3	1:B:525:VAL:HG11	2.04	0.40
1:B:541:ARG:O	1:B:581:GLY:HA3	2.22	0.40
1:B:438:VAL:HG21	1:B:455:LEU:HD22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:LEU:HD12	1:A:685:LEU:HA	1.79	0.40
1:B:593:TYR:HD1	1:B:679:ASP:HB3	1.87	0.40
1:A:551:THR:O	1:A:555:THR:HG23	2.21	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	1100/1104 (100%)	997 (91%)	95 (9%)	8 (1%)	22	60
1	B	1100/1104 (100%)	988 (90%)	99 (9%)	13 (1%)	13	48
All	All	2200/2208 (100%)	1985 (90%)	194 (9%)	21 (1%)	15	52

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	417	GLU
1	A	792	LYS
1	A	791	GLY
1	B	39	SER
1	B	562	ARG
1	B	791	GLY
1	B	792	LYS
1	A	415	ALA
1	B	30	GLU
1	B	173	ASP
1	B	415	ALA
1	B	432	LEU
1	B	538	ASP
1	B	886	SER
1	B	983	HIS

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Mol	Chain	Res	Type
1	A	173	ASP
1	A	431	HIS
1	A	983	HIS
1	A	76	GLY
1	B	76	GLY
1	B	598	LYS

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	992/993 (100%)	930 (94%)	62 (6%)	18	50
1	B	992/993 (100%)	892 (90%)	100 (10%)	7	30
All	All	1984/1986 (100%)	1822 (92%)	162 (8%)	11	39

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ARG
1	A	65	GLU
1	A	66	ASP
1	A	73	LYS
1	A	80	THR
1	A	85	LEU
1	A	90	ILE
1	A	146	ASP
1	A	158	MET
1	A	249	LYS
1	A	261	LYS
1	A	280	ARG
1	A	284	VAL
1	A	299	GLU
1	A	321	GLU
1	A	343	PHE
1	A	358	LEU

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Mol	Chain	Res	Type
1	A	364	TYR
1	A	367	LYS
1	A	376	GLU
1	A	390	ARG
1	A	396	ASP
1	A	400	ARG
1	A	410	MET
1	A	432	LEU
1	A	435	LYS
1	A	436	GLU
1	A	439	GLU
1	A	454	ASP
1	A	537	THR
1	A	555	THR
1	A	564	SER
1	A	573	VAL
1	A	619	LYS
1	A	647	THR
1	A	709	GLU
1	A	722	GLN
1	A	725	ARG
1	A	729	ASP
1	A	743	ARG
1	A	775	ASP
1	A	786	ASN
1	A	792	LYS
1	A	793	ILE
1	A	797	VAL
1	A	813	LEU
1	A	819	SER
1	A	828	LYS
1	A	877	GLU
1	A	878	ASP
1	A	881	MET
1	A	927	LEU
1	A	931	ARG
1	A	942	VAL
1	A	956	MET
1	A	958	ILE
1	A	965	LEU
1	A	978	SER
1	A	995	LYS

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Mol	Chain	Res	Type
1	A	997	HIS
1	A	1077	ASP
1	A	1101	MET
1	B	9	HIS
1	B	21	GLU
1	B	29	CYS
1	B	30	GLU
1	B	35	GLU
1	B	55	ARG
1	B	65	GLU
1	B	66	ASP
1	B	73	LYS
1	B	80	THR
1	B	85	LEU
1	B	90	ILE
1	B	115	LEU
1	B	124	SER
1	B	146	ASP
1	B	170	PHE
1	B	249	LYS
1	B	261	LYS
1	B	280	ARG
1	B	284	VAL
1	B	299	GLU
1	B	321	GLU
1	B	343	PHE
1	B	358	LEU
1	B	364	TYR
1	B	367	LYS
1	B	376	GLU
1	B	390	ARG
1	B	396	ASP
1	B	400	ARG
1	B	410	MET
1	B	412	LEU
1	B	416	GLN
1	B	418	ASN
1	B	429	LYS
1	B	430	GLU
1	B	433	THR
1	B	435	LYS
1	B	436	GLU

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Mol	Chain	Res	Type
1	B	439	GLU
1	B	454	ASP
1	B	476	LEU
1	B	492	GLU
1	B	527	GLU
1	B	528	SER
1	B	529	ARG
1	B	542	SER
1	B	543	LEU
1	B	545	ILE
1	B	547	VAL
1	B	554	GLU
1	B	564	SER
1	B	573	VAL
1	B	583	ILE
1	B	586	THR
1	B	619	LYS
1	B	629	THR
1	B	640	SER
1	B	647	THR
1	B	661	ASP
1	B	695	GLU
1	B	696	MET
1	B	702	TYR
1	B	709	GLU
1	B	722	GLN
1	B	725	ARG
1	B	729	ASP
1	B	743	ARG
1	B	764	GLU
1	B	771	LYS
1	B	775	ASP
1	B	786	ASN
1	B	792	LYS
1	B	793	ILE
1	B	797	VAL
1	B	813	LEU
1	B	819	SER
1	B	828	LYS
1	B	845	GLU
1	B	877	GLU
1	B	878	ASP

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Mol	Chain	Res	Type
1	B	881	MET
1	B	895	ARG
1	B	927	LEU
1	B	931	ARG
1	B	942	VAL
1	B	944	LYS
1	B	956	MET
1	B	958	ILE
1	B	960	GLN
1	B	961	ILE
1	B	963	GLU
1	B	965	LEU
1	B	977	VAL
1	B	995	LYS
1	B	996	LYS
1	B	1010	GLU
1	B	1052	VAL
1	B	1077	ASP
1	B	1101	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	GLN
1	A	346	ASN
1	A	431	HIS
1	A	722	GLN
1	A	834	GLN
1	B	317	GLN
1	B	346	ASN
1	B	431	HIS
1	B	722	GLN
1	B	834	GLN
1	B	960	GLN
1	B	997	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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(Å²)	Q<0.9
1	A	1102/1104 (99%)	0.79	144 (13%)	3	5	48, 100, 169, 216	0
1	B	1102/1104 (99%)	0.61	104 (9%)	8	10	25, 90, 175, 224	0
All	All	2204/2208 (99%)	0.70	248 (11%)	5	7	25, 96, 174, 224	0

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	240	LYS	11.1
1	B	236	ILE	8.9
1	B	241	ILE	8.0
1	B	228	ILE	7.5
1	A	240	LYS	7.2
1	A	239	GLY	7.1
1	A	217	THR	7.0
1	A	412	LEU	6.7
1	A	193	SER	6.6
1	A	309	ARG	6.0
1	B	239	GLY	5.9
1	B	166	PHE	5.9
1	B	242	TYR	5.7
1	A	998	THR	5.7
1	A	413	ILE	5.4
1	A	242	TYR	5.4
1	A	241	ILE	5.3
1	B	268	LEU	5.3
1	A	269	LEU	5.2
1	A	230	ARG	5.2
1	A	348	GLU	5.2
1	B	160	LYS	5.1
1	B	15	GLY	5.1
1	A	173	ASP	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	748	ASN	4.9
1	A	194	GLN	4.8
1	B	232	ALA	4.8
1	B	998	THR	4.8
1	A	220	MET	4.7
1	B	195	LYS	4.7
1	A	160	LYS	4.7
1	A	594	ASP	4.6
1	A	526	GLU	4.5
1	A	633	ASP	4.5
1	A	166	PHE	4.4
1	A	232	ALA	4.4
1	A	39	SER	4.4
1	B	193	SER	4.4
1	B	173	ASP	4.4
1	B	272	ASP	4.3
1	B	172	GLU	4.2
1	A	170	PHE	4.2
1	B	233	PHE	4.1
1	B	269	LEU	4.0
1	A	175	TYR	4.0
1	B	185	VAL	4.0
1	B	217	THR	4.0
1	A	518	TRP	3.9
1	A	214	ASN	3.9
1	A	228	ILE	3.9
1	A	236	ILE	3.9
1	A	238	GLN	3.8
1	B	443	GLU	3.8
1	A	623	ASP	3.8
1	B	245	PRO	3.8
1	A	999	VAL	3.8
1	B	151	ILE	3.8
1	B	229	ILE	3.7
1	B	238	GLN	3.7
1	B	140	ARG	3.7
1	A	783	ASN	3.7
1	A	174	ASP	3.7
1	B	152	PHE	3.6
1	A	522	VAL	3.6
1	B	640	SER	3.6
1	A	182	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	634	GLU	3.5
1	A	643	ILE	3.5
1	A	445	PHE	3.5
1	A	233	PHE	3.5
1	A	206	ASP	3.5
1	A	991	LYS	3.4
1	B	189	ARG	3.4
1	B	1063	TYR	3.4
1	A	195	LYS	3.4
1	A	254	VAL	3.3
1	A	790	GLU	3.3
1	A	533	GLU	3.3
1	B	214	ASN	3.3
1	A	196	ARG	3.3
1	A	760	GLY	3.3
1	A	764	GLU	3.2
1	B	939	ALA	3.2
1	A	219	LEU	3.2
1	A	247	ASN	3.1
1	A	224	ILE	3.1
1	A	207	ALA	3.1
1	A	425	ARG	3.1
1	A	189	ARG	3.1
1	B	533	GLU	3.1
1	A	431	HIS	3.1
1	A	747	SER	3.1
1	A	940	VAL	3.1
1	A	268	LEU	3.1
1	B	896	PRO	3.0
1	A	164	GLU	3.0
1	A	644	ASP	3.0
1	B	161	GLU	3.0
1	B	273	LEU	3.0
1	A	226	GLU	3.0
1	B	976	THR	3.0
1	A	761	TRP	3.0
1	A	38	PRO	3.0
1	A	154	PHE	3.0
1	B	133	LEU	2.9
1	A	744	PHE	2.9
1	A	426	LYS	2.9
1	A	271	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	979	PRO	2.9
1	A	641	LYS	2.9
1	B	170	PHE	2.9
1	A	172	GLU	2.9
1	B	602	HIS	2.9
1	A	976	THR	2.9
1	A	372	VAL	2.9
1	B	154	PHE	2.8
1	B	776	PHE	2.8
1	B	990	GLU	2.8
1	A	201	PHE	2.8
1	B	171	GLU	2.8
1	B	574	HIS	2.8
1	B	940	VAL	2.7
1	A	621	CYS	2.7
1	A	416	GLN	2.7
1	B	206	ASP	2.7
1	A	346	ASN	2.7
1	A	624	CYS	2.7
1	B	790	GLU	2.7
1	A	896	PRO	2.7
1	A	163	LYS	2.7
1	A	517	ASN	2.7
1	B	57	TYR	2.7
1	A	988	ILE	2.7
1	B	153	GLY	2.6
1	B	775	ASP	2.6
1	A	140	ARG	2.6
1	A	267	PRO	2.6
1	A	161	GLU	2.6
1	B	119	ARG	2.6
1	B	39	SER	2.6
1	A	167	GLU	2.6
1	B	417	GLU	2.6
1	B	216	ASP	2.6
1	B	748	ASN	2.6
1	A	310	ASP	2.5
1	B	271	ARG	2.5
1	A	176	HIS	2.5
1	A	607	GLU	2.5
1	A	767	GLU	2.5
1	A	982	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	332	PHE	2.5
1	A	880	PHE	2.5
1	B	267	PRO	2.5
1	A	1063	TYR	2.5
1	B	445	PHE	2.5
1	A	765	ARG	2.5
1	B	244	ARG	2.5
1	A	441	VAL	2.4
1	A	109	PHE	2.4
1	B	410	MET	2.4
1	A	763	VAL	2.4
1	B	441	VAL	2.4
1	A	769	TYR	2.4
1	A	216	ASP	2.4
1	B	194	GLN	2.4
1	B	887	THR	2.4
1	A	229	ILE	2.4
1	A	305	LEU	2.4
1	A	443	GLU	2.4
1	A	574	HIS	2.4
1	B	16	GLY	2.3
1	B	186	SER	2.3
1	A	177	ILE	2.3
1	B	946	ILE	2.3
1	A	282	VAL	2.3
1	B	742	LYS	2.3
1	B	752	GLY	2.3
1	A	188	ASN	2.3
1	A	152	PHE	2.3
1	B	910	GLU	2.3
1	A	775	ASP	2.3
1	B	424	LEU	2.3
1	A	352	VAL	2.3
1	B	981	PHE	2.3
1	B	177	ILE	2.3
1	B	639	SER	2.3
1	A	133	LEU	2.2
1	B	210	LYS	2.2
1	B	164	GLU	2.2
1	A	221	MET	2.2
1	A	255	VAL	2.2
1	A	355	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1008	VAL	2.2
1	A	561	GLY	2.2
1	A	423	GLU	2.2
1	A	477	ASN	2.2
1	B	783	ASN	2.2
1	B	779	LEU	2.2
1	A	291	VAL	2.2
1	B	991	LYS	2.2
1	A	805	GLU	2.2
1	B	949	VAL	2.2
1	A	889	GLY	2.2
1	B	996	LYS	2.2
1	B	518	TRP	2.2
1	A	741	GLN	2.2
1	A	190	GLU	2.2
1	A	781	LEU	2.1
1	A	975	LEU	2.1
1	B	235	THR	2.1
1	B	778	LEU	2.1
1	A	582	VAL	2.1
1	A	671	VAL	2.1
1	B	753	ARG	2.1
1	B	886	SER	2.1
1	B	163	LYS	2.1
1	A	185	VAL	2.1
1	A	797	VAL	2.1
1	A	128	PHE	2.1
1	A	435	LYS	2.1
1	A	235	THR	2.1
1	A	77	LYS	2.1
1	B	181	SER	2.1
1	B	230	ARG	2.1
1	A	668	ASP	2.1
1	A	768	GLU	2.1
1	B	458	ILE	2.1
1	A	15	GLY	2.1
1	A	155	TYR	2.1
1	B	741	GLN	2.1
1	A	35	GLU	2.1
1	B	479	VAL	2.1
1	B	141	LEU	2.1
1	A	981	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	942	VAL	2.1
1	B	159	LYS	2.0
1	A	535	GLU	2.0
1	A	410	MET	2.0
1	B	167	GLU	2.0
1	B	237	LYS	2.0
1	A	350	PHE	2.0
1	B	446	ARG	2.0
1	B	531	ARG	2.0
1	B	728	GLN	2.0
1	B	1067	GLU	2.0
1	A	178	LEU	2.0
1	B	413	ILE	2.0
1	B	731	TRP	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 monosaccharides in this entry.

6.4　Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	A	2001	1/1	0.81	0.06	137,137,137,137	0
2	ZN	B	2001	1/1	0.90	0.07	137,137,137,137	0
2	ZN	A	2002	1/1	0.98	0.12	75,75,75,75	0
2	ZN	B	2002	1/1	0.98	0.09	55,55,55,55	0

6.5　Other polymers ⓘ

There are no such residues in this entry.