Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:46 PM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

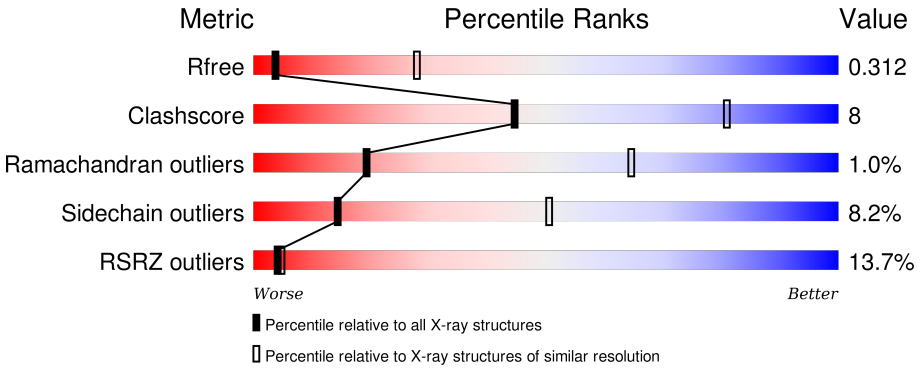
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.46 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}	91344	1000 (3.56-3.36)
Clashscore	102246	1090 (3.56-3.36)
Ramachandran outliers	100387	1057 (3.56-3.36)
Sidechain outliers	100360	1058 (3.56-3.36)
RSRZ outliers	91569	1005 (3.56-3.36)

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 <=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	16% 78% 20%
1	B	1104	12% 72% 24%

2 Entry composition (i)

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	C	N	O	S	0	0	0
			9030	5759	1563	1682	26			
1	B	1102	Total	C	N	O	S	0	0	0
			9030	5759	1563	1682	26			

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

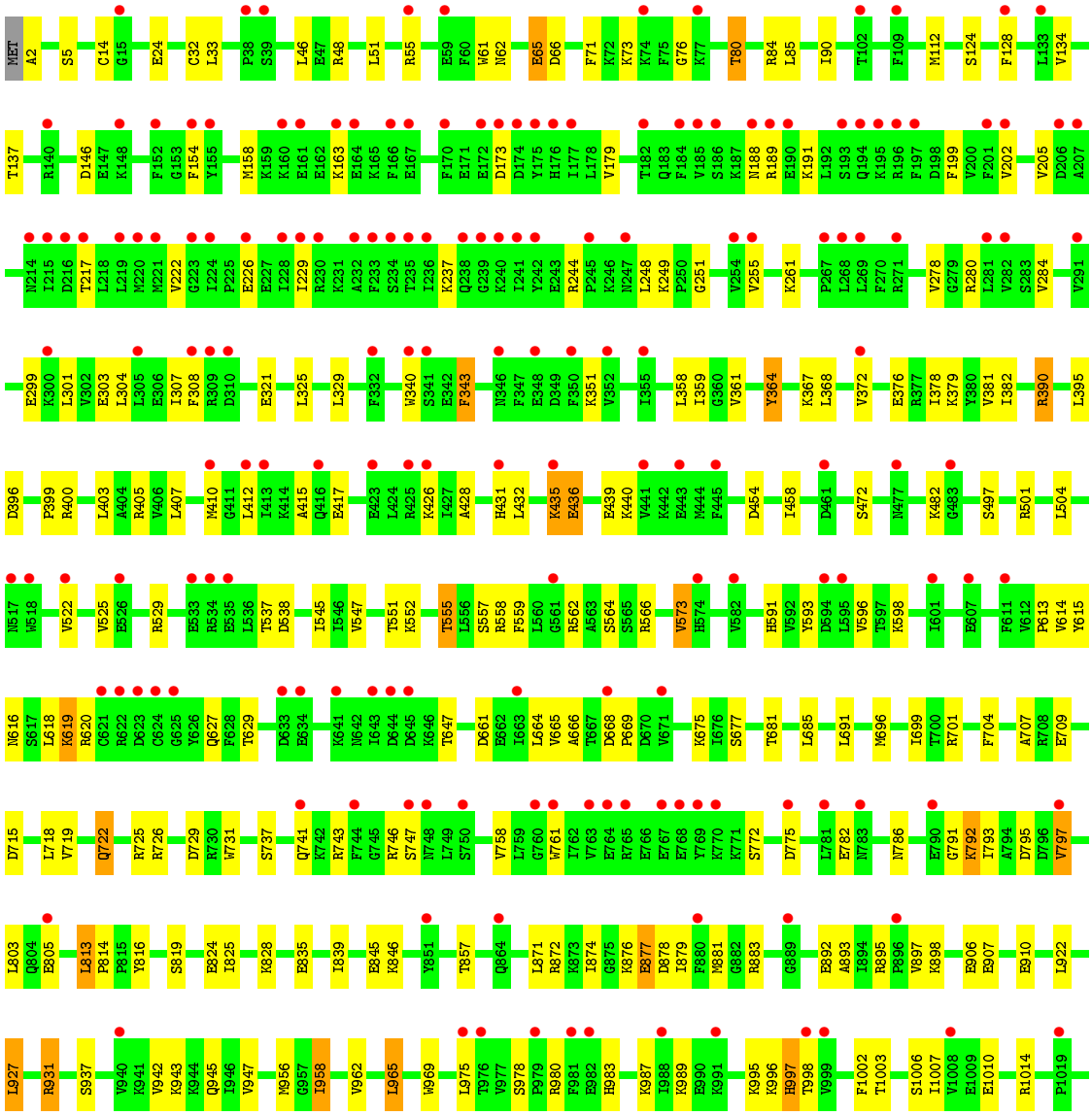
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

3 Residue-property plots (i)

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.

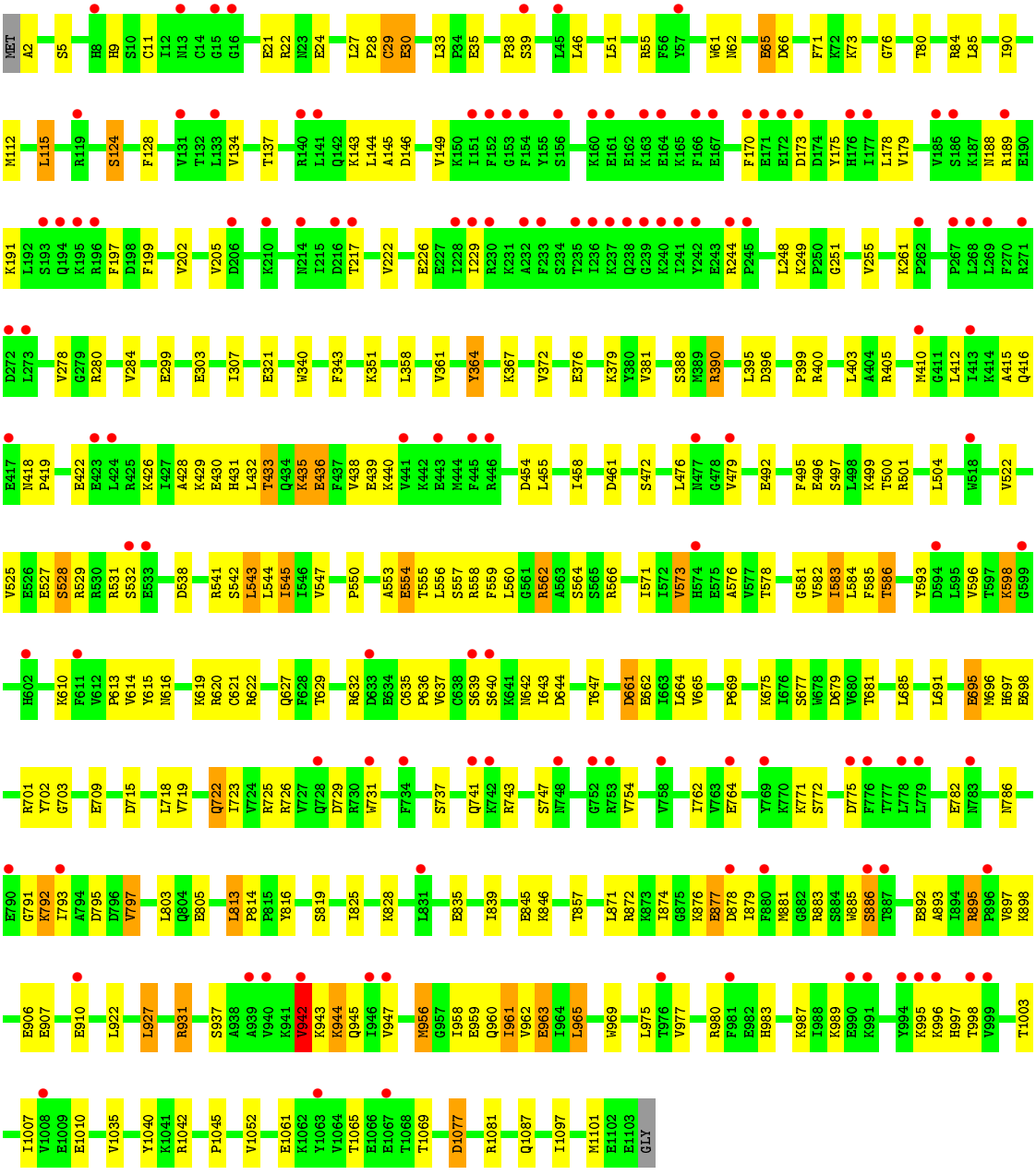
- Molecule 1: Reverse gyrase

Chain A:



- Molecule 1: Reverse gyrase

Chain B:



4 Data and refinement statistics (i)

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) 80.4 (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 0.266 , 0.312	Depositor DCC
R_{free} test set	2069 reflections (5.31%)	DCC
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 , 90.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Outliers	0 of 41025 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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.

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:CG1	1:A:958:ILE:CD1	1.77	1.57
1:B:961:ILE:CG1	1:B:961:ILE:CD1	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:B:555:THR:HG22	1:B:558:ARG:NH2	2.00	0.77
1:A:412:LEU:HD21	1:A:426:LYS:HB3	1.66	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:HA	1:A:958:ILE:CD1	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:B:772:SER:HB3	1:B:998:THR:HB	1.79	0.64
1:A:772:SER:HB3	1:A: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: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: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: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:1010:GLU:OE1	1:A:1014:ARG:NH1	2.37	0.57
1:A:969:TRP:CH2	1:A:975:LEU:HD13	2.40	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:B:816:TYR:CZ	1:B:931:ARG:HG3	2.44	0.53
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: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:B:222:VAL:HB	1:B:251:GLY:H	1.75	0.52
1:A:619:LYS:NZ	1:A:629:THR:O	2.40	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:582:VAL:HG12	1:B:583:ILE:H	1.73	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: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:B:944:LYS:HE3	1:B:959:GLU:OE1	2.11	0.50
1:A:731:TRP:HB3	1:A:1097:ILE:HG13	1.93	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:B:145:ALA:HB1	1:B:149:VAL:HG21	1.93	0.49
1:A:1061:GLU:O	1:A:1065:THR:OG1	2.30	0.49
1:B:892:GLU:OE2	1:B:895:ARG:NH1	2.45	0.49
1:B:543:LEU:HD21	1:B:664:LEU:CD1	2.37	0.49
1:A:814:PRO:O	1:A:931:ARG:NH1	2.45	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:B:943:LYS:HB2	1:B:965:LEU:CD1	2.42	0.48
1:A:596:VAL:HG12	1:A:598:LYS:H	1.78	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:479:VAL:HB	1:B:532:SER:HB3	1.94	0.48
1:B:71:PHE:CD2	1:B:112:MET:HG2	2.48	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: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:B:24:GLU:HA	1:B:685:LEU:HD23	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:675:LYS:HB2	1:A:722:GLN:HG3	1.97	0.47
1:A:390:ARG:HG3	1:A:458:ILE:HG13	1.96	0.47
1:A:205:VAL:HG21	1:A:278:VAL:HG11	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
1:A:351:LYS:NZ	1:A:372:VAL:HG11	2.29	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: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:B:22:ARG:HG2	1:B:27:LEU:HB2	1.96	0.47
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:A:547:VAL:HG12	1:A:666:ALA:HB3	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:B:961:ILE:CD1	1:B:961:ILE:CB	2.83	0.46
1:B:134:VAL:HG13	1:B:179:VAL:HG12	1.97	0.46
1:A:71:PHE:CD2	1:A:112:MET:HG2	2.50	0.46
1:A:696:MET:HG2	1:A:707:ALA:HB2	1.98	0.46
1:A:395:LEU:HD11	1:A:428:ALA:HA	1.97	0.46
1:B:754:VAL:HG22	1:B:1069:THR:CG2	2.45	0.46
1:A:958:ILE:HA	1:A:958:ILE:HD13	1.95	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: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:B:803:LEU:CD1	1:B:947:VAL:HG22	2.46	0.45
1:A:1003:THR:O	1:A:1007:ILE:HG13	2.15	0.45
1:B:1003:THR:O	1:B:1007:ILE:HG13	2.17	0.45
1:A:803:LEU:CD1	1:A:947:VAL:HG22	2.46	0.45
1:A:435:LYS:HD2	1:A:435:LYS:H	1.82	0.45
1:B:997:HIS:N	1:B:997:HIS:CD2	2.85	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:675:LYS:HB2	1:B:722:GLN:HG3	1.98	0.45
1:B:2:ALA:HB2	1:B:24:GLU:OE1	2.17	0.45
1:B:620:ARG:O	1:B:644:ASP:N	2.47	0.45
1:B:11:CYS:SG	1:B:29:CYS:HB3	2.57	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:HH11	1:B:558:ARG:HG3	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:B:816:TYR:O	1:B:893:ALA:HB1	2.18	0.44
1:A:591:HIS:HB2	1:A:618:LEU:HD12	2.00	0.44
1:B:615:TYR:OH	1:B:723:ILE:HG12	2.17	0.43
1:A:943:LYS:HB2	1:A:965:LEU:HD21	2.00	0.43
1:A:134:VAL:HG13	1:A:179:VAL:HG12	1.99	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:835:GLU:O	1:B:839:ILE:HG12	2.19	0.43
1:B:419:PRO:O	1:B:422:GLU:HB3	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:B:189:ARG:HG3	1:B:217:THR:OG1	2.18	0.43
1:A:715:ASP:OD1	1:A:718:LEU:HD13	2.19	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:B:1077:ASP:HB3	1:B:1081:ARG:HH12	1.84	0.43
1:A:805:GLU:HG2	1:A:945:GLN:HB3	2.01	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:HA	1:A:996:LYS:HD3	1.73	0.42
1:B:143:LYS:HG3	1:B:144:LEU:HG	2.02	0.42
1:A:1077:ASP:HB3	1:A:1081:ARG:HH12	1.85	0.42
1:B:943:LYS:HE3	1:B:965:LEU:HD11	2.02	0.42
1:A:189:ARG:HG3	1:A:217:THR:OG1	2.18	0.42
1:A:805:GLU:CG	1:A:945:GLN:HB3	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LEU:HA	1:A:304:LEU:HD23	1.79	0.42
1:B:956:MET:HB3	1:B:956:MET:HE3	1.86	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:301:LEU:HD23	1:A:325:LEU:HD11	2.01	0.42
1:B:1097:ILE:HD13	1:B:1097:ILE:HA	1.99	0.42
1:A:803:LEU:HD13	1:A:947:VAL:HG13	2.01	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:816:TYR:O	1:A:893:ALA:HB1	2.20	0.41
1:A:154:PHE:CE1	1:A:163:LYS:HG3	2.55	0.41
1:A:737:SER:O	1:A:741:GLN:HG3	2.20	0.41
1:B:762:ILE:HG22	1:B:1045:PRO:HD3	2.01	0.41
1:A:795:ASP:N	1:A:795:ASP:OD1	2.49	0.41
1:A:436:GLU:O	1:A:440:LYS:HG2	2.20	0.41
1:A:758:VAL:O	1:A:761:TRP:HB2	2.20	0.41
1:A:379:LYS:HB3	1:A:525:VAL:HG11	2.02	0.41
1:B:610:LYS:HG2	1:B:1087:GLN:HG2	2.02	0.41
1:B:433:THR:C	1:B:435:LYS:H	2.24	0.41
1:B:545:ILE:HD13	1:B:585:PHE:HB3	2.03	0.41
1:B:175:TYR:HB2	1:B:178:LEU:HD21	2.03	0.41
1:A:824:GLU:OE2	1:A:931:ARG:NH2	2.52	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:CA	1:A:958:ILE:CD1	2.95	0.41
1:A:1002:PHE:HD1	1:A:1006:SER:OG	2.04	0.41
1:A:5:SER:HB3	1:A:613:PRO:HD2	2.03	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:351:LYS:HZ2	1:B:372:VAL:HG11	1.86	0.41
1:B:5:SER:HB3	1:B:613:PRO:HD2	2.02	0.41
1:B:795:ASP:OD1	1:B:795:ASP:N	2.51	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:388:SER:HA	1:B:461:ASP:H	1.86	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:B:541:ARG:O	1:B:581:GLY:HA3	2.22	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: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:B:593:TYR:HD1	1:B:679:ASP:HB3	1.87	0.40
1:A:685:LEU:HD12	1:A:685:LEU:HA	1.79	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 (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	1100/1104 (100%)	997 (91%)	95 (9%)	8 (1%)	26	71
1	B	1100/1104 (100%)	988 (90%)	99 (9%)	13 (1%)	16	60
All	All	2200/2208 (100%)	1985 (90%)	194 (9%)	21 (1%)	19	64

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%)	22 62
1	B	992/993 (100%)	892 (90%)	100 (10%)	9 39
All	All	1984/1986 (100%)	1822 (92%)	162 (8%)	14 50

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

Some 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

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	1102/1104 (99%)	0.89	176 (15%)	3	3	48, 100, 169, 216	0
1	B	1102/1104 (99%)	0.72	127 (11%)	6	7	25, 90, 175, 224	0
All	All	2204/2208 (99%)	0.81	303 (13%)	4	5	25, 96, 174, 224	0

All (303) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	240	LYS	12.4
1	B	236	ILE	9.7
1	B	241	ILE	8.1
1	A	412	LEU	7.9
1	A	240	LYS	7.8
1	A	239	GLY	7.5
1	B	228	ILE	7.5
1	A	217	THR	7.4
1	A	193	SER	7.0
1	B	15	GLY	6.4
1	A	309	ARG	6.4
1	B	166	PHE	6.1
1	A	998	THR	6.0
1	B	239	GLY	6.0
1	A	241	ILE	6.0
1	B	242	TYR	5.9
1	A	413	ILE	5.7
1	B	998	THR	5.7
1	A	242	TYR	5.6
1	A	348	GLU	5.5
1	B	268	LEU	5.4
1	A	594	ASP	5.4
1	A	269	LEU	5.3
1	B	232	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	230	ARG	5.1
1	A	194	GLN	5.1
1	A	173	ASP	5.1
1	A	39	SER	5.0
1	B	195	LYS	4.9
1	A	633	ASP	4.8
1	B	160	LYS	4.8
1	A	526	GLU	4.8
1	B	272	ASP	4.8
1	A	220	MET	4.7
1	B	193	SER	4.7
1	A	748	ASN	4.7
1	A	160	LYS	4.6
1	A	166	PHE	4.6
1	A	999	VAL	4.6
1	B	185	VAL	4.4
1	B	172	GLU	4.4
1	B	173	ASP	4.4
1	B	269	LEU	4.4
1	A	518	TRP	4.3
1	A	175	TYR	4.3
1	A	170	PHE	4.2
1	B	939	ALA	4.2
1	B	140	ARG	4.2
1	B	640	SER	4.1
1	A	940	VAL	4.1
1	B	238	GLN	4.1
1	B	245	PRO	4.0
1	A	228	ILE	4.0
1	B	1063	TYR	4.0
1	A	236	ILE	4.0
1	B	233	PHE	4.0
1	A	623	ASP	4.0
1	A	174	ASP	4.0
1	A	238	GLN	3.9
1	A	232	ALA	3.9
1	B	443	GLU	3.9
1	A	214	ASN	3.8
1	B	229	ILE	3.8
1	B	217	THR	3.8
1	A	991	LYS	3.8
1	A	783	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	533	GLU	3.8
1	B	151	ILE	3.7
1	A	196	ARG	3.7
1	A	445	PHE	3.7
1	A	761	TRP	3.7
1	A	764	GLU	3.7
1	B	152	PHE	3.7
1	A	206	ASP	3.7
1	A	533	GLU	3.6
1	B	189	ARG	3.6
1	A	790	GLU	3.6
1	A	522	VAL	3.5
1	B	896	PRO	3.5
1	A	164	GLU	3.4
1	A	254	VAL	3.4
1	B	776	PHE	3.4
1	A	760	GLY	3.4
1	A	621	CYS	3.4
1	A	182	THR	3.4
1	A	643	ILE	3.4
1	A	634	GLU	3.4
1	A	219	LEU	3.4
1	A	233	PHE	3.4
1	A	271	ARG	3.3
1	A	195	LYS	3.3
1	A	979	PRO	3.3
1	A	744	PHE	3.3
1	A	224	ILE	3.3
1	B	940	VAL	3.3
1	B	133	LEU	3.2
1	B	273	LEU	3.2
1	A	747	SER	3.2
1	B	790	GLU	3.2
1	B	574	HIS	3.2
1	B	748	ASN	3.2
1	B	752	GLY	3.2
1	B	119	ARG	3.2
1	B	57	TYR	3.1
1	A	189	ARG	3.1
1	A	226	GLU	3.1
1	B	214	ASN	3.1
1	A	207	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	765	ARG	3.1
1	A	247	ASN	3.1
1	A	268	LEU	3.1
1	A	976	THR	3.1
1	B	976	THR	3.1
1	A	624	CYS	3.1
1	A	372	VAL	3.1
1	A	425	ARG	3.1
1	A	431	HIS	3.1
1	A	767	GLU	3.0
1	B	161	GLU	3.0
1	B	171	GLU	3.0
1	A	416	GLN	3.0
1	A	426	LYS	3.0
1	A	896	PRO	3.0
1	A	668	ASP	3.0
1	A	154	PHE	3.0
1	A	1063	TYR	3.0
1	A	140	ARG	3.0
1	B	981	PHE	3.0
1	A	201	PHE	2.9
1	B	602	HIS	2.9
1	A	763	VAL	2.9
1	A	644	ASP	2.9
1	B	267	PRO	2.9
1	A	310	ASP	2.9
1	A	38	PRO	2.9
1	A	172	GLU	2.9
1	B	946	ILE	2.8
1	A	769	TYR	2.8
1	B	154	PHE	2.8
1	A	988	ILE	2.8
1	B	206	ASP	2.8
1	A	641	LYS	2.8
1	A	109	PHE	2.8
1	B	417	GLU	2.8
1	A	880	PHE	2.7
1	B	445	PHE	2.7
1	A	267	PRO	2.7
1	B	210	LYS	2.7
1	B	244	ARG	2.7
1	A	332	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	346	ASN	2.7
1	B	775	ASP	2.7
1	A	975	LEU	2.7
1	B	990	GLU	2.7
1	A	574	HIS	2.7
1	A	163	LYS	2.7
1	B	742	LYS	2.7
1	B	194	GLN	2.7
1	A	352	VAL	2.7
1	A	805	GLU	2.7
1	A	981	PHE	2.7
1	B	170	PHE	2.7
1	A	517	ASN	2.7
1	A	781	LEU	2.6
1	B	163	LYS	2.6
1	A	291	VAL	2.6
1	B	942	VAL	2.6
1	B	39	SER	2.6
1	B	887	THR	2.6
1	B	441	VAL	2.6
1	A	305	LEU	2.6
1	A	534	ARG	2.6
1	A	128	PHE	2.6
1	A	161	GLU	2.6
1	A	625	GLY	2.6
1	A	282	VAL	2.6
1	A	1008	VAL	2.6
1	A	133	LEU	2.5
1	B	271	ARG	2.5
1	B	910	GLU	2.5
1	A	167	GLU	2.5
1	A	441	VAL	2.5
1	A	216	ASP	2.5
1	B	783	ASN	2.5
1	A	797	VAL	2.5
1	B	410	MET	2.5
1	A	176	HIS	2.5
1	A	775	ASP	2.5
1	B	886	SER	2.5
1	B	216	ASP	2.4
1	B	186	SER	2.4
1	B	779	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	190	GLU	2.4
1	A	152	PHE	2.4
1	B	753	ARG	2.4
1	A	59	GLU	2.4
1	A	423	GLU	2.4
1	A	229	ILE	2.4
1	A	355	ILE	2.4
1	B	996	LYS	2.4
1	A	410	MET	2.4
1	B	16	GLY	2.4
1	B	131	VAL	2.4
1	A	607	GLU	2.4
1	B	153	GLY	2.4
1	A	741	GLN	2.4
1	B	164	GLU	2.3
1	B	1067	GLU	2.3
1	A	350	PHE	2.3
1	B	424	LEU	2.3
1	B	611	PHE	2.3
1	A	255	VAL	2.3
1	B	999	VAL	2.3
1	A	768	GLU	2.3
1	B	758	VAL	2.3
1	B	639	SER	2.3
1	A	221	MET	2.3
1	B	518	TRP	2.3
1	B	731	TRP	2.3
1	B	778	LEU	2.3
1	B	446	ARG	2.3
1	A	15	GLY	2.3
1	A	185	VAL	2.3
1	B	177	ILE	2.3
1	B	878	ASP	2.3
1	A	202	VAL	2.3
1	A	55	ARG	2.2
1	A	982	GLU	2.2
1	A	435	LYS	2.2
1	B	413	ILE	2.2
1	A	186	SER	2.2
1	A	851	TYR	2.2
1	B	994	TYR	2.2
1	A	461	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1040	TYR	2.2
1	A	477	ASN	2.2
1	B	479	VAL	2.2
1	B	594	ASP	2.2
1	A	77	LYS	2.2
1	B	995	LYS	2.2
1	B	1008	VAL	2.2
1	B	230	ARG	2.2
1	B	633	ASP	2.2
1	B	947	VAL	2.2
1	A	645	ASP	2.2
1	B	167	GLU	2.1
1	A	197	PHE	2.1
1	A	864	GLN	2.1
1	A	245	PRO	2.1
1	B	13	ASN	2.1
1	B	991	LYS	2.1
1	A	341	SER	2.1
1	A	770	LYS	2.1
1	A	340	TRP	2.1
1	B	196	ARG	2.1
1	A	188	ASN	2.1
1	A	601	ILE	2.1
1	B	769	TYR	2.1
1	A	215	ILE	2.1
1	A	582	VAL	2.1
1	B	764	GLU	2.1
1	A	595	LEU	2.1
1	A	611	PHE	2.1
1	A	535	GLU	2.1
1	A	671	VAL	2.1
1	B	423	GLU	2.1
1	B	741	GLN	2.1
1	A	622	ARG	2.1
1	A	1019	PRO	2.1
1	B	141	LEU	2.1
1	B	156	SER	2.1
1	B	176	HIS	2.1
1	A	483	GLY	2.1
1	A	561	GLY	2.1
1	B	532	SER	2.1
1	B	599	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	300	LYS	2.1
1	B	793	ILE	2.1
1	B	262	PRO	2.1
1	A	443	GLU	2.1
1	B	235	THR	2.1
1	B	237	LYS	2.1
1	B	728	GLN	2.1
1	A	308	PHE	2.1
1	A	223	GLY	2.1
1	A	155	TYR	2.1
1	A	102	THR	2.0
1	A	235	THR	2.0
1	B	831	LEU	2.0
1	A	148	LYS	2.0
1	B	45	LEU	2.0
1	B	477	ASN	2.0
1	A	234	SER	2.0
1	A	750	SER	2.0
1	A	177	ILE	2.0
1	A	184	PHE	2.0
1	B	8	HIS	2.0
1	B	880	PHE	2.0
1	A	889	GLY	2.0
1	A	663	ILE	2.0
1	A	74	LYS	2.0
1	A	281	LEU	2.0
1	B	734	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	B	2002	1/1	0.98	0.09	-1.33	55,55,55,55	0
2	ZN	A	2002	1/1	0.97	0.12	-1.44	75,75,75,75	0
2	ZN	B	2001	1/1	0.90	0.08	-1.86	137,137,137,137	0
2	ZN	A	2001	1/1	0.79	0.06	-3.17	137,137,137,137	0

6.5 Other polymers (i)

There are no such residues in this entry.