



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:46 PM GMT

PDB ID : 4DDX  
Title : Thermotoga maritima reverse gyrase, primitive monoclinic form  
Authors : Rudolph, M.G.; Klostermeier, D.  
Deposited on : 2012-01-19  
Resolution : 4.17 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

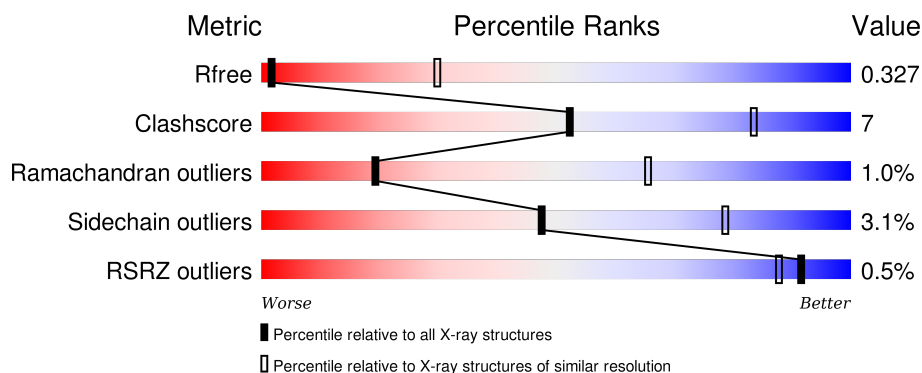
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.17 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	1030 (4.76-3.60)
Clashscore	102246	1130 (4.76-3.60)
Ramachandran outliers	100387	1076 (4.76-3.60)
Sidechain outliers	100360	1061 (4.76-3.60)
RSRZ outliers	91569	1034 (4.76-3.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1104	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>77%</span> <span>21%</span> </div> </div>
1	B	1104	<div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>77%</span> <span>21%</span> </div> </div>

## 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	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			

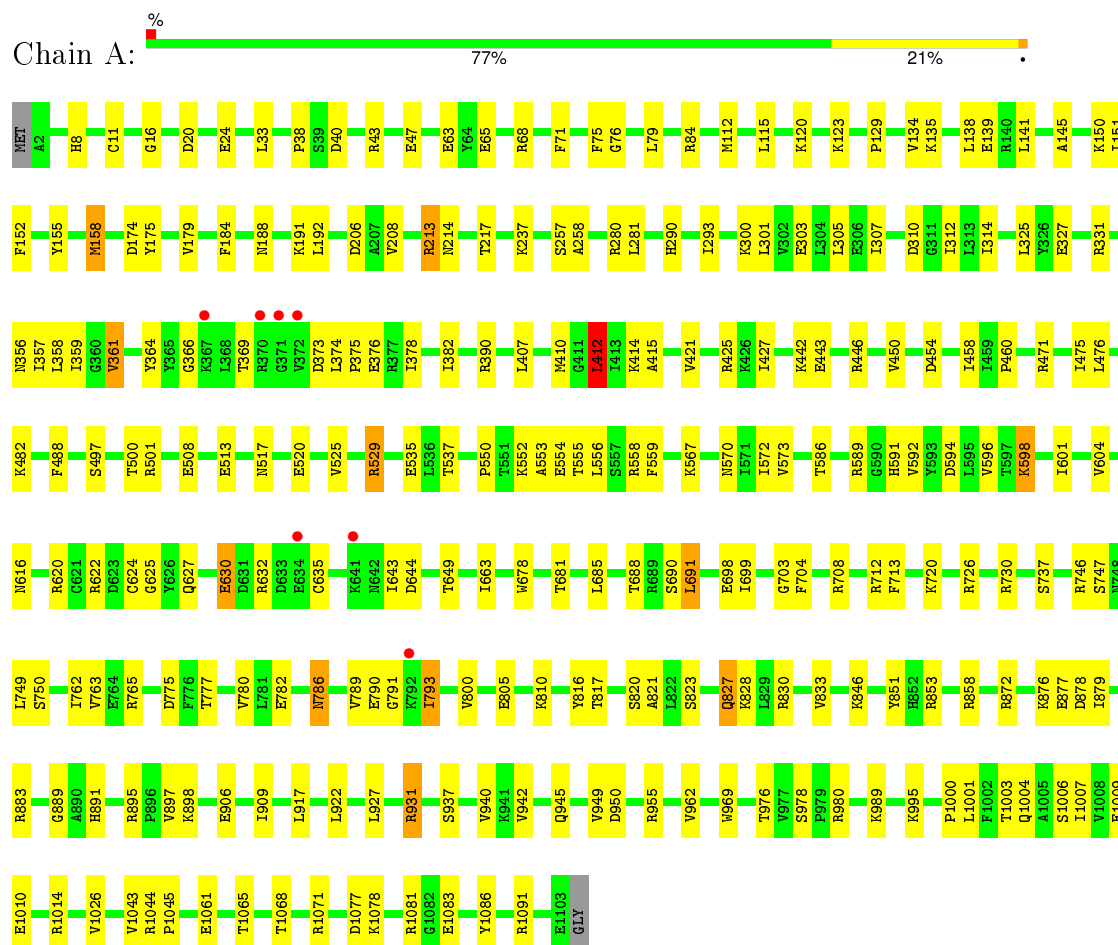
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

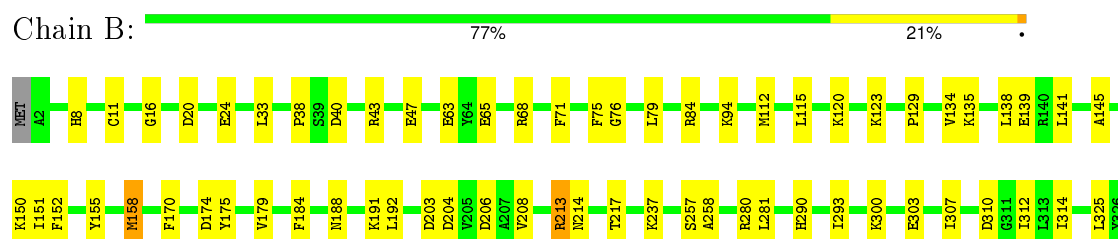
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.81Å 104.90Å 126.18Å 90.00° 91.72° 90.00°	Depositor
Resolution (Å)	48.43 – 4.17 48.43 – 4.17	Depositor EDS
% Data completeness (in resolution range)	96.8 (48.43-4.17) 87.1 (48.43-4.17)	Depositor EDS
$R_{merge}$	0.28	Depositor
$R_{sym}$	0.28	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 4.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_881)	Depositor
R, $R_{free}$	0.244 , 0.305 0.275 , 0.327	Depositor DCC
$R_{free}$ test set	1110 reflections (5.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	84.8	Xtriage
Anisotropy	0.684	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 95.6	EDS
Estimated twinning fraction	0.007 for l,k,-h 0.023 for h,-k,-l 0.239 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 23987 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	18064	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.21	0/9191	0.37	0/12356
1	B	0.21	0/9191	0.37	0/12356
All	All	0.21	0/18382	0.37	0/24712

There are no bond length outliers.

There are no bond angle outliers.

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	9186	122	0
1	B	9030	0	9186	124	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
All	All	18064	0	18372	244	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 7.

All (244) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:LEU:HA	1:B:410:MET:HB2	1.69	0.74
1:A:407:LEU:HA	1:A:410:MET:HB2	1.69	0.73
1:A:897:VAL:HG23	1:A:898:LYS:HG3	1.72	0.72
1:A:375:PRO:HG2	1:A:476:LEU:HD11	1.71	0.72
1:B:375:PRO:HG2	1:B:476:LEU:HD11	1.71	0.71
1:A:780:VAL:HA	1:A:786:ASN:HB3	1.72	0.71
1:B:620:ARG:HG3	1:B:627:GLN:HG2	1.74	0.70
1:B:780:VAL:HA	1:B:786:ASN:HB3	1.72	0.70
1:B:897:VAL:HG23	1:B:898:LYS:HG3	1.72	0.70
1:A:620:ARG:HG3	1:A:627:GLN:HG2	1.73	0.70
1:B:883:ARG:NH2	1:B:937:SER:O	2.25	0.69
1:A:883:ARG:NH2	1:A:937:SER:O	2.25	0.68
1:A:858:ARG:NH1	1:A:891:HIS:O	2.27	0.67
1:B:555:THR:HG21	1:B:846:LYS:HA	1.77	0.67
1:A:555:THR:HG21	1:A:846:LYS:HA	1.76	0.66
1:B:858:ARG:NH1	1:B:891:HIS:O	2.26	0.66
1:A:390:ARG:HG2	1:A:458:ILE:HG12	1.80	0.63
1:B:390:ARG:HG2	1:B:458:ILE:HG12	1.79	0.63
1:A:782:GLU:HA	1:A:989:LYS:HE3	1.80	0.63
1:B:782:GLU:HA	1:B:989:LYS:HE3	1.81	0.62
1:A:237:LYS:HG3	1:B:414:LYS:HE3	1.82	0.62
1:B:20:ASP:OD1	1:B:678:TRP:NE1	2.34	0.60
1:A:314:ILE:HB	1:A:359:ILE:HA	1.84	0.59
1:A:412:LEU:HD13	1:A:427:ILE:HG23	1.84	0.59
1:B:412:LEU:HD13	1:B:427:ILE:HG23	1.84	0.59
1:B:314:ILE:HB	1:B:359:ILE:HA	1.84	0.59
1:B:378:ILE:O	1:B:529:ARG:NH2	2.35	0.59
1:A:688:THR:HG22	1:A:690:SER:H	1.69	0.58
1:A:378:ILE:O	1:A:529:ARG:NH2	2.36	0.58
1:A:115:LEU:HD11	1:A:145:ALA:HB2	1.85	0.58
1:B:115:LEU:HD11	1:B:145:ALA:HB2	1.86	0.57
1:B:290:HIS:NE2	1:B:508:GLU:OE1	2.35	0.57
1:A:65:GLU:HG2	1:A:68:ARG:HH21	1.70	0.57
1:B:482:LYS:O	1:B:529:ARG:NH1	2.38	0.56
1:A:482:LYS:O	1:A:529:ARG:NH1	2.38	0.56
1:A:1061:GLU:O	1:A:1065:THR:OG1	2.22	0.56
1:B:63:GLU:OE2	1:B:120:LYS:NZ	2.38	0.56
1:B:65:GLU:HG2	1:B:68:ARG:HH21	1.70	0.56
1:B:688:THR:HG22	1:B:690:SER:H	1.69	0.56
1:A:63:GLU:OE2	1:A:120:LYS:NZ	2.38	0.56
1:B:443:GLU:O	1:B:446:ARG:NH1	2.39	0.55
1:B:663:ILE:HB	1:B:691:LEU:HG	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:ASP:OD1	1:B:356:ASN:ND2	2.38	0.55
1:A:663:ILE:HB	1:A:691:LEU:HG	1.88	0.55
1:B:1061:GLU:O	1:B:1065:THR:OG1	2.22	0.55
1:A:20:ASP:OD1	1:A:678:TRP:NE1	2.34	0.55
1:A:1001:LEU:HD11	1:A:1044:ARG:HE	1.71	0.55
1:B:762:ILE:HG22	1:B:1045:PRO:HD3	1.88	0.55
1:B:878:ASP:OD1	1:B:878:ASP:N	2.36	0.55
1:A:290:HIS:NE2	1:A:508:GLU:OE1	2.35	0.55
1:B:1001:LEU:HD11	1:B:1044:ARG:HE	1.71	0.55
1:A:443:GLU:O	1:A:446:ARG:NH1	2.39	0.54
1:A:817:THR:H	1:A:820:SER:HB2	1.72	0.54
1:B:817:THR:H	1:B:820:SER:HB2	1.73	0.54
1:A:762:ILE:HG22	1:A:1045:PRO:HD3	1.88	0.54
1:A:878:ASP:N	1:A:878:ASP:OD1	2.36	0.54
1:B:594:ASP:OD2	1:B:726:ARG:NH1	2.38	0.54
1:A:300:LYS:NZ	1:A:513:GLU:OE2	2.38	0.54
1:A:33:LEU:HD21	1:A:38:PRO:HG3	1.89	0.53
1:A:310:ASP:OD1	1:A:356:ASN:ND2	2.38	0.53
1:A:589:ARG:NH2	1:A:644:ASP:OD1	2.41	0.53
1:A:950:ASP:OD1	1:A:955:ARG:NE	2.42	0.53
1:B:33:LEU:HD21	1:B:38:PRO:HG3	1.89	0.53
1:A:553:ALA:HA	1:A:556:LEU:HB2	1.91	0.53
1:B:858:ARG:HH11	1:B:889:GLY:HA3	1.73	0.53
1:A:573:VAL:HA	1:A:586:THR:HB	1.91	0.53
1:B:421:VAL:HG12	1:B:425:ARG:HH21	1.74	0.52
1:A:555:THR:HG22	1:A:558:ARG:HH21	1.74	0.52
1:B:553:ALA:HA	1:B:556:LEU:HB2	1.90	0.52
1:B:555:THR:HG22	1:B:558:ARG:HH21	1.74	0.52
1:A:188:ASN:HB3	1:A:191:LYS:HD2	1.92	0.52
1:A:858:ARG:HH11	1:A:889:GLY:HA3	1.73	0.52
1:A:134:VAL:HG13	1:A:179:VAL:HG12	1.92	0.51
1:A:550:PRO:O	1:A:554:GLU:N	2.42	0.51
1:B:950:ASP:OD1	1:B:955:ARG:NE	2.42	0.51
1:A:421:VAL:HG12	1:A:425:ARG:HH21	1.74	0.51
1:B:460:PRO:HB2	1:B:501:ARG:HD2	1.92	0.51
1:A:765:ARG:HG3	1:A:1001:LEU:HD23	1.92	0.51
1:B:573:VAL:HA	1:B:586:THR:HB	1.91	0.50
1:B:188:ASN:HB3	1:B:191:LYS:HD2	1.93	0.50
1:B:596:VAL:HG22	1:B:616:ASN:HB2	1.92	0.50
1:B:1003:THR:H	1:B:1006:SER:HB2	1.76	0.50
1:B:213:ARG:O	1:B:217:THR:OG1	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:VAL:HG22	1:A:616:ASN:HB2	1.92	0.50
1:A:909:ILE:HD11	1:A:917:LEU:HD12	1.93	0.50
1:B:40:ASP:HB3	1:B:43:ARG:HB3	1.93	0.50
1:B:765:ARG:HG3	1:B:1001:LEU:HD23	1.92	0.50
1:B:909:ILE:HD11	1:B:917:LEU:HD12	1.92	0.50
1:A:1010:GLU:OE1	1:A:1014:ARG:NH1	2.44	0.50
1:A:460:PRO:HB2	1:A:501:ARG:HD2	1.93	0.50
1:B:134:VAL:HG13	1:B:179:VAL:HG12	1.92	0.50
1:B:184:PHE:HE2	1:B:192:LEU:HD21	1.76	0.50
1:B:366:GLY:HA2	1:B:471:ARG:HH22	1.77	0.50
1:A:800:VAL:HA	1:A:949:VAL:HG12	1.94	0.50
1:A:184:PHE:HE2	1:A:192:LEU:HD21	1.76	0.49
1:B:1010:GLU:OE1	1:B:1014:ARG:NH1	2.44	0.49
1:A:40:ASP:HB3	1:A:43:ARG:HB3	1.93	0.49
1:B:550:PRO:O	1:B:554:GLU:N	2.42	0.49
1:A:141:LEU:HB3	1:A:151:ILE:HD13	1.94	0.49
1:B:141:LEU:HB3	1:B:151:ILE:HD13	1.94	0.49
1:A:681:THR:HG22	1:A:691:LEU:HD22	1.94	0.49
1:A:1003:THR:H	1:A:1006:SER:HB2	1.76	0.49
1:A:366:GLY:HA2	1:A:471:ARG:HH22	1.77	0.49
1:B:589:ARG:NH2	1:B:644:ASP:OD1	2.42	0.49
1:B:746:ARG:HB2	1:B:749:LEU:HD11	1.94	0.49
1:A:314:ILE:HD13	1:A:382:ILE:HB	1.95	0.49
1:B:314:ILE:HD13	1:B:382:ILE:HB	1.95	0.49
1:A:594:ASP:OD2	1:A:726:ARG:NH1	2.37	0.49
1:B:79:LEU:HB2	1:B:84:ARG:HG3	1.95	0.49
1:A:293:ILE:HD12	1:A:488:PHE:CZ	2.48	0.48
1:B:800:VAL:HA	1:B:949:VAL:HG12	1.95	0.48
1:A:71:PHE:CD2	1:A:112:MET:HG2	2.48	0.48
1:A:777:THR:HG21	1:A:793:ILE:HG12	1.95	0.48
1:B:71:PHE:CD2	1:B:112:MET:HG2	2.49	0.48
1:A:79:LEU:HB2	1:A:84:ARG:HG3	1.95	0.48
1:B:777:THR:HG21	1:B:793:ILE:HG12	1.95	0.48
1:B:681:THR:HG22	1:B:691:LEU:HD22	1.95	0.48
1:B:517:ASN:HB3	1:B:520:GLU:HB3	1.95	0.48
1:A:213:ARG:O	1:A:217:THR:OG1	2.25	0.48
1:A:828:LYS:HD2	1:A:927:LEU:HD11	1.94	0.48
1:A:746:ARG:HB2	1:A:749:LEU:HD11	1.94	0.48
1:A:517:ASN:HB3	1:A:520:GLU:HB3	1.95	0.48
1:B:816:TYR:HB3	1:B:821:ALA:HB2	1.95	0.48
1:B:777:THR:HG22	1:B:791:GLY:HA2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:LYS:NZ	1:B:513:GLU:OE2	2.38	0.47
1:B:828:LYS:HD2	1:B:927:LEU:HD11	1.94	0.47
1:B:293:ILE:HD12	1:B:488:PHE:CZ	2.48	0.47
1:A:567:LYS:HG3	1:A:572:ILE:HG12	1.97	0.47
1:A:777:THR:HG22	1:A:791:GLY:HA2	1.96	0.47
1:B:805:GLU:HG2	1:B:945:GLN:HB3	1.97	0.47
1:A:208:VAL:O	1:A:214:ASN:ND2	2.44	0.47
1:A:816:TYR:HB3	1:A:821:ALA:HB2	1.96	0.47
1:B:135:LYS:O	1:B:139:GLU:N	2.44	0.47
1:B:567:LYS:HG3	1:B:572:ILE:HG12	1.97	0.47
1:B:823:SER:O	1:B:827:GLN:HB2	2.15	0.47
1:A:726:ARG:HH12	1:A:730:ARG:NH2	2.13	0.46
1:B:258:ALA:H	1:B:280:ARG:HA	1.80	0.46
1:A:823:SER:O	1:A:827:GLN:HB2	2.15	0.46
1:B:150:LYS:HB3	1:B:152:PHE:CE2	2.51	0.46
1:B:622:ARG:NH1	1:B:643:ILE:O	2.48	0.46
1:A:258:ALA:H	1:A:280:ARG:HA	1.80	0.46
1:B:720:LYS:HD3	1:B:1086:TYR:HB2	1.96	0.46
1:A:805:GLU:HG2	1:A:945:GLN:HB3	1.97	0.46
1:B:726:ARG:HH12	1:B:730:ARG:NH2	2.13	0.46
1:B:208:VAL:O	1:B:214:ASN:ND2	2.44	0.46
1:B:624:CYS:SG	1:B:625:GLY:N	2.89	0.46
1:B:737:SER:HB2	1:B:750:SER:HB3	1.97	0.45
1:B:369:THR:HG21	1:B:471:ARG:HH21	1.81	0.45
1:A:369:THR:HG21	1:A:471:ARG:HH21	1.81	0.45
1:A:737:SER:HB2	1:A:750:SER:HB3	1.98	0.45
1:B:906:GLU:HG2	1:B:922:LEU:HD13	1.99	0.45
1:A:150:LYS:HB3	1:A:152:PHE:CE2	2.51	0.45
1:A:622:ARG:NH1	1:A:643:ILE:O	2.48	0.45
1:B:876:LYS:O	1:B:879:ILE:HG12	2.16	0.45
1:A:720:LYS:HD3	1:A:1086:TYR:HB2	1.97	0.45
1:A:135:LYS:O	1:A:139:GLU:N	2.44	0.45
1:A:624:CYS:SG	1:A:625:GLY:N	2.89	0.45
1:B:816:TYR:CE1	1:B:931:ARG:HG3	2.52	0.45
1:A:906:GLU:HG2	1:A:922:LEU:HD13	1.98	0.45
1:B:1068:THR:HG22	1:B:1071:ARG:HH21	1.82	0.45
1:A:876:LYS:O	1:A:879:ILE:HG12	2.16	0.45
1:B:1078:LYS:HB3	1:B:1083:GLU:HB2	1.99	0.44
1:A:1068:THR:HG22	1:A:1071:ARG:HH21	1.82	0.44
1:A:816:TYR:CE1	1:A:931:ARG:HG3	2.52	0.44
1:B:257:SER:HB3	1:B:281:LEU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:GLU:HA	1:B:685:LEU:HD23	1.99	0.44
1:B:203:ASP:HB3	1:B:204:ASP:H	1.67	0.44
1:B:775:ASP:HA	1:B:995:LYS:HB3	2.00	0.44
1:B:816:TYR:CZ	1:B:931:ARG:HG3	2.53	0.44
1:B:833:VAL:HG21	1:B:1026:VAL:HB	2.00	0.44
1:B:303:GLU:O	1:B:307:ILE:HG12	2.18	0.44
1:B:698:GLU:HB2	1:B:703:GLY:HA3	2.00	0.44
1:A:872:ARG:HA	1:A:877:GLU:HB3	2.00	0.44
1:A:712:ARG:NH1	1:A:713:PHE:O	2.49	0.44
1:B:872:ARG:HA	1:B:877:GLU:HB3	2.00	0.43
1:A:24:GLU:HA	1:A:685:LEU:HD23	1.99	0.43
1:A:833:VAL:HG21	1:A:1026:VAL:HB	1.99	0.43
1:B:135:LYS:HE3	1:B:155:TYR:CZ	2.53	0.43
1:A:303:GLU:O	1:A:307:ILE:HG12	2.18	0.43
1:A:789:VAL:HG22	1:A:790:GLU:H	1.84	0.43
1:A:698:GLU:HB2	1:A:703:GLY:HA3	2.00	0.43
1:B:123:LYS:HD3	1:B:175:TYR:CE1	2.54	0.43
1:B:570:ASN:OD1	1:B:649:THR:OG1	2.37	0.43
1:A:816:TYR:CZ	1:A:931:ARG:HG3	2.53	0.43
1:A:775:ASP:HA	1:A:995:LYS:HB3	2.00	0.43
1:A:570:ASN:OD1	1:A:649:THR:OG1	2.37	0.43
1:A:1078:LYS:HB3	1:A:1083:GLU:HB2	1.99	0.43
1:B:789:VAL:HG22	1:B:790:GLU:H	1.84	0.43
1:A:135:LYS:HE3	1:A:155:TYR:CZ	2.54	0.43
1:A:257:SER:HB3	1:A:281:LEU:HB2	2.00	0.43
1:A:497:SER:O	1:A:500:THR:OG1	2.37	0.42
1:A:552:LYS:HE2	1:A:699:ILE:HD11	2.01	0.42
1:A:556:LEU:HA	1:A:559:PHE:CE2	2.54	0.42
1:A:414:LYS:HE3	1:B:237:LYS:HG3	2.00	0.42
1:A:685:LEU:HD12	1:A:685:LEU:HA	1.80	0.42
1:A:962:VAL:HG11	1:A:980:ARG:HG3	2.01	0.42
1:A:833:VAL:HG13	1:A:1004:GLN:HB3	2.02	0.42
1:A:123:LYS:HD3	1:A:175:TYR:CE1	2.54	0.42
1:B:552:LYS:HE2	1:B:699:ILE:HD11	2.02	0.42
1:B:556:LEU:HA	1:B:559:PHE:CE2	2.54	0.42
1:B:630:GLU:HG3	1:B:632:ARG:NH1	2.35	0.42
1:B:962:VAL:HG11	1:B:980:ARG:HG3	2.01	0.42
1:A:358:LEU:HD23	1:A:358:LEU:HA	1.89	0.42
1:B:497:SER:O	1:B:500:THR:OG1	2.37	0.42
1:B:704:PHE:CZ	1:B:708:ARG:HD2	2.55	0.42
1:A:312:ILE:HD12	1:A:357:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:PHE:CZ	1:A:708:ARG:HD2	2.55	0.42
1:A:11:CYS:HB3	1:A:16:GLY:H	1.85	0.41
1:B:482:LYS:HG2	1:B:525:VAL:HG22	2.02	0.41
1:A:374:LEU:HG	1:A:376:GLU:HG2	2.02	0.41
1:A:763:VAL:HA	1:A:1045:PRO:HG3	2.03	0.41
1:B:11:CYS:HB3	1:B:16:GLY:H	1.85	0.41
1:A:596:VAL:HG12	1:A:598:LYS:H	1.85	0.41
1:A:940:VAL:HG12	1:A:942:VAL:HG13	2.02	0.41
1:B:327:GLU:O	1:B:331:ARG:HG3	2.21	0.41
1:B:596:VAL:HG12	1:B:598:LYS:H	1.86	0.41
1:B:685:LEU:HD12	1:B:685:LEU:HA	1.81	0.41
1:A:630:GLU:HG3	1:A:632:ARG:NH1	2.35	0.41
1:B:312:ILE:HD12	1:B:357:ILE:HG12	2.01	0.41
1:B:851:TYR:CZ	1:B:853:ARG:HB2	2.56	0.41
1:A:1007:ILE:HD11	1:A:1043:VAL:HG11	2.03	0.41
1:A:482:LYS:HG2	1:A:525:VAL:HG22	2.02	0.41
1:B:155:TYR:CE1	1:B:158:MET:HA	2.56	0.41
1:A:155:TYR:CE1	1:A:158:MET:HA	2.56	0.41
1:B:833:VAL:HG13	1:B:1004:GLN:HB3	2.02	0.41
1:A:940:VAL:HG23	1:A:969:TRP:CD1	2.56	0.41
1:A:327:GLU:O	1:A:331:ARG:HG3	2.21	0.41
1:B:763:VAL:HA	1:B:1045:PRO:HG3	2.03	0.41
1:B:1018:ARG:O	1:B:1021:THR:N	2.51	0.41
1:B:601:ILE:HB	1:B:604:VAL:HB	2.02	0.41
1:B:170:PHE:HE1	1:B:191:LYS:HB3	1.86	0.41
1:B:712:ARG:NH1	1:B:713:PHE:O	2.50	0.41
1:B:1077:ASP:OD1	1:B:1081:ARG:NH2	2.54	0.41
1:B:537:THR:O	1:B:537:THR:OG1	2.39	0.41
1:A:1077:ASP:OD1	1:A:1081:ARG:NH2	2.54	0.41
1:A:851:TYR:CZ	1:A:853:ARG:HB2	2.56	0.40
1:A:601:ILE:HB	1:A:604:VAL:HB	2.02	0.40
1:B:374:LEU:HG	1:B:376:GLU:HG2	2.02	0.40
1:B:94:LYS:HD3	1:B:566:ARG:HH22	1.86	0.40
1:A:301:LEU:O	1:A:305:LEU:HG	2.21	0.40
1:B:593:TYR:HD1	1:B:679:ASP:HB3	1.86	0.40
1:B:414:LYS:O	1:B:416:GLN:N	2.54	0.40
1:B:501:ARG:HE	1:B:908:MET:HE1	1.86	0.40
1:A:442:LYS:HA	1:A:450:VAL:HG21	2.04	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%)	979 (89%)	110 (10%)	11 (1%)	19	65
1	B	1100/1104 (100%)	979 (89%)	110 (10%)	11 (1%)	19	65
All	All	2200/2208 (100%)	1958 (89%)	220 (10%)	22 (1%)	19	65

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	PRO
1	B	129	PRO
1	A	174	ASP
1	A	412	LEU
1	A	535	GLU
1	A	598	LYS
1	B	174	ASP
1	B	412	LEU
1	B	535	GLU
1	B	598	LYS
1	A	415	ALA
1	B	415	ALA
1	A	747	SER
1	B	747	SER
1	A	373	ASP
1	B	373	ASP
1	A	76	GLY
1	B	76	GLY
1	A	1000	PRO
1	B	1000	PRO
1	A	361	VAL
1	B	361	VAL

### 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%)	961 (97%)	31 (3%)	47	79
1	B	992/993 (100%)	961 (97%)	31 (3%)	47	79
All	All	1984/1986 (100%)	1922 (97%)	62 (3%)	47	79

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	47	GLU
1	A	75	PHE
1	A	138	LEU
1	A	158	MET
1	A	206	ASP
1	A	213	ARG
1	A	325	LEU
1	A	361	VAL
1	A	364	TYR
1	A	412	LEU
1	A	454	ASP
1	A	475	ILE
1	A	529	ARG
1	A	537	THR
1	A	591	HIS
1	A	592	VAL
1	A	630	GLU
1	A	635	CYS
1	A	691	LEU
1	A	786	ASN
1	A	793	ILE
1	A	810	LYS
1	A	827	GLN
1	A	830	ARG
1	A	895	ARG
1	A	931	ARG

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Mol	Chain	Res	Type
1	A	976	THR
1	A	978	SER
1	A	1009	GLU
1	A	1091	ARG
1	B	8	HIS
1	B	47	GLU
1	B	75	PHE
1	B	138	LEU
1	B	158	MET
1	B	206	ASP
1	B	213	ARG
1	B	325	LEU
1	B	361	VAL
1	B	364	TYR
1	B	412	LEU
1	B	454	ASP
1	B	475	ILE
1	B	529	ARG
1	B	537	THR
1	B	591	HIS
1	B	592	VAL
1	B	630	GLU
1	B	635	CYS
1	B	691	LEU
1	B	786	ASN
1	B	793	ILE
1	B	810	LYS
1	B	827	GLN
1	B	830	ARG
1	B	895	ARG
1	B	931	ARG
1	B	976	THR
1	B	978	SER
1	B	1009	GLU
1	B	1091	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	728	GLN
1	B	728	GLN



### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1102/1104 (99%)	-0.55	7 (0%) 90 86	23, 135, 216, 337	0
1	B	1102/1104 (99%)	-0.57	3 (0%) 94 92	41, 135, 210, 367	0
All	All	2204/2208 (99%)	-0.56	10 (0%) 91 88	23, 135, 212, 367	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	371	GLY	4.3
1	B	371	GLY	4.2
1	B	372	VAL	3.6
1	A	372	VAL	2.4
1	A	634	GLU	2.3
1	A	367	LYS	2.2
1	A	641	LYS	2.1
1	A	370	ARG	2.1
1	B	364	TYR	2.1
1	A	792	LYS	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

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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	ZN	A	1201	1/1	0.99	0.04	-1.94	203,203,203,203	0
2	ZN	A	1202	1/1	0.98	0.05	-2.14	125,125,125,125	0
2	ZN	B	1202	1/1	0.99	0.04	-2.21	101,101,101,101	0
2	ZN	B	1201	1/1	0.99	0.03	-2.86	189,189,189,189	0

## 6.5 Other polymers

There are no such residues in this entry.