



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:34 am BST

PDB ID : 2W9M
Title : Structure of family X DNA polymerase from *Deinococcus radiodurans*
Authors : Leulliot, N.; Cladiere, L.; Lecointe, F.; Durand, D.; Hubscher, U.; van Tilbeurgh, H.
Deposited on : 2009-01-27
Resolution : 2.46 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 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 : 2.11
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) : 2.11

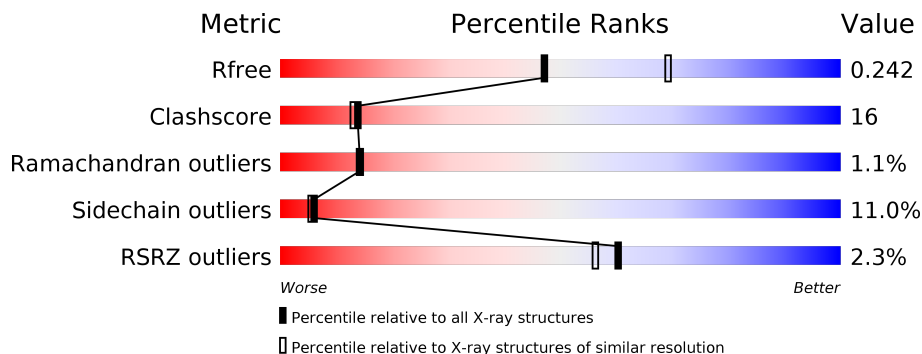
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 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	578	
1	B	578	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 8426 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 POLYMERASE X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	541	Total 4106	C 2571	N 753	O 777	S 5	0	0	0
1	B	559	Total 4234	C 2645	N 774	O 810	S 5	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	573	HIS	-	expression tag	UNP Q9RX48
A	574	HIS	-	expression tag	UNP Q9RX48
A	575	HIS	-	expression tag	UNP Q9RX48
A	576	HIS	-	expression tag	UNP Q9RX48
A	577	HIS	-	expression tag	UNP Q9RX48
A	578	HIS	-	expression tag	UNP Q9RX48
B	573	HIS	-	expression tag	UNP Q9RX48
B	574	HIS	-	expression tag	UNP Q9RX48
B	575	HIS	-	expression tag	UNP Q9RX48
B	576	HIS	-	expression tag	UNP Q9RX48
B	577	HIS	-	expression tag	UNP Q9RX48
B	578	HIS	-	expression tag	UNP Q9RX48

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total 3	Zn 3	0	0
2	A	4	Total 4	Zn 4	0	0

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Hg 1 1	0	0
3	A	1	Total Hg 1 1	0	0

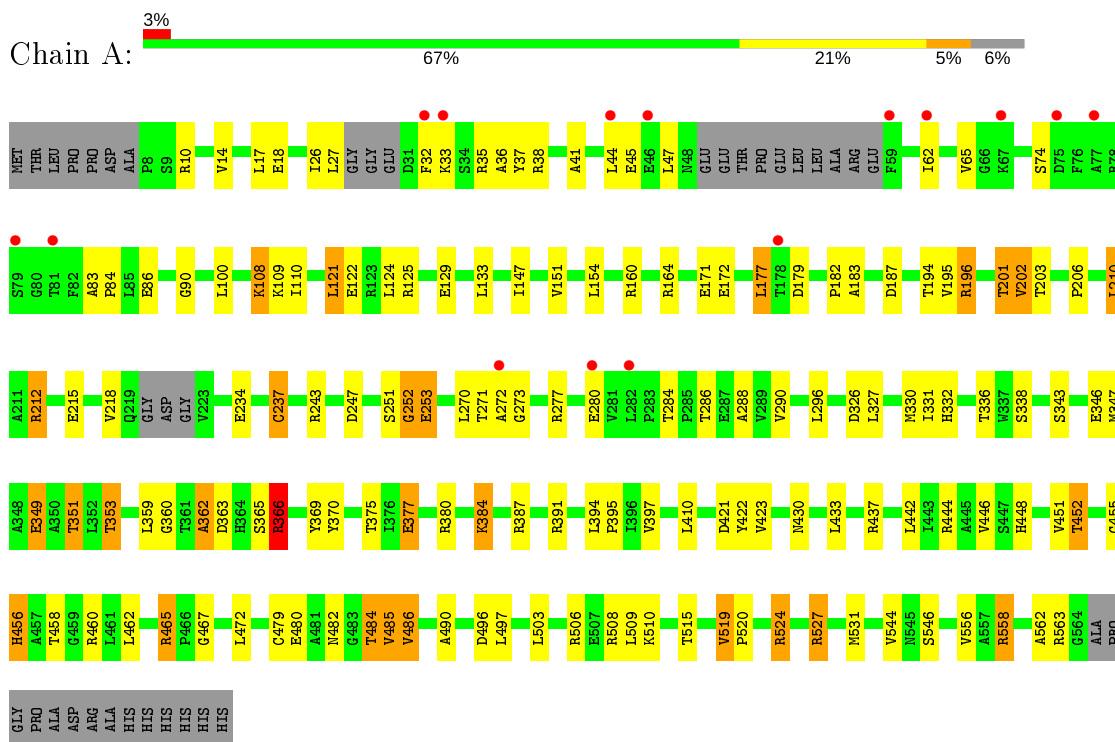
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	34	Total O 34 34	0	0
4	B	43	Total O 43 43	0	0

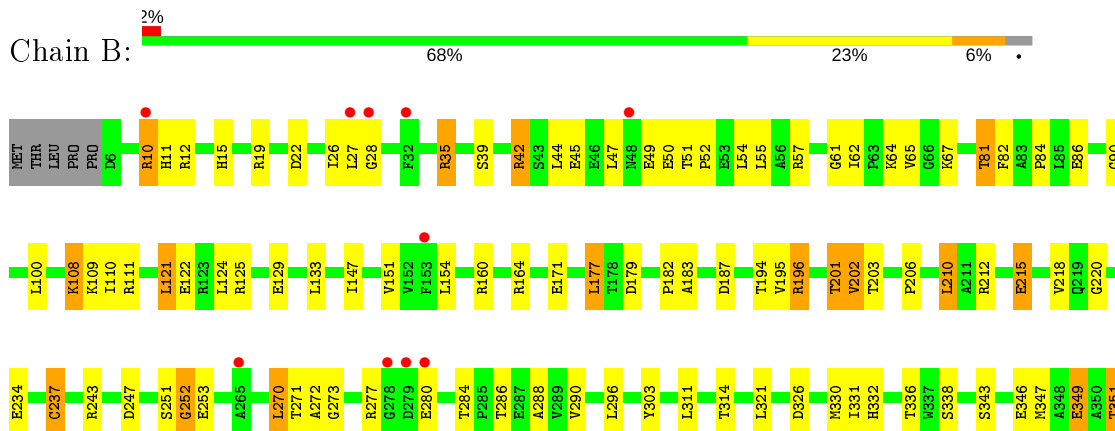
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: POLYMERASE X



- Molecule 1: POLYMERASE X





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.93Å 138.25Å 67.75Å 90.00° 92.25° 90.00°	Depositor
Resolution (Å)	45.32 – 2.46 48.37 – 2.46	Depositor EDS
% Data completeness (in resolution range)	94.2 (45.32-2.46) 95.2 (48.37-2.46)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.45Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.203 , 0.249 0.195 , 0.242	Depositor DCC
R_{free} test set	1866 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtrriage
Anisotropy	0.407	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.108 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8426	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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

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

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	0.24	0/4176	0.44	0/5666
1	B	0.24	0/4308	0.45	0/5850
All	All	0.24	0/8484	0.45	0/11516

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	4106	0	4105	114	0
1	B	4234	0	4216	151	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	34	0	0	1	0
4	B	43	0	0	1	0
All	All	8426	0	8321	264	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 16.

All (264) 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:10:ARG:HH21	1:B:11:HIS:CD2	1.76	1.03
1:B:10:ARG:HH11	1:B:47:LEU:HD11	1.26	1.00
1:B:391:ARG:HH11	1:B:391:ARG:HG3	1.28	0.99
1:B:39:SER:HA	1:B:42:ARG:HD3	1.44	0.97
1:A:391:ARG:HH11	1:A:391:ARG:HG3	1.28	0.96
1:A:271:THR:HG22	1:A:273:GLY:H	1.33	0.94
1:B:271:THR:HG22	1:B:273:GLY:H	1.33	0.93
1:B:10:ARG:HH21	1:B:11:HIS:HD2	0.97	0.89
1:B:42:ARG:HA	1:B:45:GLU:HB2	1.62	0.82
1:B:423:VAL:H	1:B:452:THR:CG2	1.93	0.81
1:B:57:ARG:HD3	1:B:61:GLY:H	1.45	0.81
1:A:423:VAL:H	1:A:452:THR:CG2	1.95	0.79
1:A:448:HIS:HB3	1:A:451:VAL:HG23	1.66	0.78
1:B:448:HIS:HB3	1:B:451:VAL:HG23	1.66	0.78
1:A:33:LYS:HB2	1:A:369:TYR:OH	1.85	0.76
1:B:10:ARG:NH2	1:B:11:HIS:HD2	1.80	0.76
1:A:44:LEU:HA	1:A:47:LEU:HD12	1.69	0.75
1:B:10:ARG:HG3	1:B:47:LEU:HD13	1.69	0.74
1:A:33:LYS:HA	1:A:36:ALA:HB3	1.70	0.74
1:A:160:ARG:HH11	1:A:194:THR:HG22	1.53	0.73
1:A:108:LYS:HZ3	1:A:108:LYS:H	1.35	0.73
1:B:391:ARG:HG3	1:B:391:ARG:NH1	1.99	0.73
1:B:160:ARG:HH11	1:B:194:THR:HG22	1.52	0.73
1:A:391:ARG:NH1	1:A:391:ARG:HG3	1.99	0.72
1:B:81:THR:HG23	1:B:86:GLU:HG3	1.71	0.71
1:B:203:THR:HG22	1:B:243:ARG:HE	1.55	0.71
1:B:10:ARG:NH1	1:B:47:LEU:HD11	2.03	0.71
1:B:108:LYS:H	1:B:108:LYS:HZ3	1.37	0.71
1:B:430:ASN:HB3	1:B:433:LEU:HD13	1.73	0.71
1:A:83:ALA:HB3	1:A:84:PRO:HD3	1.72	0.70
1:B:10:ARG:HG3	1:B:47:LEU:HD22	1.73	0.70
1:A:430:ASN:HB3	1:A:433:LEU:HD13	1.73	0.69
1:B:160:ARG:HD3	1:B:194:THR:CG2	2.23	0.69
1:B:218:VAL:HG12	1:B:220:GLY:H	1.59	0.68
1:B:39:SER:HA	1:B:42:ARG:CD	2.21	0.68
1:A:160:ARG:HD3	1:A:194:THR:CG2	2.24	0.68
1:B:10:ARG:HG3	1:B:47:LEU:CD1	2.24	0.67
1:B:160:ARG:HD3	1:B:194:THR:HG22	1.77	0.67
1:A:486:VAL:HG11	1:A:509:LEU:HD13	1.78	0.65
1:B:284:THR:O	1:B:284:THR:HG22	1.95	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:THR:O	1:A:284:THR:HG22	1.96	0.65
1:A:338:SER:HB2	1:A:363:ASP:HB3	1.78	0.65
1:B:338:SER:HB2	1:B:363:ASP:HB3	1.79	0.64
1:B:44:LEU:O	1:B:47:LEU:HB3	1.98	0.64
1:B:486:VAL:HG11	1:B:509:LEU:HD13	1.78	0.64
1:A:203:THR:HG22	1:A:243:ARG:HE	1.61	0.64
1:B:10:ARG:HG3	1:B:47:LEU:CD2	2.28	0.63
1:A:160:ARG:HD3	1:A:194:THR:HG22	1.78	0.62
1:B:42:ARG:HH12	1:B:64:LYS:HD2	1.64	0.62
1:B:349:GLU:O	1:B:353:THR:HG23	2.00	0.62
1:B:196:ARG:HH11	1:B:196:ARG:HB2	1.65	0.62
1:A:482:ASN:HB3	1:A:484:THR:HG22	1.83	0.61
1:A:62:ILE:HB	1:A:65:VAL:HG21	1.82	0.61
1:B:82:PHE:CE2	1:B:84:PRO:HG2	2.35	0.61
1:B:10:ARG:NH1	1:B:47:LEU:HD21	2.16	0.61
1:A:196:ARG:HB2	1:A:196:ARG:HH11	1.65	0.61
1:A:387:ARG:O	1:A:391:ARG:HG2	2.01	0.60
1:A:349:GLU:O	1:A:353:THR:HG23	2.01	0.60
1:B:527:ARG:O	1:B:531:MET:HG3	2.02	0.60
1:B:482:ASN:HB3	1:B:484:THR:HG22	1.84	0.60
1:A:527:ARG:O	1:A:531:MET:HG3	2.02	0.59
1:B:387:ARG:O	1:B:391:ARG:HG2	2.02	0.59
1:B:347:MET:O	1:B:351:THR:HG23	2.02	0.59
1:A:183:ALA:HB3	1:A:201:THR:HG22	1.86	0.58
1:B:54:LEU:CD2	1:B:57:ARG:HH12	2.16	0.58
1:B:203:THR:HG22	1:B:243:ARG:NE	2.19	0.58
1:A:286:THR:HG22	1:A:288:ALA:H	1.68	0.58
1:B:183:ALA:HB3	1:B:201:THR:HG22	1.85	0.58
1:A:347:MET:O	1:A:351:THR:HG23	2.03	0.58
1:B:160:ARG:HB3	1:B:194:THR:HG23	1.86	0.58
1:B:10:ARG:HE	1:B:11:HIS:HB2	1.69	0.58
1:B:26:ILE:O	1:B:111:ARG:HD2	2.04	0.57
1:A:160:ARG:HB3	1:A:194:THR:HG23	1.85	0.57
1:B:62:ILE:HB	1:B:65:VAL:HG22	1.87	0.57
1:A:422:TYR:HB2	1:A:452:THR:HG21	1.87	0.56
1:B:277:ARG:HB3	1:B:280:GLU:HB2	1.87	0.56
1:B:286:THR:HG22	1:B:288:ALA:H	1.69	0.56
1:A:479:CYS:HA	1:A:484:THR:HG23	1.87	0.56
1:B:422:TYR:HB2	1:B:452:THR:HG21	1.87	0.56
1:A:65:VAL:HG23	1:A:65:VAL:O	2.05	0.56
1:A:253:GLU:OE2	1:B:437:ARG:HD3	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:ASP:HA	1:B:497:LEU:C	2.26	0.55
1:B:479:CYS:HA	1:B:484:THR:HG23	1.87	0.55
1:A:503:LEU:O	1:A:506:ARG:HG2	2.06	0.55
1:A:108:LYS:N	1:A:108:LYS:HD2	2.22	0.55
1:A:277:ARG:HB3	1:A:280:GLU:HB2	1.87	0.55
1:B:187:ASP:HB3	1:B:195:VAL:HG22	1.89	0.55
1:B:62:ILE:HB	1:B:65:VAL:CG2	2.37	0.55
1:A:203:THR:HG22	1:A:243:ARG:NE	2.22	0.55
1:B:108:LYS:HD2	1:B:108:LYS:N	2.23	0.54
1:A:62:ILE:HB	1:A:65:VAL:CG2	2.37	0.54
1:B:448:HIS:HB3	1:B:451:VAL:CG2	2.37	0.54
1:A:187:ASP:HB3	1:A:195:VAL:HG22	1.90	0.54
1:B:503:LEU:O	1:B:506:ARG:HG2	2.07	0.54
1:A:206:PRO:O	1:A:210:LEU:HB2	2.08	0.54
1:B:90:GLY:HA2	1:B:465:ARG:HH22	1.73	0.54
1:A:202:VAL:O	1:A:237:CYS:HA	2.08	0.53
1:B:510:LYS:HB3	1:B:510:LYS:HZ2	1.74	0.53
1:A:510:LYS:HZ2	1:A:544:VAL:HG13	1.73	0.53
1:A:496:ASP:HA	1:A:497:LEU:C	2.29	0.53
1:A:448:HIS:HB3	1:A:451:VAL:CG2	2.37	0.53
1:A:510:LYS:HZ2	1:A:510:LYS:HB3	1.74	0.52
1:B:510:LYS:HZ2	1:B:544:VAL:HG13	1.74	0.52
1:B:206:PRO:O	1:B:210:LEU:HB2	2.09	0.52
1:A:377:GLU:H	1:A:377:GLU:CD	2.12	0.52
1:A:343:SER:OG	1:A:346:GLU:HG3	2.10	0.52
1:A:160:ARG:HB3	1:A:194:THR:CG2	2.39	0.52
1:A:122:GLU:HG2	1:A:164:ARG:HG2	1.92	0.52
1:B:39:SER:HB2	1:B:42:ARG:CZ	2.40	0.51
1:B:423:VAL:O	1:B:452:THR:HG23	2.10	0.51
1:A:90:GLY:HA2	1:A:465:ARG:HH22	1.74	0.51
1:B:391:ARG:CG	1:B:391:ARG:NH1	2.73	0.51
1:B:39:SER:CA	1:B:42:ARG:HD3	2.30	0.51
1:A:203:THR:N	1:A:243:ARG:HH21	2.09	0.51
1:B:446:VAL:O	1:B:484:THR:HG21	2.11	0.51
1:B:202:VAL:O	1:B:237:CYS:HA	2.11	0.51
1:B:338:SER:HB2	1:B:363:ASP:CB	2.41	0.50
1:B:51:THR:HB	1:B:52:PRO:HD3	1.94	0.50
1:B:65:VAL:O	1:B:65:VAL:HG23	2.10	0.50
1:B:122:GLU:HG2	1:B:164:ARG:HG2	1.93	0.50
1:B:54:LEU:HD23	1:B:57:ARG:HH12	1.75	0.50
1:A:187:ASP:CB	1:A:195:VAL:HG22	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:VAL:O	1:A:452:THR:HG23	2.12	0.50
1:A:84:PRO:HB3	1:A:370:TYR:OH	2.11	0.50
1:B:187:ASP:CB	1:B:195:VAL:HG22	2.41	0.50
1:B:452:THR:O	1:B:485:VAL:HG13	2.12	0.50
1:B:519:VAL:HG13	1:B:520:PRO:HD2	1.93	0.50
1:A:338:SER:HB2	1:A:363:ASP:CB	2.41	0.50
1:A:35:ARG:HG2	1:A:38:ARG:HH12	1.77	0.50
1:B:377:GLU:H	1:B:377:GLU:CD	2.14	0.50
1:B:343:SER:OG	1:B:346:GLU:HG3	2.11	0.49
1:A:452:THR:O	1:A:485:VAL:HG13	2.12	0.49
1:A:446:VAL:O	1:A:484:THR:HG21	2.11	0.49
1:B:86:GLU:HA	1:B:86:GLU:OE1	2.13	0.49
1:A:524:ARG:HB3	1:A:524:ARG:HH11	1.77	0.49
1:B:160:ARG:HB3	1:B:194:THR:CG2	2.41	0.49
1:B:510:LYS:HB3	1:B:510:LYS:NZ	2.28	0.49
1:A:86:GLU:OE1	1:A:86:GLU:HA	2.12	0.49
1:B:100:LEU:HD23	1:B:110:ILE:HD12	1.95	0.49
1:A:332:HIS:HA	1:A:362:ALA:HB3	1.94	0.49
1:B:380:ARG:HB3	1:B:380:ARG:NH1	2.28	0.49
1:A:100:LEU:HD23	1:A:110:ILE:HD12	1.94	0.48
1:A:380:ARG:NH1	1:A:380:ARG:HB3	2.28	0.48
1:B:26:ILE:HG22	1:B:27:LEU:HG	1.95	0.48
1:B:15:HIS:HB3	1:B:19:ARG:HH22	1.78	0.48
1:B:332:HIS:HA	1:B:362:ALA:HB3	1.96	0.48
1:B:338:SER:HB2	1:B:363:ASP:OD1	2.13	0.48
1:A:519:VAL:HG13	1:A:520:PRO:HD2	1.96	0.48
1:B:10:ARG:CG	1:B:47:LEU:HD22	2.40	0.48
1:A:330:MET:CE	1:A:330:MET:HA	2.43	0.48
1:B:330:MET:HA	1:B:330:MET:CE	2.43	0.48
1:B:458:THR:CG2	1:B:467:GLY:HA3	2.44	0.48
1:B:524:ARG:HB3	1:B:524:ARG:HH11	1.78	0.48
1:B:378:ARG:HD3	4:B:2025:HOH:O	2.13	0.47
1:A:351:THR:HG21	1:A:359:LEU:HD13	1.95	0.47
1:A:108:LYS:HD2	1:A:108:LYS:H	1.79	0.47
1:B:203:THR:N	1:B:243:ARG:HH21	2.11	0.47
1:A:458:THR:CG2	1:A:467:GLY:HA3	2.45	0.47
1:B:203:THR:HG23	1:B:243:ARG:NH2	2.29	0.47
1:B:203:THR:HG23	1:B:243:ARG:HH21	1.80	0.47
1:A:510:LYS:NZ	1:A:510:LYS:HB3	2.29	0.46
1:A:26:ILE:HG22	1:A:27:LEU:HD23	1.98	0.46
1:B:351:THR:HG21	1:B:359:LEU:HD13	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:LYS:H	1:B:108:LYS:NZ	2.10	0.46
1:B:455:GLY:O	1:B:456:HIS:C	2.54	0.46
1:A:442:LEU:O	1:A:446:VAL:HG22	2.16	0.46
1:B:108:LYS:HD2	1:B:109:LYS:H	1.81	0.46
1:A:196:ARG:NH2	1:A:234:GLU:OE2	2.49	0.45
1:A:496:ASP:OD2	1:A:497:LEU:HA	2.16	0.45
1:B:215:GLU:HG3	1:B:215:GLU:H	1.47	0.45
1:B:243:ARG:HD2	1:B:247:ASP:OD1	2.17	0.45
1:A:455:GLY:O	1:A:456:HIS:C	2.55	0.45
1:B:384:LYS:HD3	1:B:384:LYS:N	2.31	0.45
1:B:496:ASP:OD2	1:B:497:LEU:HA	2.16	0.45
1:A:243:ARG:HD2	1:A:247:ASP:OD1	2.16	0.45
1:A:203:THR:HG23	1:A:243:ARG:NH2	2.32	0.45
1:B:196:ARG:NH2	1:B:234:GLU:OE2	2.50	0.45
1:A:384:LYS:HD3	1:A:384:LYS:N	2.31	0.45
1:B:108:LYS:H	1:B:108:LYS:HD2	1.81	0.45
1:B:22:ASP:O	1:B:26:ILE:HG13	2.16	0.45
1:A:251:SER:N	1:A:252:GLY:CA	2.80	0.45
1:B:331:ILE:HA	1:B:360:GLY:HA3	1.99	0.45
1:B:251:SER:N	1:B:252:GLY:CA	2.80	0.44
1:B:50:GLU:HG3	1:B:51:THR:N	2.31	0.44
1:A:391:ARG:NH1	1:A:391:ARG:CG	2.73	0.44
1:A:338:SER:HB2	1:A:363:ASP:OD1	2.17	0.44
1:B:122:GLU:OE1	1:B:125:ARG:NH1	2.50	0.44
1:A:397:VAL:HG13	1:A:421:ASP:HB2	1.99	0.44
1:B:90:GLY:HA2	1:B:465:ARG:NH2	2.32	0.44
1:A:108:LYS:HD2	1:A:109:LYS:H	1.82	0.44
1:A:331:ILE:HA	1:A:360:GLY:HA3	1.99	0.44
1:B:147:ILE:O	1:B:151:VAL:HG23	2.18	0.44
1:A:18:GLU:HG3	1:A:41:ALA:HB1	1.99	0.44
1:B:15:HIS:HB3	1:B:19:ARG:NH2	2.33	0.44
1:B:203:THR:CG2	1:B:243:ARG:HE	2.27	0.43
1:A:202:VAL:HA	1:A:243:ARG:NH2	2.33	0.43
1:B:177:LEU:O	1:B:182:PRO:HG3	2.18	0.43
1:B:45:GLU:HA	1:B:45:GLU:OE2	2.18	0.43
1:A:397:VAL:HG13	1:A:421:ASP:CB	2.49	0.43
1:A:271:THR:CG2	1:A:272:ALA:N	2.82	0.43
1:A:147:ILE:O	1:A:151:VAL:HG23	2.18	0.43
1:B:397:VAL:HG13	1:B:421:ASP:CB	2.49	0.43
1:A:212:ARG:NH1	4:A:2014:HOH:O	2.51	0.43
1:A:482:ASN:OD1	1:A:563:ARG:HD2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:GLU:HB2	1:B:54:LEU:HD21	2.01	0.43
1:B:558:ARG:HH11	1:B:562:ALA:HB2	1.84	0.43
1:B:423:VAL:H	1:B:452:THR:HG22	1.82	0.42
1:B:54:LEU:HD22	1:B:57:ARG:HH12	1.84	0.42
1:A:271:THR:HG22	1:A:272:ALA:N	2.34	0.42
1:A:122:GLU:OE1	1:A:125:ARG:NH1	2.53	0.42
1:B:57:ARG:HD3	1:B:61:GLY:N	2.24	0.42
1:B:365:SER:O	1:B:366:ARG:C	2.58	0.42
1:B:187:ASP:OD2	1:B:196:ARG:HG2	2.20	0.42
1:A:203:THR:CG2	1:A:243:ARG:HE	2.31	0.42
1:A:33:LYS:O	1:A:37:TYR:HD1	2.02	0.42
1:B:271:THR:CG2	1:B:272:ALA:N	2.83	0.42
1:B:284:THR:HG23	1:B:290:VAL:CG2	2.50	0.42
1:A:201:THR:HG21	1:A:247:ASP:OD1	2.19	0.42
1:A:284:THR:HG23	1:A:290:VAL:CG2	2.50	0.42
1:B:326:ASP:O	1:B:546:SER:HA	2.20	0.42
1:B:39:SER:HB2	1:B:42:ARG:NH1	2.34	0.42
1:A:187:ASP:OD2	1:A:196:ARG:HG2	2.21	0.41
1:B:394:LEU:HA	1:B:395:PRO:HD3	1.78	0.41
1:B:397:VAL:HG13	1:B:421:ASP:HB2	2.02	0.41
1:A:10:ARG:O	1:A:14:VAL:HG23	2.20	0.41
1:A:394:LEU:HA	1:A:395:PRO:HD3	1.79	0.41
1:A:490:ALA:HB3	1:A:515:THR:HA	2.01	0.41
1:B:201:THR:HG21	1:B:247:ASP:OD1	2.20	0.41
1:B:210:LEU:HD12	1:B:210:LEU:HA	1.77	0.41
1:B:203:THR:CG2	1:B:243:ARG:NE	2.83	0.41
1:B:482:ASN:OD1	1:B:563:ARG:HD2	2.19	0.41
1:A:160:ARG:HD3	1:A:194:THR:HG21	2.02	0.41
1:A:366:ARG:HE	1:A:375:THR:HG22	1.85	0.41
1:B:311:LEU:O	1:B:314:THR:HB	2.20	0.41
1:B:528:TYR:O	1:B:532:GLN:HG2	2.21	0.41
1:A:26:ILE:CD1	1:A:100:LEU:HD21	2.50	0.41
1:A:365:SER:O	1:A:366:ARG:C	2.59	0.41
1:B:108:LYS:HB3	1:B:108:LYS:HZ2	1.85	0.41
1:A:108:LYS:NZ	1:A:108:LYS:H	2.11	0.41
1:A:326:ASP:O	1:A:546:SER:HA	2.20	0.41
1:B:284:THR:HG23	1:B:290:VAL:HG23	2.03	0.41
1:B:284:THR:O	1:B:284:THR:CG2	2.67	0.41
1:B:303:TYR:OH	1:B:321:LEU:HD11	2.20	0.41
1:B:338:SER:HB2	1:B:363:ASP:CG	2.41	0.41
1:A:203:THR:HG23	1:A:243:ARG:HH21	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LEU:HA	1:B:121:LEU:HD12	1.78	0.41
1:B:202:VAL:HA	1:B:243:ARG:NH2	2.35	0.41
1:B:65:VAL:O	1:B:65:VAL:CG2	2.68	0.41
1:B:271:THR:HG22	1:B:272:ALA:N	2.35	0.41
1:A:121:LEU:HA	1:A:121:LEU:HD12	1.77	0.41
1:A:177:LEU:O	1:A:182:PRO:HG3	2.20	0.41
1:A:284:THR:HG23	1:A:290:VAL:HG23	2.03	0.41
1:B:490:ALA:HB3	1:B:515:THR:HA	2.03	0.41
1:B:539:THR:HB	1:B:540:PRO:HD2	2.02	0.41
1:A:17:LEU:HD12	1:A:44:LEU:HD12	2.02	0.40
1:A:558:ARG:HH11	1:A:562:ALA:HB2	1.86	0.40
1:A:18:GLU:HG3	1:A:41:ALA:CB	2.52	0.40
1:A:480:GLU:OE2	1:A:508:ARG:HD2	2.21	0.40
1:A:125:ARG:NH2	1:A:172:GLU:OE2	2.54	0.40
1:B:35:ARG:O	1:B:39:SER:HB3	2.21	0.40
1:B:10:ARG:HE	1:B:11:HIS:CB	2.32	0.40
1:B:270:LEU:HA	1:B:270:LEU:HD23	1.92	0.40
1:B:330:MET:HA	1:B:330:MET:HE2	2.04	0.40
1:B:442:LEU:O	1:B:446:VAL:HG22	2.22	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	533/578 (92%)	509 (96%)	18 (3%)	6 (1%)	14 14
1	B	557/578 (96%)	538 (97%)	13 (2%)	6 (1%)	14 14
All	All	1090/1156 (94%)	1047 (96%)	31 (3%)	12 (1%)	14 14

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	366	ARG
1	B	366	ARG
1	A	253	GLU
1	A	456	HIS
1	B	456	HIS
1	B	253	GLU
1	A	45	GLU
1	B	28	GLY
1	A	362	ALA
1	B	362	ALA
1	A	252	GLY
1	B	252	GLY

5.3.2 Protein sidechains [i](#)

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	415/442 (94%)	370 (89%)	45 (11%)	6 6
1	B	427/442 (97%)	379 (89%)	48 (11%)	6 5
All	All	842/884 (95%)	749 (89%)	93 (11%)	6 5

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	PHE
1	A	74	SER
1	A	108	LYS
1	A	121	LEU
1	A	124	LEU
1	A	129	GLU
1	A	133	LEU
1	A	154	LEU
1	A	171	GLU
1	A	177	LEU
1	A	179	ASP
1	A	196	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	201	THR
1	A	202	VAL
1	A	210	LEU
1	A	212	ARG
1	A	215	GLU
1	A	218	VAL
1	A	237	CYS
1	A	270	LEU
1	A	296	LEU
1	A	327	LEU
1	A	336	THR
1	A	349	GLU
1	A	351	THR
1	A	353	THR
1	A	366	ARG
1	A	377	GLU
1	A	384	LYS
1	A	410	LEU
1	A	437	ARG
1	A	444	ARG
1	A	452	THR
1	A	460	ARG
1	A	462	LEU
1	A	465	ARG
1	A	472	LEU
1	A	484	THR
1	A	485	VAL
1	A	486	VAL
1	A	519	VAL
1	A	524	ARG
1	A	527	ARG
1	A	556	VAL
1	A	558	ARG
1	B	10	ARG
1	B	12	ARG
1	B	35	ARG
1	B	42	ARG
1	B	55	LEU
1	B	67	LYS
1	B	81	THR
1	B	108	LYS
1	B	121	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	124	LEU
1	B	129	GLU
1	B	133	LEU
1	B	154	LEU
1	B	171	GLU
1	B	177	LEU
1	B	179	ASP
1	B	196	ARG
1	B	201	THR
1	B	202	VAL
1	B	210	LEU
1	B	212	ARG
1	B	215	GLU
1	B	237	CYS
1	B	270	LEU
1	B	296	LEU
1	B	336	THR
1	B	349	GLU
1	B	351	THR
1	B	353	THR
1	B	366	ARG
1	B	377	GLU
1	B	384	LYS
1	B	410	LEU
1	B	437	ARG
1	B	444	ARG
1	B	452	THR
1	B	460	ARG
1	B	462	LEU
1	B	465	ARG
1	B	472	LEU
1	B	484	THR
1	B	485	VAL
1	B	486	VAL
1	B	519	VAL
1	B	524	ARG
1	B	527	ARG
1	B	556	VAL
1	B	558	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	GLN
1	B	11	HIS
1	B	219	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 9 ligands modelled in this entry, 9 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, 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	541/578 (93%)	-0.02	15 (2%) 53 49	20, 37, 77, 105	0
1	B	559/578 (96%)	-0.01	10 (1%) 68 65	19, 36, 65, 97	0
All	All	1100/1156 (95%)	-0.02	25 (2%) 60 56	19, 37, 72, 105	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	265	ALA	5.5
1	B	48	ASN	3.8
1	B	280	GLU	3.7
1	A	32	PHE	3.7
1	B	27	LEU	3.4
1	B	278	GLY	3.3
1	A	280	GLU	3.3
1	B	279	ASP	3.0
1	A	62	ILE	2.9
1	A	272	ALA	2.8
1	A	33	LYS	2.8
1	B	28	GLY	2.8
1	A	77	ALA	2.8
1	B	32	PHE	2.8
1	A	79	SER	2.6
1	A	67	LYS	2.5
1	A	81	THR	2.5
1	A	75	ASP	2.3
1	A	44	LEU	2.3
1	A	46	GLU	2.2
1	A	59	PHE	2.1
1	A	178	THR	2.1
1	A	282	LEU	2.1
1	B	153	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	10	ARG	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. 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(\AA^2)	Q<0.9
2	ZN	A	1569	1/1	0.89	0.22	112,112,112,112	0
3	HG	B	1568	1/1	0.98	0.10	74,74,74,74	1
2	ZN	A	1567	1/1	0.98	0.05	27,27,27,27	0
2	ZN	A	1565	1/1	0.99	0.03	34,34,34,34	0
2	ZN	B	1565	1/1	0.99	0.03	28,28,28,28	0
2	ZN	A	1566	1/1	0.99	0.05	24,24,24,24	0
2	ZN	B	1566	1/1	0.99	0.05	25,25,25,25	0
2	ZN	B	1567	1/1	0.99	0.05	32,32,32,32	0
3	HG	A	1568	1/1	0.99	0.10	88,88,88,88	1

6.5 Other polymers [i](#)

There are no such residues in this entry.