Full wwPDB X-ray Structure Validation Report (i)

Dec 5, 2016 – 09:16 PM EST

PDB ID	:	5MDN
Title	:	Structure of the family B DNA polymerase from the hyperthermophilic archaeon Pyrobaculum calidifontis
Authors	:	Guo, J.; Zhang, W.; Coker, A.R.; Wood, S.P.; Cooper, J.B.; Rashid, N.; Akhtar, M.
Deposited on	:	2016-11-12
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
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:

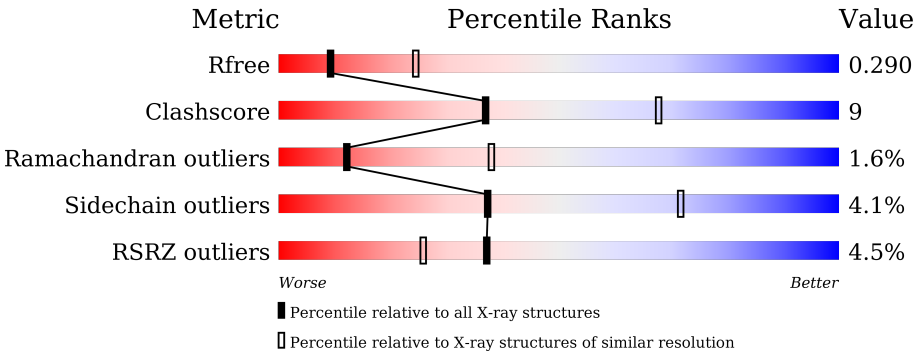
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	783	6% 73% 23%
1	B	783	2% 76% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	801	-	-	-	X
2	MG	B	801	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12315 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 DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	761	Total	C	N	O	S	0	0	0
			6130	3954	1054	1104	18			
1	B	761	Total	C	N	O	S	0	0	0
			6130	3954	1054	1104	18			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is water.

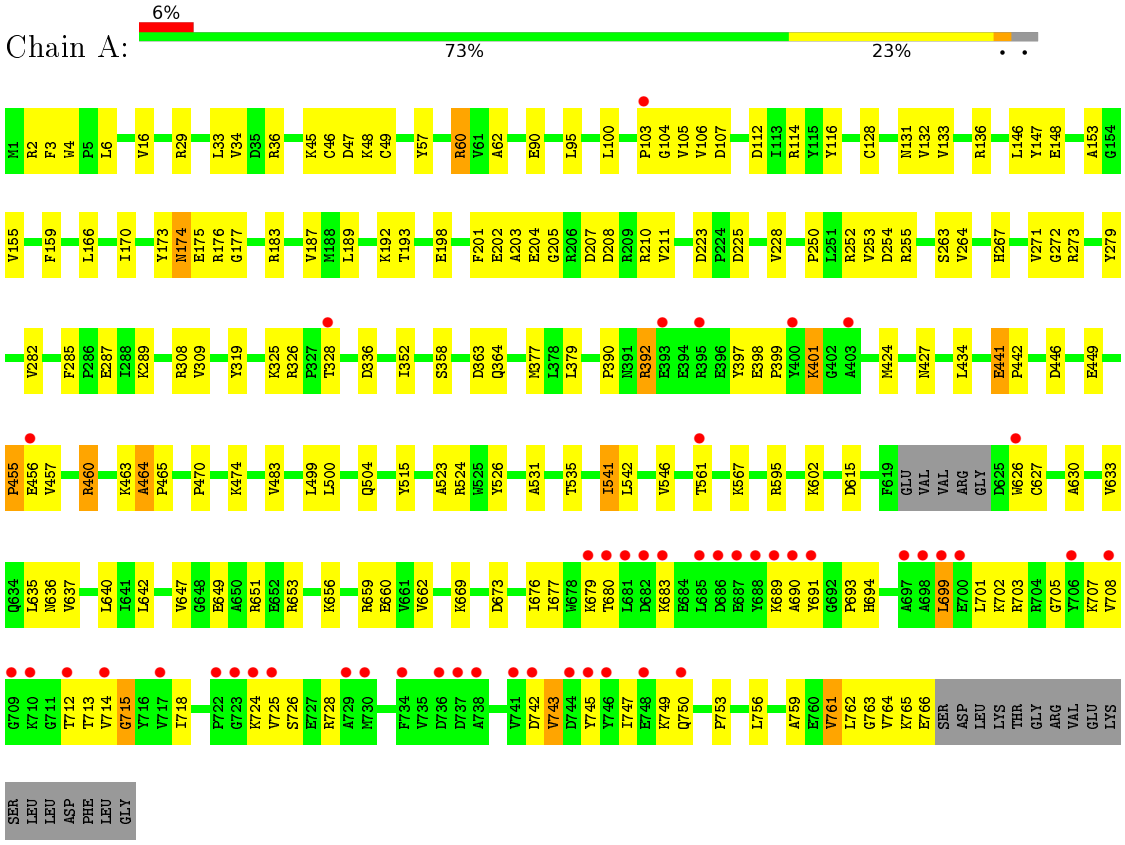
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		
3	B	30	Total	O	0	0
			30	30		

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.

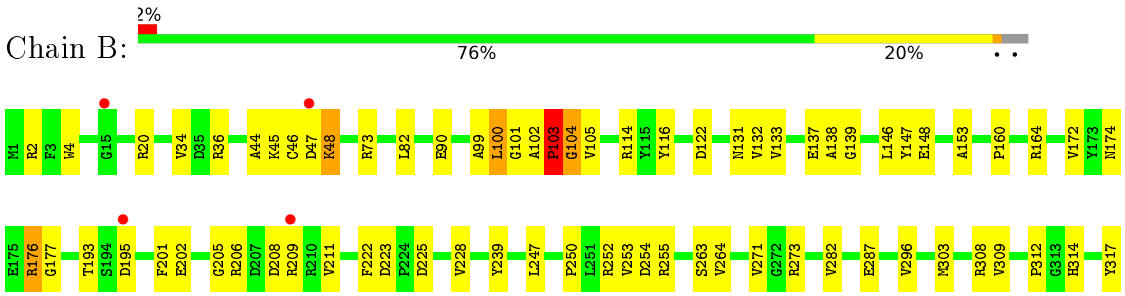
- Molecule 1: DNA polymerase

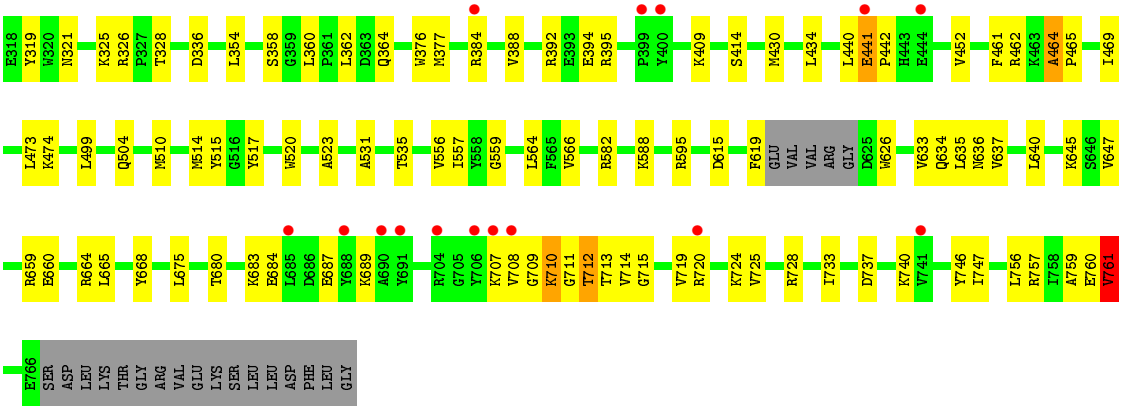
Chain A:



- Molecule 1: DNA polymerase

Chain B:




E318 Y319 W320 N321 K325 R326 P327 T328 D336 L354 S358 G359 L360 P361 L362 D363 Q364 W376 M377 R384 V388 R392 E393 E394 R395 P399 Y400 K409 S414 M430 L434 L440 E441 P442 H443 E444 V452 F461 R462 K463 A464 P465 I469
L473 K474 L499 Q504 M510 M514 Y515 G516 Y517 W520 A523 A531 T535 V556 I557 Y558 G559 L564 F565 V566 R582 K588 R595 D615 F619 GLU VAL VAL ARG GLY D625 W626 V633 Q634 L635 N636 V637 L640 K645 S646 V647
R659 E660 R664 L665 Y668 L675 T680 K683 E684 L685 D686 E687 Y688 K689 A690 Y691 R704 G705 Y706 K707 V708 G709 K710 G711 T712 T713 V714 G715 V719 R720 K724 V725 R728 I733 D737 K740 V741 Y746 I747 L756 R757 I758 A759 E760 V761
E766 SER ASP LEU LYS THR GLY ARG VAL GLU LYS SER LEU LEU ASP PHE LEU GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.19Å 100.74Å 119.33Å 90.00° 94.72° 90.00°	Depositor
Resolution (Å)	65.25 – 2.80 65.25 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.9 (65.25-2.80) 96.9 (65.25-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.11rc3_2553: ???)	Depositor
R, R_{free}	0.252 , 0.290 0.250 , 0.290	Depositor DCC
R_{free} test set	2131 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	66.8	Xtriage
Anisotropy	0.688	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12315	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: MG

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	0.31	0/6275	0.52	3/8505 (0.0%)
1	B	0.33	0/6275	0.50	1/8505 (0.0%)
All	All	0.32	0/12550	0.51	4/17010 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	104	GLY	N-CA-C	-8.44	92.00	113.10
1	A	463	LYS	C-N-CA	5.77	136.12	121.70
1	B	104	GLY	N-CA-C	-5.25	99.97	113.10
1	A	699	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	399	PRO	Peptide
1	A	455	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	B	394	GLU	Peptide

5.2 Too-close contacts (i)

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	6130	0	6193	133	0
1	B	6130	0	6193	98	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	19	0	0	2	0
3	B	30	0	0	0	0
All	All	12315	0	12386	231	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 9.

All (231) 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:464:ALA:CB	1:B:465:PRO:HD2	1.54	1.31
1:A:464:ALA:CB	1:A:465:PRO:CD	2.07	1.30
1:B:464:ALA:CB	1:B:465:PRO:CD	2.08	1.27
1:A:464:ALA:HB1	1:A:465:PRO:CD	1.65	1.22
1:A:464:ALA:HB3	1:A:465:PRO:HD2	1.22	1.19
1:B:464:ALA:HB1	1:B:465:PRO:CD	1.75	1.11
1:B:464:ALA:HB1	1:B:465:PRO:HD3	1.34	1.10
1:A:659:ARG:NH2	1:A:766:GLU:HG3	1.73	1.03
1:A:464:ALA:CB	1:A:465:PRO:HD3	1.80	1.02
1:A:45:LYS:O	1:A:105:VAL:HG23	1.61	1.01
1:A:464:ALA:HB1	1:A:465:PRO:HD3	0.99	0.99
1:A:464:ALA:CB	1:A:465:PRO:HD2	1.80	0.98
1:B:464:ALA:HB3	1:B:465:PRO:HD2	0.98	0.95
1:B:626:TRP:CH2	1:B:634:GLN:OE1	2.18	0.95
1:A:659:ARG:HH22	1:A:766:GLU:HG3	1.37	0.89
1:B:464:ALA:HB3	1:B:465:PRO:CD	1.87	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:626:TRP:HH2	1:B:634:GLN:OE1	1.59	0.86
1:A:105:VAL:HG22	1:A:106:VAL:N	1.91	0.85
1:B:99:ALA:C	1:B:101:GLY:H	1.78	0.83
1:A:173:TYR:O	1:A:174:ASN:ND2	2.11	0.83
1:B:99:ALA:O	1:B:101:GLY:N	2.17	0.77
1:B:308:ARG:NH1	1:B:309:VAL:O	2.17	0.76
1:B:626:TRP:HZ3	1:B:634:GLN:HE22	1.33	0.75
1:B:45:LYS:O	1:B:105:VAL:HA	1.88	0.74
1:B:441:GLU:HB3	1:B:442:PRO:HD2	1.70	0.72
1:A:398:GLU:OE2	1:A:401:LYS:NZ	2.24	0.71
1:A:455:PRO:O	1:A:457:VAL:N	2.25	0.69
1:A:441:GLU:HB3	1:A:442:PRO:HD2	1.73	0.69
1:B:626:TRP:CZ3	1:B:634:GLN:NE2	2.61	0.68
1:B:99:ALA:C	1:B:101:GLY:N	2.44	0.67
1:A:659:ARG:HH12	1:A:766:GLU:HG2	1.60	0.67
1:B:36:ARG:NH1	1:B:148:GLU:OE2	2.25	0.65
1:A:45:LYS:C	1:A:105:VAL:HG23	2.18	0.64
1:A:659:ARG:CZ	1:A:766:GLU:HG3	2.28	0.64
1:B:308:ARG:NH2	1:B:336:ASP:OD1	2.30	0.64
1:B:253:VAL:O	1:B:273:ARG:NH1	2.30	0.64
1:A:745:TYR:CE2	1:A:749:LYS:HD3	2.34	0.63
1:A:105:VAL:CG2	1:A:106:VAL:N	2.58	0.62
1:B:684:GLU:HG2	1:B:710:LYS:HE2	1.80	0.62
1:B:473:LEU:HD21	1:B:514:MET:HG3	1.82	0.62
1:A:764:VAL:O	1:A:764:VAL:HG23	1.97	0.62
1:B:201:PHE:HB2	1:B:211:VAL:HG23	1.82	0.62
1:A:449:GLU:HG3	1:A:464:ALA:HA	1.83	0.61
1:A:47:ASP:OD1	1:A:48:LYS:N	2.33	0.61
1:B:47:ASP:OD1	1:B:48:LYS:N	2.35	0.60
1:A:105:VAL:HG22	1:A:107:ASP:H	1.65	0.60
1:A:2:ARG:NH1	3:A:901:HOH:O	2.34	0.60
1:A:253:VAL:O	1:A:273:ARG:NH1	2.34	0.59
1:A:749:LYS:O	1:A:750:GLN:NE2	2.36	0.59
1:A:390:PRO:O	1:A:392:ARG:NH2	2.32	0.59
1:A:524:ARG:NH2	3:A:902:HOH:O	2.35	0.59
1:B:556:VAL:HG22	1:B:566:VAL:HG12	1.85	0.59
1:A:725:VAL:O	1:A:726:SER:OG	2.21	0.58
1:A:680:THR:HA	1:A:713:THR:HG22	1.86	0.57
1:A:201:PHE:HB2	1:A:211:VAL:HG23	1.85	0.57
1:A:192:LYS:HG3	1:A:198:GLU:HG2	1.86	0.57
1:A:90:GLU:N	1:A:90:GLU:OE1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:LEU:HD11	1:A:524:ARG:NH1	2.20	0.56
1:A:693:PRO:HD3	1:A:726:SER:HB2	1.86	0.56
1:A:105:VAL:HG22	1:A:106:VAL:H	1.68	0.56
1:A:279:TYR:HA	1:A:282:VAL:HG22	1.87	0.56
1:B:225:ASP:OD1	1:B:255:ARG:NH2	2.38	0.56
1:B:102:ALA:N	1:B:103:PRO:HD3	2.21	0.56
1:A:595:ARG:NH1	1:A:642:LEU:O	2.38	0.55
1:A:132:VAL:HB	1:A:153:ALA:HB3	1.88	0.55
1:A:659:ARG:NH1	1:A:766:GLU:HG2	2.20	0.55
1:B:114:ARG:NH2	1:B:364:GLN:OE1	2.40	0.55
1:A:105:VAL:HG22	1:A:107:ASP:N	2.22	0.55
1:B:132:VAL:HB	1:B:153:ALA:HB3	1.88	0.55
1:A:112:ASP:OD1	1:A:392:ARG:NH1	2.40	0.55
1:B:116:TYR:OH	1:B:364:GLN:NE2	2.41	0.54
1:B:20:ARG:HG2	1:B:34:VAL:HG12	1.90	0.54
1:A:424:MET:SD	1:A:541:ILE:HD11	2.48	0.53
1:A:441:GLU:HB3	1:A:442:PRO:CD	2.39	0.53
1:A:636:ASN:O	1:A:640:LEU:N	2.38	0.53
1:A:659:ARG:NH1	1:A:766:GLU:CG	2.70	0.53
1:B:668:TYR:OH	1:B:720:ARG:NH2	2.41	0.53
1:A:29:ARG:NH2	1:A:147:TYR:OH	2.42	0.53
1:A:105:VAL:CG2	1:A:106:VAL:H	2.22	0.53
1:A:225:ASP:OD1	1:A:255:ARG:NH2	2.35	0.53
1:A:449:GLU:HG3	1:A:464:ALA:CA	2.40	0.52
1:A:651:ARG:HH21	1:A:761:VAL:HG22	1.74	0.52
1:B:465:PRO:O	1:B:465:PRO:HG2	2.10	0.52
1:A:46:CYS:HA	1:A:105:VAL:HA	1.91	0.52
1:A:308:ARG:NH2	1:A:336:ASP:OD1	2.42	0.52
1:A:176:ARG:HH22	1:A:183:ARG:HG3	1.75	0.52
1:B:209:ARG:NH2	1:B:247:LEU:O	2.43	0.51
1:A:223:ASP:OD1	1:A:273:ARG:NH2	2.43	0.51
1:A:651:ARG:HE	1:A:761:VAL:HG22	1.75	0.51
1:B:626:TRP:CH2	1:B:634:GLN:CD	2.83	0.51
1:A:45:LYS:O	1:A:105:VAL:CG2	2.46	0.51
1:A:702:LYS:HE2	1:A:708:VAL:HG23	1.92	0.51
1:B:635:LEU:O	1:B:637:VAL:N	2.44	0.51
1:A:662:VAL:HG13	1:A:747:ILE:HG12	1.92	0.51
1:B:559:GLY:HA2	1:B:564:LEU:HA	1.93	0.50
1:A:659:ARG:CZ	1:A:766:GLU:CG	2.89	0.50
1:B:358:SER:HA	1:B:377:MET:HB2	1.94	0.50
1:B:44:ALA:HB1	1:B:105:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:TYR:CD2	1:A:325:LYS:HB3	2.48	0.49
1:A:358:SER:HA	1:A:377:MET:HB2	1.95	0.49
1:B:469:ILE:HD12	1:B:514:MET:HE1	1.94	0.49
1:B:287:GLU:HB3	1:B:615:ASP:HB2	1.94	0.49
1:A:635:LEU:O	1:A:637:VAL:N	2.43	0.49
1:B:176:ARG:NH1	1:B:712:THR:OG1	2.37	0.49
1:A:651:ARG:NH2	1:A:761:VAL:HG22	2.27	0.49
1:B:122:ASP:O	1:B:384:ARG:NH2	2.46	0.49
1:B:441:GLU:HB3	1:B:442:PRO:CD	2.39	0.49
1:B:756:LEU:HA	1:B:759:ALA:HB2	1.95	0.49
1:B:708:VAL:HG22	1:B:709:GLY:H	1.78	0.48
1:A:626:TRP:NE1	1:A:750:GLN:OE1	2.45	0.48
1:B:2:ARG:HA	1:B:131:ASN:O	2.13	0.48
1:B:193:THR:HG22	1:B:195:ASP:H	1.77	0.48
1:A:398:GLU:OE1	1:A:401:LYS:HG3	2.14	0.48
1:B:102:ALA:N	1:B:103:PRO:CD	2.76	0.48
1:B:317:TYR:O	1:B:321:ASN:ND2	2.46	0.48
1:B:164:ARG:HB3	1:B:222:PHE:CZ	2.48	0.48
1:B:392:ARG:HH22	1:B:395:ARG:CZ	2.27	0.48
1:B:395:ARG:O	1:B:520:TRP:NE1	2.43	0.47
1:B:707:LYS:HD3	1:B:712:THR:OG1	2.15	0.47
1:A:651:ARG:NH2	1:A:761:VAL:O	2.48	0.47
1:A:718:ILE:HG22	1:A:742:ASP:HB3	1.96	0.47
1:A:100:LEU:HD23	1:A:100:LEU:HA	1.72	0.47
1:A:166:LEU:HD12	1:A:193:THR:HG22	1.97	0.47
1:B:312:PRO:HB2	1:B:314:HIS:CE1	2.50	0.47
1:B:680:THR:HA	1:B:713:THR:HG22	1.95	0.46
1:A:679:LYS:HD2	1:A:679:LYS:HA	1.81	0.46
1:B:105:VAL:O	1:B:105:VAL:HG13	2.14	0.46
1:A:651:ARG:NE	1:A:761:VAL:HG22	2.30	0.46
1:A:649:GLU:OE2	1:A:653:ARG:NH1	2.49	0.46
1:A:204:GLU:CG	1:A:210:ARG:HH11	2.29	0.46
1:B:44:ALA:HB1	1:B:105:VAL:CG2	2.46	0.45
1:A:159:PHE:CD1	1:A:499:LEU:HD13	2.50	0.45
1:A:702:LYS:HA	1:A:702:LYS:HD3	1.68	0.45
1:A:250:PRO:HB2	1:A:252:ARG:HG3	1.99	0.45
1:A:3:PHE:CE1	1:A:33:LEU:HD13	2.51	0.45
1:A:627:CYS:HB3	1:A:677:ILE:HG12	1.98	0.45
1:A:263:SER:OG	1:A:264:VAL:N	2.45	0.45
1:A:287:GLU:HB3	1:A:615:ASP:HB2	1.97	0.45
1:A:308:ARG:HG2	1:A:309:VAL:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:636:ASN:O	1:B:640:LEU:N	2.40	0.45
1:A:114:ARG:NH2	1:A:264:VAL:HG21	2.32	0.45
1:A:208:ASP:OD1	1:A:208:ASP:N	2.50	0.45
1:A:743:VAL:O	1:A:747:ILE:HD12	2.17	0.45
1:A:204:GLU:HG2	1:A:210:ARG:HH11	1.82	0.45
1:A:647:VAL:CG1	1:A:761:VAL:HG21	2.47	0.45
1:B:414:SER:OG	1:B:595:ARG:NH1	2.50	0.45
1:A:34:VAL:HB	1:A:146:LEU:HD11	1.98	0.44
1:A:659:ARG:NH2	1:A:766:GLU:CG	2.64	0.44
1:B:208:ASP:N	1:B:208:ASP:OD1	2.50	0.44
1:A:116:TYR:OH	1:A:364:GLN:OE1	2.30	0.44
1:A:470:PRO:O	1:A:474:LYS:HG3	2.18	0.44
1:B:250:PRO:HB2	1:B:252:ARG:HG3	1.99	0.44
1:B:90:GLU:N	1:B:90:GLU:OE1	2.42	0.44
1:B:711:GLY:O	1:B:712:THR:HG22	2.17	0.44
1:A:626:TRP:HB3	1:A:630:ALA:HB3	1.99	0.44
1:A:693:PRO:HB3	1:A:726:SER:O	2.18	0.44
1:A:630:ALA:HA	1:A:633:VAL:HG22	2.00	0.44
1:A:703:ARG:O	1:A:705:GLY:N	2.47	0.43
1:B:303:MET:SD	1:B:308:ARG:HG3	2.59	0.43
1:B:626:TRP:HZ3	1:B:634:GLN:NE2	2.03	0.43
1:B:223:ASP:OD1	1:B:273:ARG:NH2	2.51	0.43
1:B:531:ALA:O	1:B:535:THR:HG23	2.18	0.43
1:B:665:LEU:HD23	1:B:747:ILE:HG13	2.00	0.43
1:B:263:SER:OG	1:B:264:VAL:N	2.46	0.43
1:A:2:ARG:HA	1:A:131:ASN:O	2.18	0.43
1:A:128:CYS:HB3	1:A:352:ILE:HG23	2.00	0.43
1:B:160:PRO:HD2	1:B:499:LEU:HD23	2.00	0.43
1:A:449:GLU:HG3	1:A:464:ALA:CB	2.48	0.43
1:B:139:GLY:O	1:B:146:LEU:HB3	2.18	0.43
1:A:531:ALA:O	1:A:535:THR:HG23	2.18	0.43
1:A:57:TYR:O	1:A:60:ARG:HG2	2.18	0.43
1:B:319:TYR:CD2	1:B:325:LYS:HB3	2.53	0.43
1:B:660:GLU:O	1:B:664:ARG:HG2	2.19	0.43
1:A:724:LYS:HZ3	1:A:725:VAL:HG22	1.84	0.43
1:A:203:ALA:HB1	1:A:207:ASP:O	2.19	0.43
1:A:756:LEU:HA	1:A:759:ALA:HB2	2.01	0.43
1:A:763:GLY:O	1:A:765:LYS:HG3	2.18	0.43
1:B:689:LYS:HA	1:B:689:LYS:HD3	1.89	0.43
1:B:430:MET:HE3	1:B:474:LYS:HG2	2.01	0.42
1:A:750:GLN:C	1:A:753:PRO:HD2	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:PRO:HA	1:A:756:LEU:HB2	2.00	0.42
1:B:619:PHE:C	1:B:757:ARG:HH22	2.22	0.42
1:A:483:VAL:HG13	1:A:500:LEU:HD22	2.01	0.42
1:A:282:VAL:HA	1:A:285:PHE:CD2	2.54	0.42
1:A:656:LYS:NZ	1:A:660:GLU:OE2	2.32	0.42
1:A:254:ASP:HB2	1:A:271:VAL:O	2.20	0.42
1:A:762:LEU:HB2	1:A:765:LYS:HE3	2.01	0.42
1:A:36:ARG:NH1	1:A:148:GLU:OE2	2.52	0.42
1:B:461:PHE:N	1:B:461:PHE:CD1	2.86	0.42
1:A:673:ASP:HA	1:A:676:ILE:HD13	2.02	0.42
1:B:73:ARG:O	1:B:388:VAL:HG22	2.19	0.42
1:B:193:THR:HG23	1:B:222:PHE:CZ	2.54	0.42
1:B:172:VAL:HG11	1:B:239:TYR:CZ	2.54	0.42
1:B:360:LEU:HD21	1:B:376:TRP:CD1	2.55	0.42
1:B:193:THR:HG22	1:B:195:ASP:N	2.34	0.42
1:A:46:CYS:SG	1:A:49:CYS:HB3	2.59	0.41
1:B:724:LYS:HG3	1:B:725:VAL:H	1.85	0.41
1:A:136:ARG:NH1	1:A:148:GLU:OE1	2.53	0.41
1:A:724:LYS:HG3	1:A:725:VAL:N	2.35	0.41
1:B:137:GLU:HA	1:B:147:TYR:CD2	2.55	0.41
1:A:170:ILE:HG22	1:A:189:LEU:HG	2.02	0.41
1:A:6:LEU:HD11	1:A:225:ASP:HB3	2.02	0.41
1:A:679:LYS:HB3	1:A:694:HIS:CE1	2.55	0.41
1:B:647:VAL:HG11	1:B:761:VAL:HG11	2.01	0.41
1:A:714:VAL:HG13	1:A:715:GLY:N	2.35	0.41
1:B:254:ASP:HB2	1:B:271:VAL:O	2.20	0.41
1:A:263:SER:HB3	1:A:267:HIS:CE1	2.56	0.41
1:A:446:ASP:OD1	1:A:460:ARG:NH2	2.49	0.41
1:B:46:CYS:HA	1:B:104:GLY:O	2.21	0.41
1:B:687:GLU:O	1:B:689:LYS:N	2.45	0.41
1:A:669:LYS:HB3	1:A:669:LYS:HE2	1.93	0.41
1:B:515:TYR:OH	1:B:535:THR:HG22	2.21	0.41
1:B:517:TYR:CZ	1:B:523:ALA:HB1	2.55	0.41
1:B:675:LEU:HD22	1:B:746:TYR:CD2	2.56	0.41
1:A:542:LEU:O	1:A:546:VAL:HG13	2.21	0.41
1:A:62:ALA:HB3	1:A:95:LEU:HD21	2.02	0.41
1:A:449:GLU:HG3	1:A:464:ALA:HB2	2.03	0.41
1:A:392:ARG:HE	1:A:524:ARG:HG2	1.86	0.41
1:B:714:VAL:HG13	1:B:715:GLY:N	2.36	0.41
1:B:282:VAL:HG11	1:B:296:VAL:HG21	2.04	0.40
1:B:440:LEU:HD21	1:B:462:ARG:HH11	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:LEU:HD11	1:B:510:MET:HE3	2.03	0.40
1:B:588:LYS:HB2	1:B:588:LYS:HE2	1.89	0.40
1:B:760:GLU:HG3	1:B:760:GLU:H	1.72	0.40
1:A:173:TYR:CE2	1:A:175:GLU:HB2	2.56	0.40
1:A:255:ARG:NH1	1:A:272:GLY:O	2.55	0.40
1:A:690:ALA:O	1:A:691:TYR:HB2	2.21	0.40
1:A:363:ASP:OD1	1:A:364:GLN:HG3	2.22	0.40
1:A:523:ALA:HB3	1:A:526:TYR:HB2	2.04	0.40
1:B:719:VAL:HG13	1:B:740:LYS:O	2.21	0.40
1:A:515:TYR:OH	1:A:535:THR: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	757/783 (97%)	694 (92%)	51 (7%)	12 (2%)	12	38
1	B	757/783 (97%)	697 (92%)	48 (6%)	12 (2%)	12	38
All	All	1514/1566 (97%)	1391 (92%)	99 (6%)	24 (2%)	12	38

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	GLY
1	A	397	TYR
1	A	456	GLU
1	A	464	ALA
1	B	100	LEU
1	B	464	ALA
1	B	710	LYS
1	B	737	ASP

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Mol	Chain	Res	Type
1	A	177	GLY
1	A	441	GLU
1	A	689	LYS
1	A	761	VAL
1	B	103	PRO
1	B	177	GLY
1	B	205	GLY
1	B	712	THR
1	A	103	PRO
1	B	138	ALA
1	B	761	VAL
1	A	401	LYS
1	B	441	GLU
1	A	4	TRP
1	B	4	TRP
1	A	715	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	649/668 (97%)	622 (96%)	27 (4%)	36	71
1	B	649/668 (97%)	623 (96%)	26 (4%)	38	73
All	All	1298/1336 (97%)	1245 (96%)	53 (4%)	37	72

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	60	ARG
1	A	133	VAL
1	A	155	VAL
1	A	174	ASN
1	A	187	VAL
1	A	202	GLU

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Mol	Chain	Res	Type
1	A	228	VAL
1	A	289	LYS
1	A	326	ARG
1	A	328	THR
1	A	392	ARG
1	A	427	ASN
1	A	434	LEU
1	A	460	ARG
1	A	504	GLN
1	A	541	ILE
1	A	561	THR
1	A	567	LYS
1	A	602	LYS
1	A	683	LYS
1	A	699	LEU
1	A	701	LEU
1	A	707	LYS
1	A	712	THR
1	A	728	ARG
1	A	743	VAL
1	B	48	LYS
1	B	82	LEU
1	B	100	LEU
1	B	103	PRO
1	B	133	VAL
1	B	174	ASN
1	B	176	ARG
1	B	202	GLU
1	B	206	ARG
1	B	228	VAL
1	B	326	ARG
1	B	328	THR
1	B	362	LEU
1	B	409	LYS
1	B	434	LEU
1	B	452	VAL
1	B	504	GLN
1	B	557	ILE
1	B	582	ARG
1	B	633	VAL
1	B	645	LYS
1	B	659	ARG

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Mol	Chain	Res	Type
1	B	683	LYS
1	B	728	ARG
1	B	733	ILE
1	B	761	VAL

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

Mol	Chain	Res	Type
1	B	512	ASN
1	B	634	GLN

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 6 ligands modelled in this entry, 6 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	761/783 (97%)	0.36	49 (6%)	23	14	45, 71, 139, 166	0
1	B	761/783 (97%)	0.18	19 (2%)	61	48	43, 68, 106, 137	0
All	All	1522/1566 (97%)	0.27	68 (4%)	37	26	43, 70, 120, 166	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	688	TYR	7.0
1	A	698	ALA	6.5
1	A	685	LEU	5.8
1	A	699	LEU	5.7
1	A	697	ALA	5.7
1	A	748	GLU	5.7
1	A	712	THR	5.6
1	A	395	ARG	5.4
1	A	680	THR	5.3
1	B	691	TYR	5.1
1	B	706	TYR	5.0
1	A	681	LEU	5.0
1	A	686	ASP	4.8
1	A	746	TYR	4.8
1	B	444	GLU	4.8
1	A	737	ASP	4.5
1	A	708	VAL	4.3
1	B	685	LEU	4.2
1	A	688	TYR	4.0
1	A	741	VAL	3.9
1	A	690	ALA	3.8
1	A	722	PRO	3.7
1	B	400	TYR	3.6
1	A	714	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	724	LYS	3.5
1	A	736	ASP	3.5
1	A	729	ALA	3.4
1	A	683	LYS	3.4
1	A	626	TRP	3.3
1	A	682	ASP	3.1
1	A	561	THR	3.1
1	A	717	VAL	3.0
1	B	704	ARG	3.0
1	A	400	TYR	2.9
1	B	708	VAL	2.9
1	A	723	GLY	2.9
1	B	47	ASP	2.9
1	A	691	TYR	2.9
1	A	706	TYR	2.9
1	A	709	GLY	2.8
1	A	742	ASP	2.8
1	A	734	PHE	2.7
1	A	725	VAL	2.6
1	B	209	ARG	2.6
1	A	710	LYS	2.6
1	A	679	LYS	2.6
1	A	689	LYS	2.6
1	A	403	ALA	2.6
1	A	687	GLU	2.5
1	A	730	MET	2.5
1	A	738	ALA	2.4
1	B	399	PRO	2.4
1	A	328	THR	2.4
1	A	750	GLN	2.3
1	A	393	GLU	2.3
1	B	15	GLY	2.2
1	B	720	ARG	2.2
1	A	700	GLU	2.2
1	A	103	PRO	2.2
1	A	745	TYR	2.2
1	B	384	ARG	2.2
1	B	441	GLU	2.2
1	B	741	VAL	2.1
1	A	744	ASP	2.0
1	B	690	ALA	2.0
1	A	456	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	195	ASP	2.0
1	B	707	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 (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	MG	B	801	1/1	0.98	0.40	23.81	44,44,44,44	0
2	MG	A	801	1/1	0.98	0.45	14.59	35,35,35,35	0
2	MG	A	802	1/1	0.93	0.57	-	82,82,82,82	0
2	MG	B	802	1/1	0.90	0.56	-	66,66,66,66	0
2	MG	A	803	1/1	0.87	0.55	-	90,90,90,90	0
2	MG	B	803	1/1	0.90	0.54	-	72,72,72,72	0

6.5 Other polymers (i)

There are no such residues in this entry.