



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:15 PM GMT

PDB ID : 1JIH
Title : Yeast DNA Polymerase ETA
Authors : Trincao, J.; Johnson, R.E.; Escalante, C.R.; Prakash, S.; Prakash, L.; Aggarwal, A.K.
Deposited on : 2001-07-02
Resolution : 2.25 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 ⓘ symbol.

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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

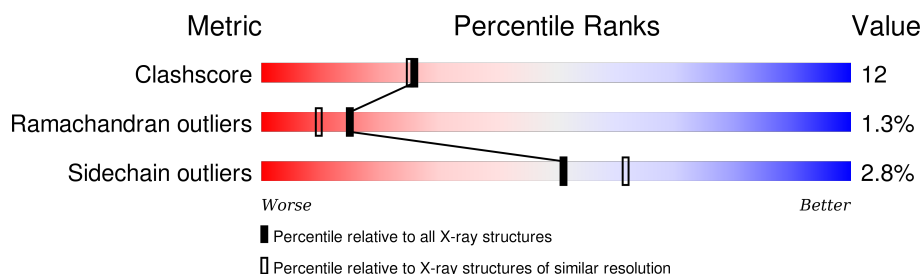
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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))
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)

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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	513	 78% 19% ..
1	B	513	 77% 19% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8410 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 ETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			3911	2487	651	749	24			
1	B	509	Total	C	N	O	S	0	0	0
			3983	2539	668	752	24			

- Molecule 2 is water.

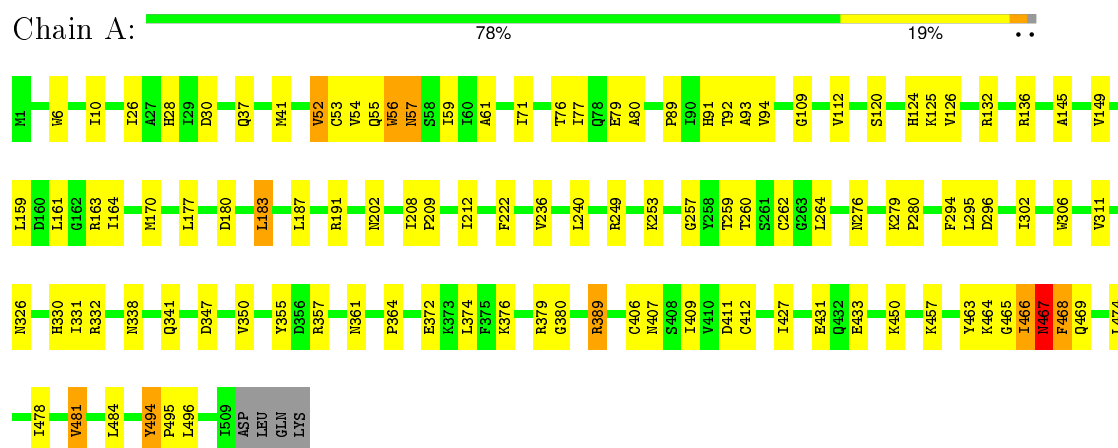
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	262	Total	O	0	0
			262	262		
2	B	254	Total	O	0	0
			254	254		

3 Residue-property plots

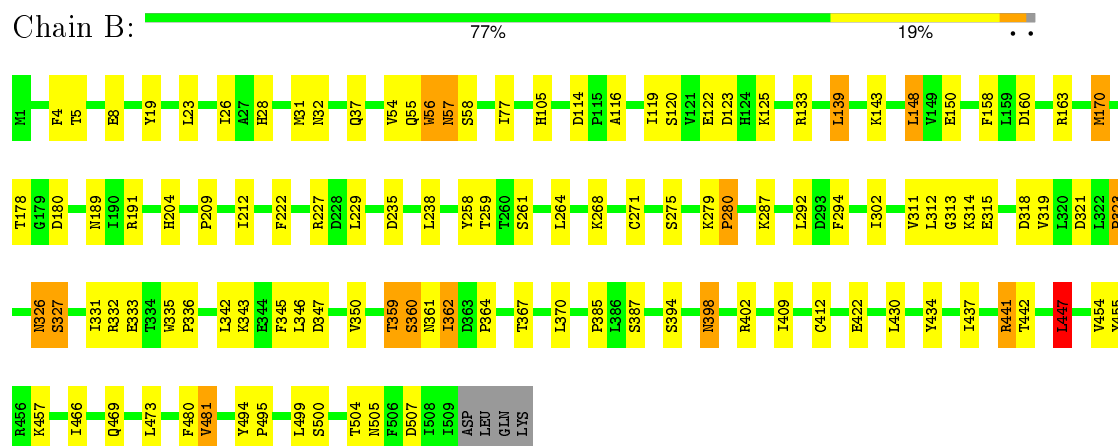
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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.

Note EDS was not executed.

• Molecule 1: DNA Polymerase ETA



• Molecule 1: DNA Polymerase ETA



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.10 Å 105.10 Å 292.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.25	Depositor
% Data completeness (in resolution range)	87.4 (50.00-2.25)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.215 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8410	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.44	1/3988 (0.0%)	0.66	5/5402 (0.1%)
1	B	0.48	2/4060 (0.0%)	0.65	8/5483 (0.1%)
All	All	0.46	3/8048 (0.0%)	0.65	13/10885 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	327	SER	N-CA	16.23	1.78	1.46
1	A	57	ASN	N-CA	15.24	1.76	1.46
1	B	57	ASN	N-CA	12.36	1.71	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	ASN	N-CA-CB	-11.61	89.71	110.60
1	B	327	SER	N-CA-CB	-9.89	95.67	110.50
1	B	326	ASN	C-N-CA	-9.67	97.53	121.70
1	B	57	ASN	N-CA-CB	-9.63	93.26	110.60
1	A	56	TRP	C-N-CA	-9.26	98.56	121.70
1	B	494	TYR	N-CA-CB	8.90	126.62	110.60
1	B	56	TRP	C-N-CA	-8.82	99.66	121.70
1	A	57	ASN	N-CA-C	8.70	134.50	111.00
1	A	494	TYR	N-CA-C	6.97	129.81	111.00
1	B	494	TYR	N-CA-C	-6.75	92.79	111.00
1	B	447	LEU	CA-CB-CG	6.29	129.77	115.30
1	B	57	ASN	N-CA-C	5.85	126.79	111.00
1	A	494	TYR	C-N-CD	5.19	139.30	128.40

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	3911	0	3799	90	0
1	B	3983	0	3971	104	0
2	A	262	0	0	7	0
2	B	254	0	0	6	0
All	All	8410	0	7770	194	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 12.

All (194) 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:57:ASN:N	1:B:57:ASN:CA	1.71	1.48
1:A:57:ASN:CA	1:A:57:ASN:N	1.76	1.47
1:B:327:SER:N	1:B:327:SER:CA	1.78	1.44
1:A:37:GLN:HE22	1:A:259:THR:H	1.13	0.96
1:B:346:LEU:HD23	1:B:367:THR:HG23	1.45	0.96
1:B:56:TRP:C	1:B:57:ASN:CA	2.33	0.96
1:A:170:MET:HE1	1:A:191:ARG:HA	1.48	0.94
1:A:350:VAL:HG21	1:A:364:PRO:HB3	1.49	0.93
1:A:56:TRP:C	1:A:57:ASN:CA	2.36	0.93
1:A:57:ASN:N	1:A:57:ASN:CB	2.33	0.91
1:B:326:ASN:C	1:B:327:SER:CA	2.40	0.90
1:B:57:ASN:N	1:B:57:ASN:CB	2.36	0.87
1:B:170:MET:HA	1:B:170:MET:HE3	1.61	0.81
1:B:394:SER:HB3	1:B:504:THR:HG22	1.63	0.80
1:B:37:GLN:HE22	1:B:259:THR:H	1.30	0.80
1:A:170:MET:CE	1:A:191:ARG:HA	2.13	0.78
1:B:454:VAL:HG12	2:B:609:HOH:O	1.85	0.77
1:B:327:SER:N	1:B:327:SER:CB	2.48	0.75
1:A:94:VAL:HG21	1:A:124:HIS:HB3	1.67	0.75
1:A:466:ILE:O	1:A:467:ASN:C	2.27	0.72
1:B:56:TRP:O	1:B:57:ASN:CA	2.37	0.72
1:B:56:TRP:O	1:B:57:ASN:HA	1.90	0.71
1:A:54:VAL:HG11	1:A:77:ILE:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:THR:HG21	1:A:126:VAL:HG13	1.70	0.71
1:A:54:VAL:CG1	1:A:77:ILE:HD11	2.21	0.70
1:A:109:GLY:O	1:A:112:VAL:HG22	1.91	0.69
1:A:170:MET:HE3	1:A:191:ARG:HG2	1.73	0.69
1:B:170:MET:CE	1:B:191:ARG:HG2	2.22	0.69
1:A:260:THR:HG21	2:A:618:HOH:O	1.93	0.69
1:A:494:TYR:O	1:A:496:LEU:N	2.27	0.68
1:A:56:TRP:O	1:A:57:ASN:CA	2.41	0.67
1:A:56:TRP:O	1:A:57:ASN:HA	1.95	0.67
1:A:37:GLN:HE22	1:A:259:THR:N	1.88	0.66
1:B:343:LYS:HG3	1:B:367:THR:HG22	1.77	0.65
1:A:364:PRO:HA	2:A:609:HOH:O	1.95	0.65
1:B:54:VAL:HG11	1:B:77:ILE:CD1	2.25	0.65
1:A:41:MET:HE3	1:A:257:GLY:HA3	1.79	0.65
1:A:427:ILE:O	1:A:431:GLU:HG3	1.97	0.65
1:B:394:SER:CB	1:B:504:THR:HG22	2.26	0.64
1:B:31:MET:HE1	1:B:258:TYR:CD2	2.32	0.64
1:B:54:VAL:HG11	1:B:77:ILE:HD11	1.80	0.63
1:B:398:ASN:C	1:B:398:ASN:HD22	2.02	0.63
1:B:326:ASN:O	1:B:327:SER:CA	2.47	0.62
1:A:132:ARG:NH1	2:A:514:HOH:O	2.30	0.62
1:A:76:THR:OG1	1:A:79:GLU:HG3	1.99	0.62
1:B:447:LEU:HD22	1:B:455:TYR:HB2	1.82	0.62
1:A:37:GLN:NE2	1:A:259:THR:H	1.92	0.62
1:B:150:GLU:HG3	1:B:387:SER:O	1.99	0.61
1:B:170:MET:HE1	1:B:191:ARG:HA	1.83	0.60
1:B:347:ASP:OD2	1:B:367:THR:HG21	2.01	0.59
1:A:311:VAL:HG12	1:A:361:ASN:OD1	2.04	0.57
1:A:41:MET:HE2	1:A:257:GLY:O	2.04	0.57
1:B:170:MET:CE	1:B:170:MET:HA	2.34	0.57
1:B:347:ASP:O	1:B:350:VAL:HG12	2.05	0.57
1:B:311:VAL:HB	2:B:758:HOH:O	2.05	0.57
1:B:314:LYS:HE2	1:B:318:ASP:OD2	2.05	0.56
1:A:54:VAL:HG11	1:A:77:ILE:CD1	2.35	0.56
1:A:26:ILE:O	1:A:264:LEU:HD12	2.06	0.56
1:A:52:VAL:HG12	1:A:89:PRO:HA	1.86	0.56
1:A:350:VAL:HG23	1:A:355:TYR:CE2	2.39	0.56
1:B:333:GLU:O	1:B:336:PRO:HD3	2.06	0.56
1:A:54:VAL:CG1	1:A:55:GLN:N	2.69	0.55
1:B:430:LEU:HD22	1:B:434:TYR:CE2	2.41	0.55
1:B:54:VAL:CG1	1:B:77:ILE:HD11	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:VAL:HA	1:B:345:PHE:HE2	1.72	0.54
1:B:170:MET:CE	1:B:191:ARG:HA	2.37	0.54
1:A:94:VAL:CG2	1:A:124:HIS:HB3	2.37	0.54
1:A:94:VAL:HG23	1:A:125:LYS:C	2.28	0.54
1:B:314:LYS:HD3	1:B:362:ILE:HD11	1.89	0.54
1:B:120:SER:HB2	1:B:122:GLU:OE1	2.07	0.53
1:B:170:MET:CA	1:B:170:MET:HE3	2.37	0.53
1:B:402:ARG:HG2	1:B:402:ARG:HH11	1.72	0.53
1:A:450:LYS:HD2	1:A:495:PRO:HD2	1.90	0.53
1:B:398:ASN:HB3	1:B:500:SER:CB	2.38	0.53
1:A:28:HIS:CE1	1:A:30:ASP:OD2	2.61	0.53
1:A:53:CYS:HB3	1:A:61:ALA:HB3	1.89	0.53
1:B:133:ARG:HH11	1:B:133:ARG:HG2	1.74	0.52
1:A:406:CYS:HA	1:A:411:ASP:HB3	1.92	0.52
1:B:105:HIS:HE1	2:B:533:HOH:O	1.91	0.52
1:B:32:ASN:HD21	1:B:261:SER:HB3	1.74	0.52
1:B:31:MET:HE1	1:B:258:TYR:CB	2.39	0.52
1:B:495:PRO:HG2	2:B:716:HOH:O	2.09	0.52
1:B:56:TRP:HZ3	1:B:119:ILE:HG22	1.75	0.52
1:A:466:ILE:O	1:A:468:PHE:N	2.43	0.52
1:A:412:CYS:HB3	1:A:481:VAL:HG21	1.90	0.52
1:A:389:ARG:N	2:A:744:HOH:O	2.39	0.52
1:B:209:PRO:O	1:B:212:ILE:HG22	2.10	0.51
1:B:170:MET:HE3	1:B:191:ARG:HG2	1.92	0.50
1:B:412:CYS:HB3	1:B:481:VAL:HG21	1.93	0.50
1:B:398:ASN:C	1:B:398:ASN:ND2	2.65	0.50
1:B:447:LEU:CD2	1:B:455:TYR:HB2	2.41	0.50
1:A:338:ASN:OD1	1:A:341:GLN:HG3	2.12	0.50
1:A:6:TRP:O	1:A:10:ILE:HG12	2.12	0.50
1:B:229:LEU:HD22	1:B:229:LEU:N	2.26	0.50
1:A:94:VAL:HG23	1:A:125:LYS:O	2.11	0.49
1:A:357:ARG:HG2	1:A:357:ARG:HH11	1.76	0.49
1:A:149:VAL:HG22	1:A:159:LEU:HD22	1.95	0.49
1:B:31:MET:HE1	1:B:258:TYR:CG	2.48	0.49
1:B:370:LEU:HD13	1:B:370:LEU:O	2.13	0.49
1:A:57:ASN:N	1:A:57:ASN:CG	2.65	0.49
1:B:139:LEU:CD2	1:B:143:LYS:HE2	2.43	0.49
1:A:136:ARG:HD3	1:A:433:GLU:HG3	1.94	0.49
1:B:279:LYS:O	1:B:280:PRO:O	2.31	0.48
1:A:302:ILE:HD12	1:A:331:ILE:HD11	1.94	0.48
1:B:54:VAL:HG12	1:B:55:GLN:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:VAL:HG22	1:A:59:ILE:HG23	1.94	0.48
1:B:350:VAL:HG21	1:B:364:PRO:HB3	1.96	0.48
1:A:350:VAL:CG2	1:A:364:PRO:HB3	2.32	0.48
1:B:28:HIS:HD2	1:B:275:SER:OG	1.97	0.48
1:A:276:ASN:OD1	1:A:279:LYS:HE3	2.14	0.47
1:A:92:THR:HG23	1:A:93:ALA:O	2.14	0.47
1:B:31:MET:CE	1:B:258:TYR:HB2	2.44	0.47
1:B:466:ILE:HA	1:B:469:GLN:HE21	1.77	0.47
1:B:32:ASN:ND2	1:B:279:LYS:O	2.48	0.47
1:B:321:ASP:O	1:B:323:PRO:HD3	2.15	0.47
1:B:229:LEU:HD22	1:B:229:LEU:H	1.80	0.47
1:A:326:ASN:HA	2:A:567:HOH:O	2.15	0.47
1:B:150:GLU:OE1	1:B:268:LYS:NZ	2.48	0.47
1:B:19:TYR:CE2	1:B:385:PRO:HB3	2.50	0.47
1:A:409:ILE:HD11	1:A:481:VAL:HG13	1.96	0.46
1:B:319:VAL:HG23	1:B:321:ASP:OD2	2.15	0.46
1:B:409:ILE:HD11	1:B:481:VAL:HG13	1.97	0.46
1:B:466:ILE:HG13	2:B:624:HOH:O	2.15	0.46
1:A:350:VAL:HG21	1:A:364:PRO:CB	2.33	0.46
1:A:372:GLU:CG	1:A:376:LYS:HE2	2.46	0.46
1:A:52:VAL:HG13	1:A:54:VAL:HG23	1.97	0.46
1:B:315:GLU:O	1:B:319:VAL:HG22	2.16	0.46
1:A:222:PHE:CE2	1:A:294:PHE:HA	2.51	0.46
1:B:5:THR:OG1	1:B:8:GLU:HG3	2.15	0.46
1:B:5:THR:HG22	1:B:204:HIS:CD2	2.51	0.46
1:B:148:LEU:HB3	1:B:160:ASP:HB3	1.98	0.45
1:A:170:MET:HE3	1:A:170:MET:HA	1.98	0.45
1:B:26:ILE:O	1:B:264:LEU:HD12	2.17	0.45
1:A:54:VAL:HG12	1:A:55:GLN:N	2.32	0.45
1:B:292:LEU:HD22	1:B:332:ARG:CZ	2.46	0.45
1:A:149:VAL:HG22	1:A:159:LEU:CD2	2.47	0.45
1:B:335:TRP:CD2	1:B:342:LEU:HD13	2.51	0.45
1:B:139:LEU:HD22	1:B:143:LYS:HE2	1.98	0.45
1:B:302:ILE:HD13	1:B:331:ILE:HD12	1.98	0.45
1:B:54:VAL:CG1	1:B:55:GLN:N	2.80	0.45
1:A:380:GLY:HA2	2:A:545:HOH:O	2.16	0.45
1:A:347:ASP:O	1:A:350:VAL:HG12	2.17	0.45
1:B:441:ARG:HE	1:B:507:ASP:HB2	1.81	0.45
1:B:319:VAL:HA	1:B:345:PHE:CE2	2.51	0.45
1:A:463:TYR:C	1:A:465:GLY:H	2.19	0.45
1:A:209:PRO:O	1:A:212:ILE:HG22	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:LYS:HE3	1:B:422:GLU:OE1	2.17	0.44
1:B:457:LYS:HG2	1:B:480:PHE:CG	2.53	0.44
1:B:398:ASN:HB3	1:B:500:SER:HB3	1.99	0.44
1:A:54:VAL:HG13	1:A:77:ILE:HD11	1.96	0.44
1:B:178:THR:C	1:B:180:ASP:H	2.20	0.43
1:B:222:PHE:CE2	1:B:294:PHE:HA	2.53	0.43
1:B:170:MET:CE	1:B:170:MET:CA	2.95	0.43
1:B:398:ASN:HB3	1:B:500:SER:HB2	2.00	0.43
1:B:437:ILE:N	1:B:437:ILE:HD12	2.33	0.43
1:B:150:GLU:HB3	1:B:158:PHE:HB2	2.00	0.43
1:A:276:ASN:OD1	1:A:279:LYS:CE	2.67	0.43
1:A:474:LEU:O	1:A:478:ILE:HG13	2.19	0.42
1:B:398:ASN:CB	1:B:500:SER:HB3	2.49	0.42
1:A:52:VAL:HG22	1:A:59:ILE:CG2	2.49	0.42
1:A:236:VAL:O	1:A:240:LEU:HG	2.18	0.42
1:B:4:PHE:CD2	1:B:23:LEU:HD21	2.53	0.42
1:B:314:LYS:HZ1	1:B:360:SER:CB	2.33	0.42
1:A:92:THR:HG21	1:A:126:VAL:HG22	2.01	0.42
1:A:91:HIS:CE1	1:A:92:THR:HG22	2.55	0.42
1:B:442:THR:CB	1:B:505:ASN:HD22	2.32	0.42
1:A:92:THR:CG2	1:A:126:VAL:HG13	2.46	0.42
1:B:359:THR:O	1:B:361:ASN:N	2.53	0.42
1:B:139:LEU:HD22	1:B:143:LYS:HG3	2.02	0.42
1:A:52:VAL:HG21	1:A:59:ILE:HD13	2.02	0.42
1:B:235:ASP:OD1	1:B:287:LYS:HE2	2.20	0.42
1:A:92:THR:HG21	1:A:126:VAL:CG1	2.47	0.41
1:B:311:VAL:C	1:B:313:GLY:H	2.23	0.41
1:B:26:ILE:O	1:B:271:CYS:SG	2.78	0.41
1:A:202:ASN:HA	1:A:202:ASN:HD22	1.67	0.41
1:A:208:ILE:HG13	1:A:208:ILE:O	2.18	0.41
1:B:54:VAL:HG13	1:B:58:SER:O	2.20	0.41
1:A:183:LEU:HD22	1:A:187:LEU:HD12	2.03	0.41
1:A:145:ALA:O	1:A:164:ILE:HD11	2.20	0.41
1:A:466:ILE:O	1:A:468:PHE:HD1	2.04	0.41
1:A:249:ARG:HD2	1:A:262:CYS:HB2	2.03	0.41
1:B:314:LYS:NZ	1:B:360:SER:CB	2.84	0.41
1:A:120:SER:O	1:A:124:HIS:HD2	2.04	0.41
1:A:71:ILE:HD13	1:A:80:ALA:HB1	2.03	0.41
1:B:227:ARG:HG2	1:B:227:ARG:HH11	1.85	0.40
1:A:253:LYS:O	1:A:257:GLY:HA2	2.21	0.40
1:A:457:LYS:HB2	1:A:484:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASN:N	1:A:57:ASN:ND2	2.69	0.40
1:A:332:ARG:HD2	1:A:379:ARG:NH1	2.36	0.40
1:B:466:ILE:HG23	1:B:469:GLN:NE2	2.37	0.40
1:A:296:ASP:OD2	1:A:332:ARG:NH2	2.48	0.40
1:B:114:ASP:OD1	1:B:116:ALA:HB3	2.21	0.40
1:A:330:HIS:HE1	2:A:611:HOH:O	2.04	0.40
1:B:189:ASN:HB2	2:B:583:HOH:O	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	507/513 (99%)	479 (94%)	21 (4%)	7 (1%)	14	9
1	B	507/513 (99%)	478 (94%)	23 (4%)	6 (1%)	16	11
All	All	1014/1026 (99%)	957 (94%)	44 (4%)	13 (1%)	15	10

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	PRO
1	A	389	ARG
1	B	280	PRO
1	B	359	THR
1	A	306	TRP
1	A	467	ASN
1	B	323	PRO
1	B	360	SER
1	A	469	GLN
1	A	464	LYS
1	B	312	LEU

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Mol	Chain	Res	Type
1	A	466	ILE
1	B	362	ILE

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	422/460 (92%)	410 (97%)	12 (3%)	51	62
1	B	439/460 (95%)	427 (97%)	12 (3%)	52	63
All	All	861/920 (94%)	837 (97%)	24 (3%)	51	62

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	161	LEU
1	A	163	ARG
1	A	177	LEU
1	A	180	ASP
1	A	183	LEU
1	A	295	LEU
1	A	374	LEU
1	A	407	ASN
1	A	467	ASN
1	A	468	PHE
1	A	481	VAL
1	B	123	ASP
1	B	139	LEU
1	B	148	LEU
1	B	163	ARG
1	B	170	MET
1	B	238	LEU
1	B	398	ASN
1	B	441	ARG
1	B	447	LEU

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Mol	Chain	Res	Type
1	B	473	LEU
1	B	481	VAL
1	B	499	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	28	HIS
1	A	37	GLN
1	A	57	ASN
1	A	78	GLN
1	A	103	GLN
1	A	124	HIS
1	A	173	ASN
1	A	202	ASN
1	A	204	HIS
1	A	283	GLN
1	A	288	ASN
1	A	330	HIS
1	A	352	GLN
1	A	400	ASN
1	A	407	ASN
1	A	428	GLN
1	A	432	GLN
1	A	505	ASN
1	B	28	HIS
1	B	32	ASN
1	B	37	GLN
1	B	78	GLN
1	B	103	GLN
1	B	105	HIS
1	B	118	GLN
1	B	288	ASN
1	B	398	ASN
1	B	428	GLN
1	B	432	GLN
1	B	469	GLN
1	B	505	ASN

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](#)

There are no ligands in this entry.

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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.