



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:37 PM GMT

PDB ID : 1BPB
Title : CRYSTAL STRUCTURE OF RAT DNA POLYMERASE BETA: EVIDENCE FOR A COMMON POLYMERASE MECHANISM
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Deposited on : 1994-04-12
Resolution : 2.30 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

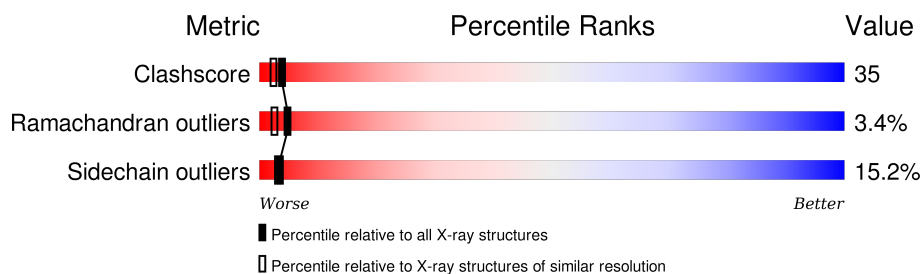
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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	248	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2024 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 BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	1	0
			1934	1218	341	367	8			

- Molecule 2 is water.

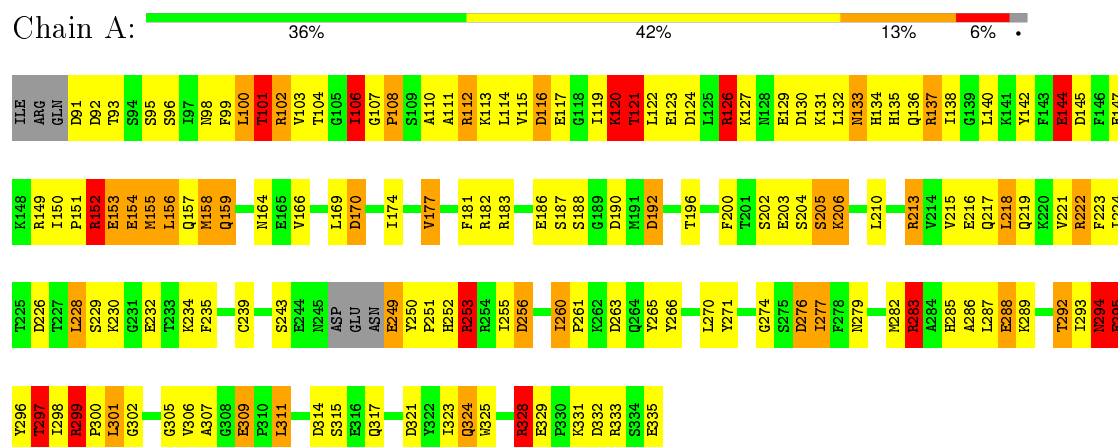
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	90	Total	O	1	0
			90	90		

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 BETA



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	120.58Å 63.52Å 38.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.193 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2024	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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	1.23	14/1972 (0.7%)	1.81	71/2661 (2.7%)

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	1	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	GLU	CD-OE1	6.58	1.32	1.25
1	A	154	GLU	CD-OE1	6.54	1.32	1.25
1	A	309	GLU	CD-OE1	6.33	1.32	1.25
1	A	232	GLU	CD-OE1	6.26	1.32	1.25
1	A	203	GLU	CD-OE1	6.13	1.32	1.25
1	A	144	GLU	CD-OE1	5.96	1.32	1.25
1	A	186	GLU	CD-OE1	5.86	1.32	1.25
1	A	153	GLU	CD-OE2	5.65	1.31	1.25
1	A	335	GLU	CD-OE1	5.45	1.31	1.25
1	A	249	GLU	CD-OE1	5.43	1.31	1.25
1	A	147	GLU	CD-OE1	5.34	1.31	1.25
1	A	295	GLU	CD-OE2	5.30	1.31	1.25
1	A	329	GLU	CD-OE1	5.15	1.31	1.25
1	A	129	GLU	CD-OE2	-5.04	1.20	1.25

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ARG	NE-CZ-NH1	13.55	127.08	120.30
1	A	253	ARG	NE-CZ-NH2	-11.34	114.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ARG	C-N-CA	-11.26	93.55	121.70
1	A	120	LYS	O-C-N	-10.83	105.37	122.70
1	A	126	ARG	O-C-N	9.74	138.29	122.70
1	A	112	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	A	299[A]	ARG	NE-CZ-NH1	9.65	125.12	120.30
1	A	299[B]	ARG	NE-CZ-NH1	9.65	125.12	120.30
1	A	314	ASP	CB-CG-OD1	-9.20	110.02	118.30
1	A	182	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	A	190	ASP	CB-CG-OD2	-8.48	110.67	118.30
1	A	190	ASP	CB-CG-OD1	8.43	125.89	118.30
1	A	126	ARG	CA-C-N	-8.16	99.24	117.20
1	A	192	ASP	CB-CG-OD1	-7.98	111.11	118.30
1	A	321	ASP	CB-CG-OD1	-7.98	111.11	118.30
1	A	283	ARG	NE-CZ-NH1	7.47	124.04	120.30
1	A	276	ASP	CB-CG-OD1	-7.08	111.93	118.30
1	A	170	ASP	CB-CG-OD1	-6.95	112.05	118.30
1	A	137	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	A	266	TYR	CB-CG-CD1	-6.83	116.90	121.00
1	A	112	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	137	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	152	ARG	N-CA-CB	6.69	122.65	110.60
1	A	299[A]	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	299[B]	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	213	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	182	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	A	314	ASP	CB-CG-OD2	6.49	124.14	118.30
1	A	130	ASP	CB-CG-OD1	-6.44	112.51	118.30
1	A	145	ASP	CB-CG-OD1	-6.38	112.56	118.30
1	A	183	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	299[A]	ARG	CD-NE-CZ	6.31	132.44	123.60
1	A	299[B]	ARG	CD-NE-CZ	6.31	132.44	123.60
1	A	149	ARG	NE-CZ-NH2	6.24	123.42	120.30
1	A	102	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	A	192	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	166	VAL	CA-CB-CG1	6.07	120.01	110.90
1	A	294	ASN	N-CA-CB	5.94	121.30	110.60
1	A	132	LEU	CB-CA-C	-5.88	99.03	110.20
1	A	222	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	283	ARG	N-CA-CB	5.83	121.08	110.60
1	A	112	ARG	CD-NE-CZ	5.82	131.75	123.60
1	A	260	ILE	CB-CA-C	-5.79	100.01	111.60
1	A	155	MET	CA-CB-CG	-5.72	103.58	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	155	MET	CG-SD-CE	5.64	109.22	100.20
1	A	145	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	297	THR	CA-C-N	-5.61	104.85	117.20
1	A	116	ASP	CB-CG-OD2	-5.57	113.28	118.30
1	A	249	GLU	N-CA-CB	5.57	120.63	110.60
1	A	328	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	A	101	THR	CA-CB-CG2	-5.56	104.62	112.40
1	A	263	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	A	102	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	253	ARG	CD-NE-CZ	5.41	131.18	123.60
1	A	263	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	226	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	A	170	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	293	ILE	CB-CA-C	-5.31	100.98	111.60
1	A	106	ILE	CG1-CB-CG2	-5.26	99.82	111.40
1	A	151	PRO	CB-CA-C	-5.25	98.88	112.00
1	A	226	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	131	LYS	CB-CA-C	5.18	120.77	110.40
1	A	286	ALA	CB-CA-C	-5.17	102.34	110.10
1	A	332	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	166	VAL	CG1-CB-CG2	5.14	119.13	110.90
1	A	256	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	332	ASP	CB-CG-OD1	-5.06	113.75	118.30
1	A	166	VAL	CA-CB-CG2	5.05	118.47	110.90
1	A	222	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	120	LYS	CA-C-N	5.01	128.23	117.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	249	GLU	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	LYS	Mainchain
1	A	297	THR	Mainchain

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	1934	0	1863	132	1
2	A	90	0	0	5	1
All	All	2024	0	1863	132	2

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 35.

All (132) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:O	1:A:126:ARG:HG3	1.54	1.07
1:A:294:ASN:HD22	1:A:296:TYR:H	1.17	0.90
1:A:270:LEU:HD21	1:A:282:MET:CE	2.01	0.90
1:A:270:LEU:HD21	1:A:282:MET:HE1	1.51	0.90
1:A:159:GLN:HB2	1:A:177:VAL:HG11	1.59	0.85
1:A:294:ASN:ND2	1:A:296:TYR:H	1.75	0.85
1:A:154:GLU:O	1:A:158:MET:HG2	1.84	0.76
1:A:133:ASN:ND2	1:A:136:GLN:H	1.84	0.76
1:A:138:ILE:HB	1:A:228:LEU:CD1	2.17	0.74
1:A:121:THR:O	1:A:124:ASP:HB2	1.86	0.74
1:A:104:THR:HG22	2:A:435:HOH:O	1.89	0.73
1:A:98:ASN:O	1:A:101:THR:HG22	1.88	0.72
1:A:92:ASP:O	1:A:95:SER:HB3	1.90	0.71
1:A:288:GLU:N	1:A:288:GLU:OE1	2.24	0.71
1:A:315:SER:HB2	1:A:317:GLN:NE2	2.08	0.69
1:A:111:ALA:O	1:A:115:VAL:HG23	1.94	0.67
1:A:270:LEU:HD12	1:A:333:ARG:NH1	2.10	0.66
1:A:243:SER:CB	1:A:249:GLU:HG2	2.26	0.66
1:A:305:GLY:O	1:A:307:ALA:N	2.30	0.65
1:A:108:PRO:O	1:A:111:ALA:N	2.31	0.64
1:A:295:GLU:OE1	1:A:295:GLU:N	2.29	0.64
1:A:100:LEU:O	1:A:103:VAL:HG23	1.97	0.64
1:A:133:ASN:HD21	1:A:135:HIS:HB3	1.62	0.64
1:A:133:ASN:H	1:A:136:GLN:NE2	1.96	0.63
1:A:140:LEU:HD23	2:A:472:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:LEU:HB2	1:A:224:ILE:HD12	1.83	0.61
1:A:204:SER:O	1:A:206:LYS:HD3	2.02	0.60
1:A:274:GLY:HA2	1:A:279:ASN:OD1	2.02	0.59
1:A:279:ASN:O	1:A:283:ARG:HG2	2.03	0.59
1:A:144:GLU:OE1	1:A:144:GLU:N	2.35	0.59
1:A:133:ASN:HD22	1:A:133:ASN:C	2.07	0.58
1:A:299[A]:ARG:HG3	1:A:299[A]:ARG:HH11	1.68	0.58
1:A:113:LYS:O	1:A:117:GLU:HG2	2.04	0.58
1:A:174:ILE:HB	1:A:196:THR:HG22	1.85	0.58
1:A:155:MET:HE2	1:A:188:SER:HB2	1.85	0.57
1:A:315:SER:HB2	1:A:317:GLN:HE22	1.69	0.57
1:A:215:VAL:O	1:A:219:GLN:HG3	2.03	0.57
1:A:138:ILE:HB	1:A:228:LEU:HD11	1.86	0.56
1:A:295:GLU:H	1:A:295:GLU:CD	2.08	0.56
1:A:292:THR:HG22	1:A:301:LEU:CD1	2.35	0.56
1:A:251:PRO:HG2	1:A:253:ARG:CZ	2.35	0.56
1:A:122:LEU:HD13	1:A:126:ARG:CZ	2.34	0.56
1:A:285:HIS:O	1:A:288:GLU:N	2.39	0.56
1:A:150:ILE:HD12	1:A:155:MET:CE	2.35	0.55
1:A:123:GLU:O	1:A:127:LYS:HG2	2.06	0.55
1:A:159:GLN:HB2	1:A:177:VAL:CG1	2.32	0.55
1:A:270:LEU:HD21	1:A:282:MET:HE3	1.82	0.55
1:A:122:LEU:O	1:A:126:ARG:CG	2.44	0.54
1:A:150:ILE:HD12	1:A:155:MET:HE2	1.89	0.54
1:A:255:ILE:HG12	1:A:256:ASP:N	2.22	0.53
1:A:205:SER:C	1:A:206:LYS:HG2	2.29	0.53
1:A:271:TYR:CG	1:A:295:GLU:HB3	2.43	0.53
1:A:213:ARG:NH1	2:A:477:HOH:O	2.42	0.53
1:A:133:ASN:HD21	1:A:136:GLN:H	1.57	0.52
1:A:91:ASP:CB	1:A:93:THR:HG22	2.39	0.52
1:A:119:ILE:HA	1:A:124:ASP:OD2	2.10	0.52
1:A:169:LEU:O	1:A:170:ASP:HB2	2.09	0.51
1:A:217:GLN:O	1:A:221:VAL:HG22	2.11	0.51
1:A:99:PHE:O	1:A:102:ARG:HB2	2.11	0.51
1:A:289:LYS:HD2	1:A:323:ILE:O	2.11	0.50
1:A:93:THR:O	1:A:96:SER:HB2	2.11	0.50
1:A:298:ILE:O	1:A:298:ILE:HG23	2.11	0.50
1:A:221:VAL:O	1:A:222:ARG:HB2	2.11	0.50
1:A:93:THR:O	1:A:96:SER:N	2.43	0.50
1:A:134:HIS:O	1:A:138:ILE:HG12	2.12	0.49
1:A:292:THR:O	1:A:292:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:MET:HA	1:A:158:MET:CG	2.42	0.49
1:A:292:THR:CG2	1:A:301:LEU:HD11	2.42	0.49
1:A:202:SER:N	1:A:261:PRO:HB3	2.28	0.49
1:A:294:ASN:ND2	1:A:297:THR:H	2.11	0.49
1:A:155:MET:HA	1:A:158:MET:HG3	1.95	0.49
1:A:135:HIS:CD2	1:A:228:LEU:HG	2.47	0.49
1:A:174:ILE:HG21	1:A:265:TYR:CE2	2.48	0.49
1:A:153:GLU:O	1:A:157:GLN:HG3	2.13	0.49
1:A:106:ILE:HG23	1:A:106:ILE:HD13	1.43	0.48
1:A:103:VAL:HB	1:A:106:ILE:CD1	2.43	0.48
1:A:110:ALA:HA	1:A:113:LYS:HE3	1.96	0.48
1:A:223:PHE:O	1:A:239:CYS:HA	2.14	0.47
1:A:133:ASN:ND2	1:A:135:HIS:HB3	2.29	0.47
1:A:113:LYS:HG3	1:A:114:LEU:N	2.29	0.47
1:A:107:GLY:O	1:A:111:ALA:N	2.46	0.47
1:A:114:LEU:O	1:A:119:ILE:N	2.42	0.46
1:A:294:ASN:HD22	1:A:295:GLU:N	2.14	0.46
1:A:120:LYS:N	1:A:124:ASP:OD2	2.39	0.46
1:A:133:ASN:H	1:A:136:GLN:HE21	1.62	0.45
1:A:294:ASN:C	1:A:294:ASN:HD22	2.19	0.45
1:A:315:SER:CB	1:A:317:GLN:NE2	2.79	0.45
1:A:299[B]:ARG:HB3	1:A:300:PRO:HD2	1.97	0.45
1:A:152:ARG:NH2	1:A:181:PHE:O	2.50	0.45
1:A:101:THR:HA	1:A:106:ILE:O	2.18	0.44
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.54	0.44
1:A:126:ARG:O	1:A:127:LYS:C	2.51	0.44
1:A:297:THR:O	1:A:299[A]:ARG:NH1	2.50	0.44
1:A:113:LYS:HG3	1:A:114:LEU:HD12	1.99	0.44
1:A:282:MET:HB3	1:A:282:MET:HE2	1.72	0.44
1:A:142:TYR:CE1	1:A:252:HIS:CG	3.06	0.43
1:A:120:LYS:C	1:A:121:THR:O	2.57	0.43
1:A:328:ARG:NE	2:A:430:HOH:O	2.52	0.43
1:A:255:ILE:CG1	1:A:256:ASP:N	2.81	0.43
1:A:137:ARG:NE	2:A:450:HOH:O	2.49	0.43
1:A:323:ILE:O	1:A:324:GLN:HG2	2.19	0.43
1:A:159:GLN:HG3	1:A:159:GLN:O	2.17	0.43
1:A:93:THR:C	1:A:96:SER:H	2.21	0.43
1:A:177:VAL:HG22	1:A:181:PHE:CD2	2.54	0.42
1:A:150:ILE:HG12	1:A:253:ARG:HG2	2.00	0.42
1:A:234:LYS:HG3	1:A:235:PHE:N	2.33	0.42
1:A:106:ILE:HG21	1:A:106:ILE:HD12	1.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LEU:CD1	1:A:311:LEU:N	2.82	0.42
1:A:249:GLU:OE2	1:A:250:TYR:HD1	2.02	0.42
1:A:302:GLY:N	1:A:307:ALA:HB3	2.35	0.42
1:A:287:LEU:HB3	1:A:288:GLU:OE1	2.20	0.42
1:A:92:ASP:C	1:A:95:SER:HB3	2.39	0.42
1:A:108:PRO:O	1:A:112:ARG:N	2.39	0.42
1:A:205:SER:O	1:A:206:LYS:HB3	2.20	0.42
1:A:255:ILE:O	1:A:256:ASP:OD1	2.36	0.42
1:A:234:LYS:CG	1:A:235:PHE:N	2.80	0.42
1:A:122:LEU:C	1:A:122:LEU:HD12	2.40	0.41
1:A:200:PHE:HE1	1:A:205:SER:HA	1.85	0.41
1:A:230:LYS:O	1:A:230:LYS:HG2	2.20	0.41
1:A:156:LEU:HA	1:A:156:LEU:HD12	1.61	0.41
1:A:150:ILE:O	1:A:187:SER:HA	2.21	0.41
1:A:260:ILE:CG2	1:A:261:PRO:HD2	2.51	0.41
1:A:277:ILE:HD13	1:A:277:ILE:HG23	1.80	0.41
1:A:218:LEU:CB	1:A:224:ILE:HD12	2.49	0.41
1:A:210:LEU:HD23	1:A:210:LEU:HA	1.95	0.41
1:A:150:ILE:CD1	1:A:155:MET:CE	2.99	0.41
1:A:218:LEU:HA	1:A:221:VAL:CG2	2.51	0.41
1:A:138:ILE:HG23	1:A:138:ILE:HD12	1.73	0.41
1:A:142:TYR:CE1	1:A:252:HIS:CD2	3.09	0.41
1:A:294:ASN:HB2	1:A:295:GLU:OE1	2.21	0.40
1:A:218:LEU:HA	1:A:221:VAL:HG22	2.02	0.40
1:A:106:ILE:HG22	1:A:136:GLN:HG2	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:468:HOH:O	2:A:468:HOH:O[2_565]	0.30	1.90
1:A:204:SER:OG	1:A:206:LYS:CE[2_555]	2.17	0.03

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	239/248 (96%)	214 (90%)	17 (7%)	8 (3%)	5 3

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	THR
1	A	206	LYS
1	A	306	VAL
1	A	309	GLU
1	A	205	SER
1	A	108	PRO
1	A	144	GLU
1	A	324	GLN

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	205/226 (91%)	173 (84%)	32 (16%)	3 3

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	LEU
1	A	101	THR
1	A	106	ILE
1	A	116	ASP
1	A	121	THR
1	A	126	ARG
1	A	133	ASN
1	A	152	ARG
1	A	156	LEU
1	A	158	MET
1	A	159	GLN

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Mol	Chain	Res	Type
1	A	164	ASN
1	A	177	VAL
1	A	192	ASP
1	A	218	LEU
1	A	228	LEU
1	A	229	SER
1	A	253	ARG
1	A	276	ASP
1	A	277	ILE
1	A	283	ARG
1	A	288	GLU
1	A	292	THR
1	A	294	ASN
1	A	295	GLU
1	A	299[A]	ARG
1	A	299[B]	ARG
1	A	301	LEU
1	A	311	LEU
1	A	325	TRP
1	A	328	ARG
1	A	331	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	ASN
1	A	135	HIS
1	A	136	GLN
1	A	157	GLN
1	A	217	GLN
1	A	219	GLN
1	A	252	HIS
1	A	281	ASN
1	A	285	HIS
1	A	294	ASN
1	A	317	GLN

5.3.3 RNA ⓘ

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

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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