



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:34 AM GMT

PDB ID : 2HPI
Title : Eubacterial and Eukaryotic Replicative DNA Polymerases are not Homologous: X-ray Structure of DNA Polymerase III
Authors : Bailey, S.; Wing, R.A.; Steitz, T.A.
Deposited on : 2006-07-17
Resolution : 3.00 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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

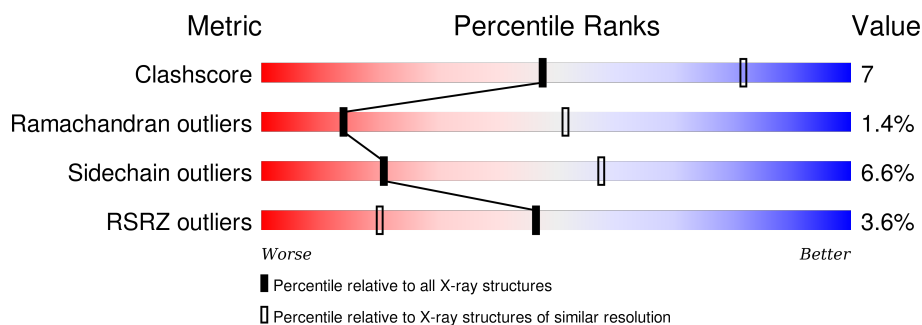
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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.

Mol	Chain	Length	Quality of chain
1	A	1220	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9155 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 III alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1143	Total	C	N	O	S	0	0	0
			9127	5820	1598	1681	28			

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

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total	O	0	0
			22	22		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	175.15Å 186.88Å 125.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 19.93 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-3.00) 97.5 (19.93-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.275 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	100.1	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 116.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 40263 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9155	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.37	0/9307	0.55	0/12562

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	337	LEU	Mainchain

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	9127	0	9158	136	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	0	0	0	0
4	A	2	0	0	0	0
5	A	22	0	0	2	0
All	All	9155	0	9158	136	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (136) 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:321:ARG:HH22	1:A:440:ASN:ND2	1.65	0.94
1:A:1143:LYS:HA	1:A:1147:ARG:HB2	1.50	0.92
1:A:321:ARG:HH22	1:A:440:ASN:HD21	1.11	0.92
1:A:743:TYR:H	1:A:746:GLN:HE21	1.30	0.78
1:A:1013:HIS:HD2	1:A:1015:VAL:H	1.30	0.78
1:A:8:ALA:H	1:A:274:THR:HG21	1.49	0.77
1:A:439:THR:HG21	5:A:1248:HOH:O	1.83	0.77
1:A:667:VAL:HA	1:A:828:THR:HG21	1.69	0.74
1:A:835:TYR:HB3	1:A:838:GLU:CG	2.18	0.74
1:A:8:ALA:H	1:A:274:THR:CG2	2.01	0.73
1:A:407:GLN:HG3	1:A:436:VAL:HG12	1.72	0.71
1:A:660:SER:HB3	1:A:683:LYS:HD3	1.71	0.71
1:A:835:TYR:HB3	1:A:838:GLU:HG2	1.74	0.69
1:A:1159:LEU:HD11	1:A:1183:GLU:HG2	1.72	0.69
1:A:1176:LEU:HD23	1:A:1179:VAL:HB	1.75	0.69
1:A:602:THR:HG22	1:A:604:TYR:H	1.59	0.67
1:A:840:MET:HA	1:A:840:MET:HE2	1.75	0.67
1:A:951:ALA:HB2	1:A:993:LEU:HG	1.78	0.66
1:A:77:ALA:O	1:A:129:ARG:NH2	2.28	0.66
1:A:1019:PRO:O	1:A:1023:GLU:HG2	1.96	0.66
1:A:1053:GLU:HB3	1:A:1068:PHE:HA	1.80	0.64
1:A:662:GLY:HA3	1:A:680:ARG:HG3	1.82	0.62
1:A:504:LEU:HD12	1:A:525:ILE:HD11	1.81	0.62
1:A:1039:LEU:HB3	1:A:1040:PRO:HD2	1.82	0.61
1:A:742:VAL:H	1:A:746:GLN:NE2	1.99	0.61
1:A:170:LEU:HD21	1:A:205:LEU:HD21	1.83	0.60
1:A:665:LYS:HB2	1:A:832:LYS:HZ1	1.65	0.60
1:A:402:TYR:HE1	1:A:615:LEU:HD11	1.65	0.60
1:A:186:LEU:HD21	1:A:245:PRO:HB2	1.85	0.59
1:A:743:TYR:HB2	1:A:746:GLN:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:VAL:HA	1:A:828:THR:CG2	2.31	0.59
1:A:447:GLY:H	1:A:815:LYS:NZ	2.00	0.59
1:A:148:ALA:O	1:A:152:GLN:HB2	2.03	0.57
1:A:406:VAL:HA	1:A:409:TYR:CE2	2.40	0.57
1:A:591:PRO:HG2	1:A:603:GLN:HB2	1.86	0.56
1:A:897:VAL:HG21	1:A:938:LEU:HD13	1.87	0.56
1:A:402:TYR:HE1	1:A:615:LEU:CD1	2.19	0.56
1:A:1143:LYS:HG2	1:A:1147:ARG:HD2	1.88	0.55
1:A:441:ILE:HD12	1:A:823:LEU:HD12	1.88	0.55
1:A:238:ASP:HB3	1:A:239:PRO:CA	2.36	0.55
1:A:703:GLU:O	1:A:706:PRO:HD2	2.06	0.55
1:A:407:GLN:HG3	1:A:436:VAL:CG1	2.36	0.54
1:A:590:VAL:CG1	1:A:602:THR:HG23	2.38	0.54
1:A:321:ARG:NH2	1:A:440:ASN:ND2	2.48	0.54
1:A:15:GLN:HE21	1:A:25:LEU:HB2	1.74	0.53
1:A:920:ASP:HA	1:A:923:LYS:HE2	1.90	0.53
1:A:840:MET:HG2	1:A:861:ALA:HB2	1.91	0.53
1:A:982:VAL:HG13	1:A:982:VAL:O	2.09	0.53
1:A:788:ALA:HB1	1:A:793:VAL:HG23	1.90	0.52
1:A:399:PHE:N	1:A:400:PRO:CD	2.72	0.52
1:A:1039:LEU:HB3	1:A:1040:PRO:CD	2.39	0.52
1:A:238:ASP:HB3	1:A:239:PRO:C	2.29	0.52
1:A:239:PRO:O	1:A:240:GLU:CB	2.58	0.52
1:A:862:ARG:HH22	1:A:1011:SER:H	1.57	0.52
1:A:788:ALA:HB1	1:A:793:VAL:CG2	2.40	0.52
1:A:549:MET:HG2	1:A:559:ILE:HD12	1.92	0.51
1:A:439:THR:CG2	5:A:1248:HOH:O	2.50	0.51
1:A:675:MET:O	1:A:679:VAL:HG23	2.10	0.51
1:A:447:GLY:H	1:A:815:LYS:HZ1	1.59	0.51
1:A:80:ARG:N	1:A:128:ASP:OD1	2.44	0.51
1:A:727:GLU:OE2	1:A:731:ARG:NH1	2.43	0.50
1:A:627:PHE:HA	1:A:846:VAL:HG21	1.93	0.50
1:A:1140:LEU:H	1:A:1143:LYS:HD2	1.77	0.50
1:A:128:ASP:H	1:A:131:ILE:HG12	1.77	0.50
1:A:1181:VAL:HG11	1:A:1185:ALA:HB3	1.93	0.49
1:A:473:ARG:NH1	1:A:477:ILE:HD11	2.26	0.49
1:A:840:MET:HE2	1:A:843:LEU:HD12	1.94	0.49
1:A:1039:LEU:HG	1:A:1040:PRO:HD3	1.95	0.49
1:A:286:PRO:HA	1:A:290:LYS:HG3	1.95	0.49
1:A:1039:LEU:CB	1:A:1040:PRO:CD	2.91	0.49
1:A:1029:ILE:HG12	1:A:1072:ASP:CG	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1173:LEU:HD13	1:A:1202:ARG:HH22	1.78	0.49
1:A:367:LYS:O	1:A:368:ARG:HG2	2.13	0.48
1:A:1050:MET:O	1:A:1070:LEU:HA	2.13	0.48
1:A:521:LEU:HD21	1:A:548:GLU:HG2	1.95	0.48
1:A:181:ILE:HD13	1:A:266:TRP:CZ3	2.48	0.48
1:A:379:THR:HG23	1:A:382:ALA:H	1.79	0.48
1:A:1053:GLU:CB	1:A:1068:PHE:HA	2.44	0.48
1:A:425:GLY:H	1:A:817:HIS:CD2	2.32	0.48
1:A:1105:VAL:HG22	1:A:1113:VAL:HG22	1.96	0.47
1:A:1140:LEU:HD12	1:A:1143:LYS:HE3	1.96	0.47
1:A:590:VAL:HG11	1:A:602:THR:HG23	1.95	0.47
1:A:776:GLU:HG2	1:A:779:LYS:HD2	1.97	0.47
1:A:595:ASP:OD2	1:A:599:ARG:HD2	2.13	0.47
1:A:319:LEU:HD13	1:A:347:GLU:HG3	1.95	0.47
1:A:215:TYR:HB2	1:A:220:ASP:HB2	1.97	0.47
1:A:364:GLU:HA	1:A:367:LYS:HE2	1.96	0.47
1:A:402:TYR:CE2	1:A:462:PRO:HG2	2.50	0.46
1:A:236:LEU:O	1:A:241:ARG:NE	2.48	0.46
1:A:835:TYR:HB3	1:A:838:GLU:HG3	1.95	0.45
1:A:151:PRO:HB3	1:A:192:VAL:HG11	1.99	0.45
1:A:470:ASP:OD2	1:A:623:ARG:HA	2.16	0.45
1:A:1046:LEU:HA	1:A:1101:VAL:O	2.16	0.45
1:A:1036:VAL:HG13	1:A:1043:PRO:HG2	1.97	0.45
1:A:139:LEU:O	1:A:176:ARG:HD2	2.16	0.45
1:A:57:TYR:O	1:A:61:THR:HB	2.17	0.45
1:A:528:GLN:HB3	1:A:533:LYS:HE3	2.00	0.44
1:A:785:VAL:HG13	1:A:795:GLU:HB2	1.99	0.44
1:A:257:MET:HA	1:A:257:MET:HE2	1.99	0.44
1:A:570:ARG:HA	1:A:570:ARG:HD3	1.84	0.44
1:A:321:ARG:HG2	1:A:434:TYR:CE2	2.52	0.44
1:A:290:LYS:HG2	1:A:290:LYS:H	1.47	0.44
1:A:269:GLU:HB2	1:A:270:PRO:HD3	1.99	0.44
1:A:45:THR:HG22	1:A:70:GLY:HA3	1.99	0.44
1:A:800:ARG:O	1:A:803:ASP:HB2	2.17	0.44
1:A:1102:LEU:HD12	1:A:1119:TRP:HH2	1.83	0.43
1:A:838:GLU:CD	1:A:838:GLU:H	2.20	0.43
1:A:795:GLU:HA	1:A:798:ALA:HB3	2.00	0.43
1:A:443:PRO:O	1:A:446:PHE:O	2.36	0.43
1:A:226:VAL:HG21	1:A:561:VAL:HG11	2.01	0.42
1:A:1039:LEU:HG	1:A:1040:PRO:CD	2.50	0.42
1:A:1101:VAL:HG22	1:A:1118:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LYS:HB3	1:A:256:GLU:HB2	2.02	0.42
1:A:431:LEU:HA	1:A:443:PRO:HG3	2.01	0.42
1:A:252:LYS:HD2	1:A:257:MET:HE2	2.02	0.42
1:A:752:SER:HA	1:A:757:TYR:HB2	2.01	0.42
1:A:402:TYR:CE1	1:A:615:LEU:CD1	3.01	0.42
1:A:384:LEU:HD23	1:A:384:LEU:HA	1.91	0.42
1:A:257:MET:CE	1:A:257:MET:HA	2.50	0.42
1:A:915:PHE:HA	1:A:924:ARG:HH21	1.85	0.41
1:A:1072:ASP:C	1:A:1074:THR:H	2.23	0.41
1:A:1026:SER:HA	1:A:1202:ARG:NH2	2.34	0.41
1:A:1014:PRO:HB2	1:A:1050:MET:CE	2.50	0.41
1:A:1036:VAL:O	1:A:1037:ARG:C	2.58	0.41
1:A:594:ARG:HH11	1:A:594:ARG:HG3	1.84	0.41
1:A:313:LEU:HB3	1:A:436:VAL:HG13	2.01	0.41
1:A:252:LYS:HD2	1:A:257:MET:CE	2.50	0.41
1:A:1182:GLY:O	1:A:1183:GLU:HB2	2.21	0.41
1:A:321:ARG:CG	1:A:434:TYR:CE2	3.04	0.41
1:A:316:LEU:HD21	1:A:348:ARG:HA	2.02	0.41
1:A:602:THR:HG21	1:A:609:VAL:CG2	2.51	0.41
1:A:402:TYR:CE1	1:A:615:LEU:HD11	2.52	0.41
1:A:1181:VAL:CG1	1:A:1185:ALA:HB3	2.51	0.41
1:A:725:HIS:HD2	1:A:797:GLU:OE2	2.03	0.41
1:A:27:ASP:HA	1:A:30:LYS:HG2	2.03	0.40
1:A:1042:LYS:HG2	1:A:1106:GLU:HG2	2.03	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	1123/1220 (92%)	1029 (92%)	78 (7%)	16 (1%)	14 51

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	774	VAL
1	A	1039	LEU
1	A	1176	LEU
1	A	290	LYS
1	A	291	MET
1	A	570	ARG
1	A	792	GLY
1	A	975	LEU
1	A	976	VAL
1	A	1177	ARG
1	A	53	ALA
1	A	238	ASP
1	A	736	GLU
1	A	977	GLY
1	A	1193	GLY
1	A	399	PHE

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	949/1009 (94%)	886 (93%)	63 (7%)	21	57

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	61	THR
1	A	75	VAL
1	A	85	ARG
1	A	132	LEU
1	A	165	ARG
1	A	207	MET
1	A	211	ASN
1	A	215	TYR

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Mol	Chain	Res	Type
1	A	222	ARG
1	A	235	THR
1	A	253	THR
1	A	274	THR
1	A	276	GLU
1	A	290	LYS
1	A	300	LEU
1	A	305	THR
1	A	319	LEU
1	A	321	ARG
1	A	326	ILE
1	A	368	ARG
1	A	407	GLN
1	A	424	ARG
1	A	439	THR
1	A	440	ASN
1	A	444	LEU
1	A	452	ARG
1	A	463	ASP
1	A	498	LEU
1	A	519	GLU
1	A	545	LEU
1	A	580	VAL
1	A	587	THR
1	A	616	LYS
1	A	617	MET
1	A	622	LEU
1	A	625	LEU
1	A	670	LEU
1	A	672	SER
1	A	707	THR
1	A	719	SER
1	A	736	GLU
1	A	786	ARG
1	A	795	GLU
1	A	823	LEU
1	A	840	MET
1	A	903	ARG
1	A	927	GLU
1	A	958	GLU
1	A	997	THR
1	A	1018	TYR

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Mol	Chain	Res	Type
1	A	1027	CYS
1	A	1028	THR
1	A	1032	LEU
1	A	1045	VAL
1	A	1046	LEU
1	A	1074	THR
1	A	1095	GLU
1	A	1096	ASP
1	A	1104	GLU
1	A	1169	PHE
1	A	1184	GLU
1	A	1192	GLU

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	9	HIS
1	A	15	GLN
1	A	440	ASN
1	A	575	HIS
1	A	715	GLN
1	A	725	HIS
1	A	746	GLN
1	A	814	ASN
1	A	817	HIS
1	A	1013	HIS
1	A	1155	HIS

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, 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	1143/1220 (93%)	0.07	41 (3%) 46 20	103, 126, 144, 167	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1116	GLN	5.8
1	A	571	HIS	4.6
1	A	775	GLU	4.5
1	A	1195	ARG	4.2
1	A	85	ARG	4.2
1	A	1094	LYS	4.1
1	A	459	VAL	3.2
1	A	531	LYS	3.1
1	A	553	GLU	3.0
1	A	64	GLY	3.0
1	A	324	ASP	3.0
1	A	530	GLY	3.0
1	A	297	ARG	2.9
1	A	974	GLY	2.9
1	A	1080	VAL	2.8
1	A	6	LYS	2.7
1	A	596	GLN	2.7
1	A	1048	SER	2.7
1	A	364	GLU	2.7
1	A	811	TYR	2.6
1	A	911	ARG	2.6
1	A	916	LYS	2.6
1	A	520	GLU	2.5
1	A	377	GLU	2.4
1	A	242	TRP	2.4
1	A	912	GLY	2.3
1	A	91	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	969	GLU	2.3
1	A	973	SER	2.3
1	A	39	ASP	2.3
1	A	773	ARG	2.2
1	A	527	VAL	2.2
1	A	515	HIS	2.2
1	A	1160	PRO	2.1
1	A	63	MET	2.1
1	A	975	LEU	2.1
1	A	359	GLU	2.1
1	A	264	ALA	2.1
1	A	914	PRO	2.1
1	A	1016	LEU	2.1
1	A	1037	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. 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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	MG	A	1223	1/1	0.85	0.17	-0.66	125,125,125,125	0
3	MG	A	1224	1/1	0.95	0.13	-1.06	83,83,83,83	0
2	ZN	A	1222	1/1	0.97	0.10	-1.48	102,102,102,102	0
2	ZN	A	1221	1/1	0.99	0.11	-	96,96,96,96	0
4	CL	A	1225	1/1	0.80	0.11	-	118,118,118,118	0
4	CL	A	1226	1/1	0.90	0.35	-	112,112,112,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.