



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:03 PM UTC

PDB ID : 2HNH / pdb_00002hnh
Title : Crystal structure of the catalytic alpha subunit of E. coli replicative DNA polymerase III
Authors : Meindert, M.H.; Georgescu, R.E.; Lee, S.; O'Donnell, M.; Kuriyan, J.
Deposited on : 2006-07-12
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

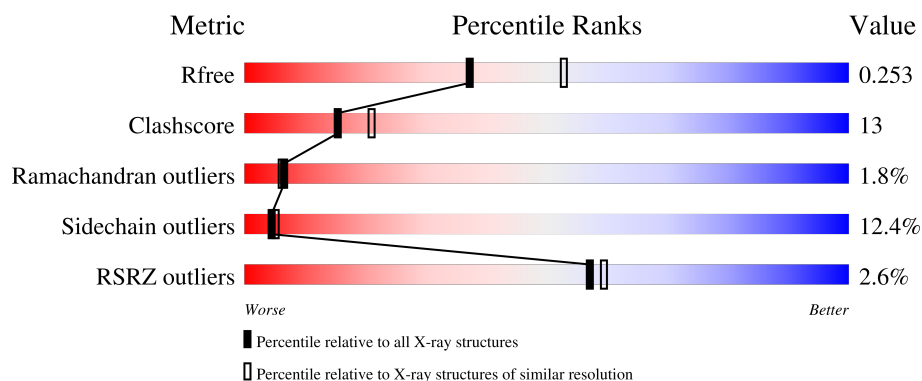
1 Overall quality at a glance

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))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 of 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	910	3% 70% 24% 6%

2 Entry composition [i](#)

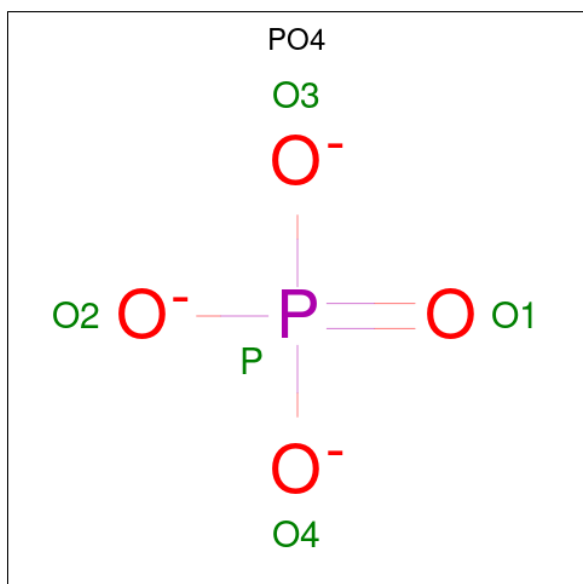
There are 3 unique types of molecules in this entry. The entry contains 7621 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	910	Total	C	N	O	S	0	9	0
			7207	4588	1229	1347	43			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

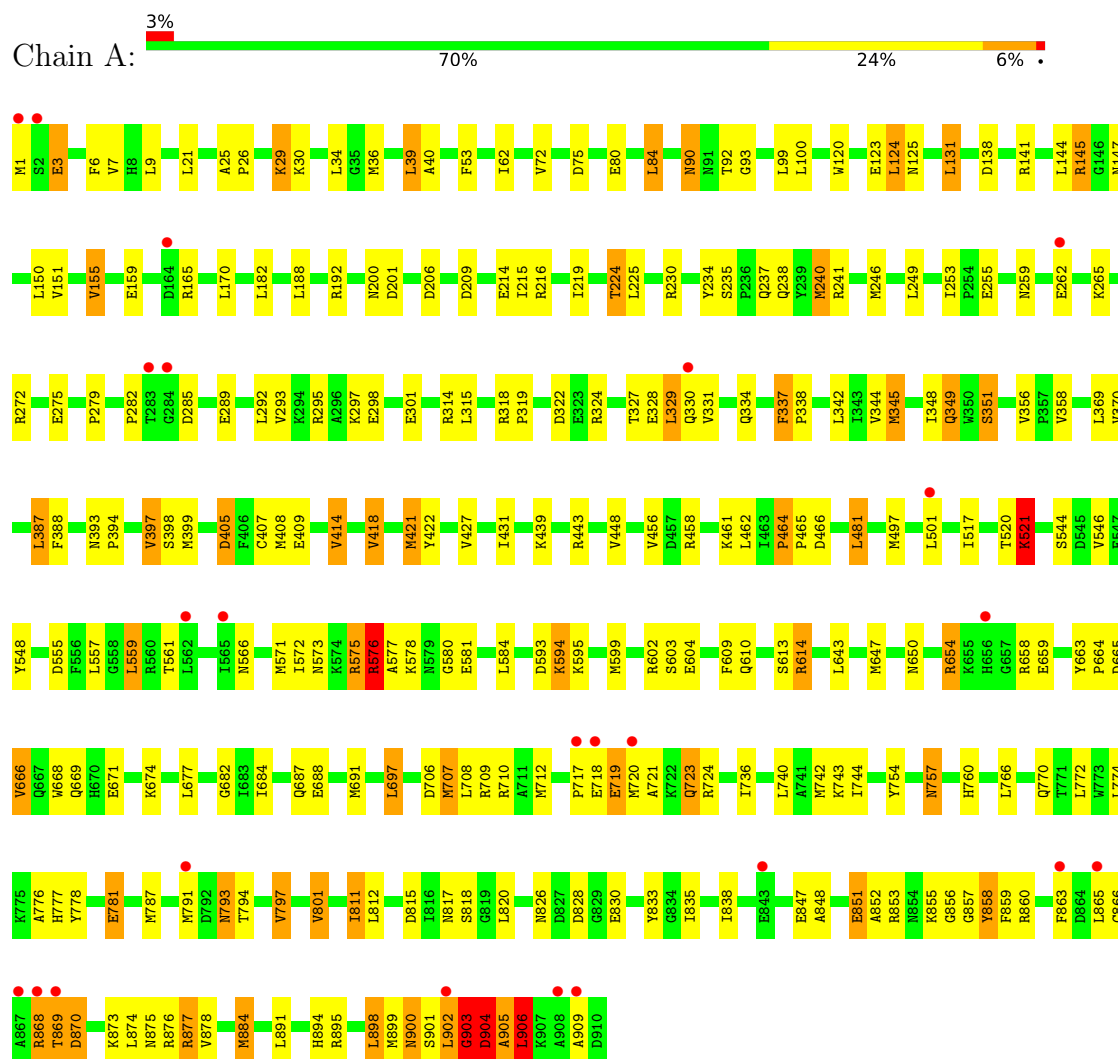
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	399	Total 399	O 399	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: DNA polymerase III alpha subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.58Å 92.60Å 130.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.8 (20.00-2.30) 89.6 (20.00-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.30Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.186 , 0.258 0.184 , 0.253	Depositor DCC
R_{free} test set	2021 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7621	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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: PO4

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	0.77	3/7381 (0.0%)	1.02	5/9975 (0.1%)

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	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	895	ARG	C-N	8.03	1.43	1.33
1	A	684	ILE	CA-CB	5.57	1.59	1.53
1	A	431	ILE	CA-CB	5.55	1.60	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	666	VAL	CB-CA-C	-6.18	103.97	111.88
1	A	414	VAL	N-CA-C	5.73	116.51	110.72
1	A	464	PRO	CA-C-N	5.58	125.25	119.05
1	A	464	PRO	C-N-CA	5.58	125.25	119.05
1	A	895	ARG	O-C-N	5.42	128.35	122.11

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	LEU	Peptide
1	A	901	SER	Peptide
1	A	903	GLY	Peptide
1	A	905	ALA	Peptide

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	7207	0	7162	194	0
2	A	15	0	0	0	0
3	A	399	0	0	11	0
All	All	7621	0	7162	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 13.

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:A:857:GLY:HA2	1:A:858:TYR:CB	1.67	1.17
1:A:857:GLY:CA	1:A:858:TYR:HB2	1.75	1.12
1:A:903:GLY:CA	1:A:904:ASP:HB2	1.76	1.12
1:A:863:PHE:CE1	1:A:905:ALA:HB3	1.87	1.10
1:A:614:ARG:HH11	1:A:614:ARG:HG2	1.20	1.07
1:A:708:LEU:HD13	1:A:723:GLN:HG2	1.36	1.06
1:A:863:PHE:CD1	1:A:905:ALA:HB3	1.91	1.05
1:A:863:PHE:CD1	1:A:905:ALA:CB	2.40	1.05
1:A:902:LEU:HD12	1:A:902:LEU:O	1.57	1.02
1:A:863:PHE:CE1	1:A:905:ALA:CB	2.41	1.02
1:A:857:GLY:HA2	1:A:858:TYR:HB2	1.03	1.01
1:A:576:ARG:HB2	3:A:1244:HOH:O	1.61	1.00
1:A:903:GLY:HA3	1:A:904:ASP:CB	1.90	1.00
1:A:903:GLY:HA3	1:A:904:ASP:HB2	0.99	0.97
1:A:576:ARG:HG3	1:A:577:ALA:N	1.81	0.95
1:A:331:VAL:HG11	1:A:388:PHE:HE1	1.33	0.93
1:A:330:GLN:O	1:A:334[A]:GLN:HG3	1.70	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:VAL:HG12	1:A:427:VAL:HG21	1.53	0.91
1:A:573:ASN:O	1:A:576:ARG:HB3	1.75	0.87
1:A:902:LEU:N	1:A:903:GLY:CA	2.38	0.87
1:A:331:VAL:HG11	1:A:388:PHE:CE1	2.12	0.84
1:A:720[B]:MET:HG3	1:A:721:ALA:N	1.95	0.81
1:A:345:MET:SD	3:A:1240:HOH:O	2.38	0.80
1:A:724:ARG:HD2	1:A:742:MET:HE2	1.65	0.78
1:A:742:MET:HE3	1:A:742:MET:HA	1.64	0.78
1:A:853:ARG:HB2	1:A:859:PHE:CE1	2.19	0.77
1:A:216:ARG:HB2	1:A:501:LEU:HD11	1.67	0.77
1:A:418:VAL:HG12	1:A:427:VAL:CG2	2.16	0.75
1:A:863:PHE:CD1	1:A:905:ALA:HB1	2.21	0.75
1:A:314:ARG:O	1:A:318:ARG:HB2	1.87	0.74
1:A:224:THR:HG23	3:A:971:HOH:O	1.86	0.73
1:A:614:ARG:HG2	1:A:614:ARG:NH1	1.92	0.73
1:A:215:ILE:CD1	1:A:497:MET:HG2	2.18	0.73
1:A:708:LEU:CD1	1:A:723:GLN:HG2	2.17	0.70
1:A:826:ASN:HD21	1:A:828:ASP:HB2	1.57	0.70
1:A:219:ILE:HG13	1:A:448:VAL:HG21	1.74	0.69
1:A:39:LEU:O	1:A:53:PHE:HZ	1.75	0.69
1:A:857:GLY:CA	1:A:858:TYR:CB	2.52	0.69
1:A:650:ASN:O	1:A:654:ARG:HG2	1.93	0.69
1:A:235:SER:H	1:A:238:GLN:HE21	1.41	0.68
1:A:787:MET:HE1	1:A:811:ILE:HD13	1.76	0.68
1:A:724:ARG:CD	1:A:742:MET:HE2	2.25	0.67
1:A:614:ARG:HH11	1:A:614:ARG:CG	2.05	0.66
1:A:902:LEU:N	1:A:903:GLY:HA3	2.09	0.65
1:A:650:ASN:O	1:A:654:ARG:CG	2.44	0.65
1:A:902:LEU:N	1:A:903:GLY:HA2	2.12	0.64
1:A:853:ARG:HB2	1:A:859:PHE:CZ	2.33	0.64
1:A:594:LYS:HG3	1:A:595:LYS:H	1.62	0.63
1:A:863:PHE:CG	1:A:905:ALA:HB1	2.33	0.63
1:A:609:PHE:O	1:A:610:GLN:HB2	1.98	0.63
1:A:869:THR:HA	1:A:870:ASP:HB2	1.81	0.62
1:A:599:MET:HE3	1:A:772:LEU:HD12	1.82	0.62
1:A:170:LEU:HD22	1:A:182:LEU:HG	1.82	0.62
1:A:331:VAL:CG1	1:A:388:PHE:CE1	2.81	0.62
1:A:301:GLU:OE2	1:A:318:ARG:NH2	2.32	0.61
1:A:902:LEU:HD12	1:A:902:LEU:C	2.25	0.61
1:A:125:ASN:O	1:A:165:ARG:NH2	2.34	0.61
1:A:902:LEU:H	1:A:903:GLY:HA2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:VAL:CG1	1:A:388:PHE:HE1	2.11	0.60
1:A:869:THR:HA	1:A:870:ASP:CB	2.32	0.60
1:A:863:PHE:CE1	1:A:905:ALA:HB2	2.33	0.60
1:A:324:ARG:HD2	1:A:328:GLU:OE1	2.01	0.59
1:A:697:LEU:HD22	1:A:736:ILE:HD13	1.84	0.59
1:A:647:MET:HE1	1:A:754:TYR:HD1	1.66	0.59
1:A:902:LEU:H	1:A:903:GLY:CA	2.15	0.59
1:A:215:ILE:HD13	1:A:497:MET:HG2	1.83	0.59
1:A:576:ARG:HD2	1:A:581:GLU:O	2.03	0.59
1:A:319:PRO:HA	3:A:1188:HOH:O	2.03	0.57
1:A:215:ILE:HD12	1:A:497:MET:HG2	1.85	0.57
1:A:318:ARG:NH1	1:A:322:ASP:OD1	2.37	0.57
1:A:9:LEU:HA	1:A:40:ALA:HB3	1.87	0.56
1:A:863:PHE:CZ	1:A:905:ALA:HB2	2.40	0.56
1:A:572:ILE:HG13	1:A:781:GLU:HG3	1.86	0.56
1:A:691:MET:HE3	1:A:706:ASP:HB2	1.88	0.56
1:A:279:PRO:HG3	1:A:517:ILE:HG22	1.86	0.55
1:A:903:GLY:H	1:A:906:LEU:HB2	1.71	0.54
1:A:712:MET:HG2	1:A:720[A]:MET:HE1	1.88	0.54
1:A:337:PHE:N	1:A:338:PRO:CD	2.71	0.54
1:A:687:GLN:HG2	1:A:709:ARG:HD2	1.90	0.54
1:A:665:ASP:O	1:A:669:GLN:HB3	2.08	0.54
1:A:237:GLN:NE2	1:A:241:ARG:HH22	2.05	0.53
1:A:677:LEU:HB3	1:A:682:GLY:HA2	1.90	0.53
1:A:237:GLN:HE21	1:A:241:ARG:HH22	1.57	0.53
1:A:724:ARG:HD3	1:A:742:MET:CE	2.39	0.53
1:A:289:GLU:O	1:A:293:VAL:HG23	2.08	0.53
1:A:594:LYS:HG3	1:A:595:LYS:N	2.23	0.53
1:A:766:LEU:O	1:A:770:GLN:HG3	2.07	0.53
1:A:899:MET:O	1:A:902:LEU:HB2	2.09	0.53
1:A:34:LEU:HD12	1:A:240:MET:CE	2.39	0.52
1:A:399:MET:HE1	1:A:548:TYR:HA	1.90	0.52
1:A:778:TYR:HB3	1:A:781:GLU:HG2	1.90	0.52
1:A:664:PRO:HD2	1:A:668:TRP:O	2.10	0.51
1:A:863:PHE:HB3	3:A:1145:HOH:O	2.11	0.51
1:A:863:PHE:CZ	1:A:905:ALA:CB	2.94	0.51
1:A:418:VAL:CG1	1:A:427:VAL:CG2	2.85	0.51
1:A:90:ASN:ND2	1:A:93:GLY:H	2.09	0.51
1:A:650:ASN:O	1:A:654:ARG:HG3	2.11	0.51
1:A:724:ARG:CD	1:A:742:MET:CE	2.88	0.50
1:A:25:ALA:HB3	1:A:26:PRO:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:ARG:O	1:A:869:THR:HB	2.12	0.50
1:A:599:MET:HE2	1:A:776:ALA:HB2	1.94	0.49
1:A:707:MET:HE3	1:A:710:ARG:HD2	1.94	0.49
1:A:462:LEU:HD13	1:A:481:LEU:HD13	1.93	0.49
1:A:815:ASP:HB3	1:A:818:SER:HB3	1.95	0.49
1:A:80:GLU:OE2	1:A:141:ARG:HD3	2.13	0.49
1:A:787:MET:CE	1:A:801:VAL:HG12	2.43	0.48
1:A:865:LEU:HD11	1:A:874:LEU:HD21	1.95	0.48
1:A:329:LEU:HD13	1:A:370:VAL:HG21	1.96	0.48
1:A:272:ARG:CZ	1:A:275:GLU:HB2	2.44	0.48
1:A:877:ARG:HG2	1:A:878:VAL:N	2.27	0.48
1:A:72:VAL:HG21	1:A:84:LEU:HB2	1.96	0.48
1:A:757:ASN:C	1:A:757:ASN:HD22	2.22	0.47
1:A:90:ASN:C	1:A:90:ASN:HD22	2.21	0.47
1:A:318:ARG:N	1:A:319:PRO:HD2	2.29	0.47
1:A:724:ARG:HD3	1:A:742:MET:HE1	1.95	0.47
1:A:295[A]:ARG:NH2	1:A:345:MET:HE1	2.30	0.47
1:A:593:ASP:OD1	1:A:777:HIS:HE1	1.97	0.47
1:A:835:ILE:HG23	1:A:838:ILE:HD12	1.97	0.47
1:A:868:ARG:O	1:A:869:THR:CB	2.61	0.47
1:A:900:ASN:ND2	3:A:1146:HOH:O	2.29	0.47
1:A:120:TRP:O	1:A:124:LEU:HB2	2.15	0.46
1:A:387:LEU:HD22	1:A:688:GLU:HB3	1.98	0.46
1:A:848:ALA:HB2	1:A:873:LYS:HD3	1.97	0.46
1:A:826:ASN:OD1	1:A:830:GLU:HB2	2.14	0.46
1:A:36:MET:O	1:A:62:ILE:CD1	2.63	0.46
1:A:458:ARG:HA	1:A:461:LYS:HE3	1.98	0.46
1:A:279:PRO:HG3	1:A:517:ILE:CG2	2.46	0.46
1:A:866:CYS:O	1:A:909:ALA:HB2	2.16	0.46
1:A:884:MET:HG3	1:A:899:MET:HE2	1.98	0.46
1:A:826:ASN:ND2	1:A:828:ASP:H	2.13	0.45
1:A:572:ILE:O	1:A:575:ARG:HB2	2.16	0.45
1:A:576:ARG:O	1:A:580:GLY:N	2.49	0.45
1:A:418:VAL:CG1	1:A:418:VAL:O	2.61	0.44
1:A:200:ASN:O	1:A:201:ASP:C	2.58	0.44
1:A:718:GLU:O	1:A:719:GLU:C	2.61	0.44
1:A:151:VAL:O	1:A:155:VAL:HG22	2.17	0.44
1:A:206:ASP:O	1:A:209:ASP:HB2	2.17	0.44
1:A:847:GLU:O	1:A:851:GLU:HB2	2.17	0.44
1:A:599:MET:CE	1:A:776:ALA:HB2	2.47	0.44
1:A:520:THR:O	1:A:521:LYS:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:ASN:HB2	3:A:1002:HOH:O	2.18	0.44
1:A:793:ASN:O	1:A:797:VAL:HG12	2.17	0.44
1:A:30:LYS:HG3	1:A:240:MET:HE2	2.00	0.44
1:A:145:ARG:NH1	1:A:150:LEU:HD22	2.33	0.44
1:A:344:VAL:O	1:A:348:ILE:HG12	2.19	0.43
1:A:757:ASN:HB3	1:A:760[B]:HIS:HB2	2.00	0.43
1:A:576:ARG:CG	1:A:577:ALA:N	2.59	0.43
1:A:147:ASN:O	1:A:151:VAL:HG23	2.19	0.43
1:A:214:GLU:OE1	1:A:230:ARG:NH2	2.51	0.43
1:A:708:LEU:HD13	1:A:723:GLN:CG	2.26	0.43
1:A:902:LEU:O	1:A:902:LEU:CD1	2.48	0.43
1:A:255:GLU:HG2	1:A:259:ASN:ND2	2.34	0.43
1:A:464:PRO:HA	1:A:465:PRO:HD3	1.90	0.43
1:A:817:ASN:ND2	1:A:891:LEU:HD21	2.33	0.43
1:A:869:THR:HG23	1:A:870:ASP:HB2	2.01	0.42
1:A:159:GLU:OE1	1:A:192:ARG:NH1	2.52	0.42
1:A:421:MET:HB3	1:A:422:TYR:CD1	2.54	0.42
1:A:857:GLY:N	1:A:858:TYR:HB2	2.28	0.42
1:A:234:TYR:HA	1:A:238:GLN:HE22	1.85	0.42
1:A:393:ASN:HA	1:A:394:PRO:HD2	1.93	0.42
1:A:418:VAL:CG1	1:A:427:VAL:HG22	2.49	0.42
1:A:349:GLN:HG3	3:A:1014:HOH:O	2.20	0.42
1:A:358:VAL:HG23	3:A:1289:HOH:O	2.20	0.42
1:A:602:ARG:NH1	1:A:604:GLU:OE1	2.52	0.42
1:A:858:TYR:CD1	1:A:859:PHE:CD2	3.07	0.42
1:A:301:GLU:CD	1:A:318:ARG:HH21	2.28	0.41
1:A:6:PHE:CZ	1:A:246:MET:HE2	2.55	0.41
1:A:292:LEU:CD2	1:A:338:PRO:HB3	2.49	0.41
1:A:663:TYR:CZ	1:A:674:LYS:HG3	2.56	0.41
1:A:25:ALA:O	1:A:29:LYS:HD3	2.20	0.41
1:A:405:ASP:HB3	1:A:555:ASP:HB2	2.01	0.41
1:A:826:ASN:ND2	1:A:828:ASP:HB2	2.32	0.41
1:A:654:ARG:HD3	1:A:659:GLU:OE2	2.21	0.41
1:A:559:LEU:HD12	1:A:561:THR:H	1.86	0.41
1:A:351:SER:HB2	1:A:356:VAL:O	2.20	0.41
1:A:858:TYR:HA	1:A:859:PHE:HA	1.90	0.41
1:A:147:ASN:C	1:A:147:ASN:HD22	2.28	0.41
1:A:345:MET:HE3	1:A:345:MET:HB2	1.73	0.41
1:A:215:ILE:HD12	1:A:497:MET:CG	2.49	0.41
1:A:297:LYS:O	1:A:301:GLU:HG2	2.21	0.41
1:A:324:ARG:NH2	3:A:945:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:PHE:O	1:A:610:GLN:CB	2.68	0.41
1:A:852:ALA:O	1:A:855:LYS:HG2	2.20	0.41
1:A:898:LEU:HD13	1:A:898:LEU:HA	1.84	0.41
1:A:292:LEU:HD22	1:A:338:PRO:HB3	2.02	0.41
1:A:397:VAL:HG12	3:A:989:HOH:O	2.20	0.41
1:A:407[B]:CYS:HB2	1:A:409:GLU:HG2	2.02	0.41
1:A:90:ASN:HD21	1:A:92:THR:HB	1.86	0.40
1:A:599:MET:HE1	1:A:772:LEU:O	2.21	0.40
1:A:793:ASN:HD22	1:A:793:ASN:C	2.29	0.40
1:A:812:LEU:O	1:A:833:TYR:HB2	2.21	0.40
1:A:145:ARG:NH1	1:A:150:LEU:CD2	2.84	0.40
1:A:740:LEU:O	1:A:744:ILE:HG13	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	917/910 (101%)	864 (94%)	37 (4%)	16 (2%)	7 7

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	466	ASP
1	A	869	THR
1	A	904	ASP
1	A	906	LEU
1	A	576	ARG
1	A	870	ASP
1	A	903	GLY
1	A	138	ASP

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Mol	Chain	Res	Type
1	A	856	GLY
1	A	717	PRO
1	A	719	GLU
1	A	282	PRO
1	A	521	LYS
1	A	575	ARG
1	A	337	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	762/753 (101%)	669 (88%)	93 (12%)	5 5

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	GLU
1	A	7	VAL
1	A	21	LEU
1	A	29	LYS
1	A	39	LEU
1	A	75	ASP
1	A	84	LEU
1	A	90	ASN
1	A	99	LEU
1	A	100	LEU
1	A	123	GLU
1	A	124	LEU
1	A	131	LEU
1	A	144	LEU
1	A	145	ARG
1	A	155	VAL
1	A	188	LEU
1	A	224	THR

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Mol	Chain	Res	Type
1	A	225	LEU
1	A	240	MET
1	A	249	LEU
1	A	253	ILE
1	A	262	GLU
1	A	265	LYS
1	A	285	ASP
1	A	298	GLU
1	A	315	LEU
1	A	327	THR
1	A	329	LEU
1	A	342	LEU
1	A	345	MET
1	A	349	GLN
1	A	351	SER
1	A	369	LEU
1	A	387	LEU
1	A	397	VAL
1	A	398	SER
1	A	405	ASP
1	A	408	MET
1	A	414	VAL
1	A	418	VAL
1	A	421	MET
1	A	439	LYS
1	A	443	ARG
1	A	456	VAL
1	A	481	LEU
1	A	521	LYS
1	A	544	SER
1	A	546	VAL
1	A	557	LEU
1	A	559	LEU
1	A	571	MET
1	A	576	ARG
1	A	578	LYS
1	A	584	LEU
1	A	594	LYS
1	A	603	SER
1	A	613	SER
1	A	614	ARG
1	A	643	LEU

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Mol	Chain	Res	Type
1	A	654	ARG
1	A	658	ARG
1	A	666	VAL
1	A	671	GLU
1	A	697	LEU
1	A	707	MET
1	A	723	GLN
1	A	743	LYS
1	A	757	ASN
1	A	774	LEU
1	A	781	GLU
1	A	791	MET
1	A	793	ASN
1	A	794	THR
1	A	797	VAL
1	A	801	VAL
1	A	811	ILE
1	A	820	LEU
1	A	851	GLU
1	A	858	TYR
1	A	860	ARG
1	A	868	ARG
1	A	875	ASN
1	A	876	ARG
1	A	877	ARG
1	A	884	MET
1	A	894	HIS
1	A	898	LEU
1	A	900	ASN
1	A	902	LEU
1	A	904	ASP
1	A	906	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	125	ASN
1	A	161	HIS
1	A	183	HIS
1	A	220	HIS
1	A	233	ASN

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Mol	Chain	Res	Type
1	A	237	GLN
1	A	238	GLN
1	A	507	ASN
1	A	566	ASN
1	A	601	GLN
1	A	650	ASN
1	A	695	GLN
1	A	723	GLN
1	A	737	ASN
1	A	757	ASN
1	A	777	HIS
1	A	826	ASN
1	A	875	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	A	913	-	4,4,4	0.94	0	6,6,6	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	A	912	-	4,4,4	0.98	0	6,6,6	0.65	0
2	PO4	A	911	-	4,4,4	0.87	0	6,6,6	1.09	1 (16%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	911	PO4	O3-P-O2	2.22	114.81	107.91

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 ⓘ

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	910/910 (100%)	0.31	24 (2%) 57 59	19, 41, 49, 76	9 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	SER	4.3
1	A	656[A]	HIS	4.0
1	A	902	LEU	3.9
1	A	867	ALA	3.7
1	A	1	MET	3.5
1	A	908	ALA	3.4
1	A	863	PHE	3.4
1	A	717	PRO	3.2
1	A	283	THR	2.6
1	A	284	GLY	2.6
1	A	718	GLU	2.5
1	A	909	ALA	2.5
1	A	330	GLN	2.4
1	A	562	LEU	2.4
1	A	868	ARG	2.3
1	A	262	GLU	2.3
1	A	720[A]	MET	2.3
1	A	869	THR	2.2
1	A	164	ASP	2.2
1	A	791	MET	2.1
1	A	565	ILE	2.1
1	A	843	GLU	2.0
1	A	501	LEU	2.0
1	A	865	LEU	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	PO4	A	913	5/5	0.90	0.23	73,75,76,76	0
2	PO4	A	912	5/5	0.92	0.18	58,59,60,61	0
2	PO4	A	911	5/5	0.94	0.18	46,47,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.