



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:26 PM GMT

PDB ID : 2HNH
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 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/ValidationPDFNotes.html>

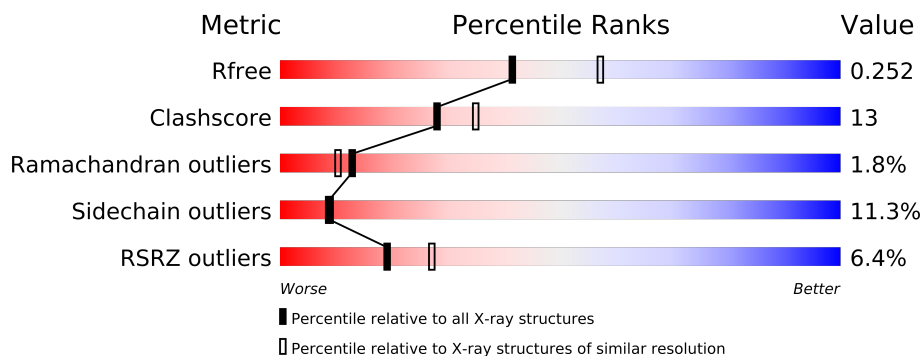
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	910	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	PO4	A	912	-	X
2	PO4	A	913	-	X

2 Entry composition i

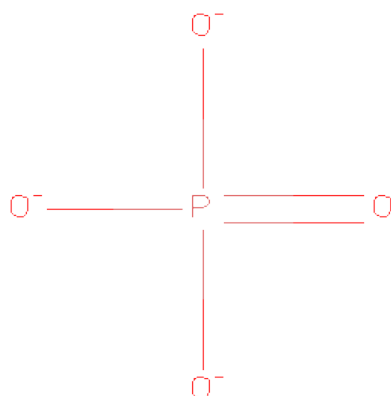
There are 3 unique types of molecules in this entry. The entry contains 7621 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 2 is PHOSPHATE ION (three-letter code: 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		

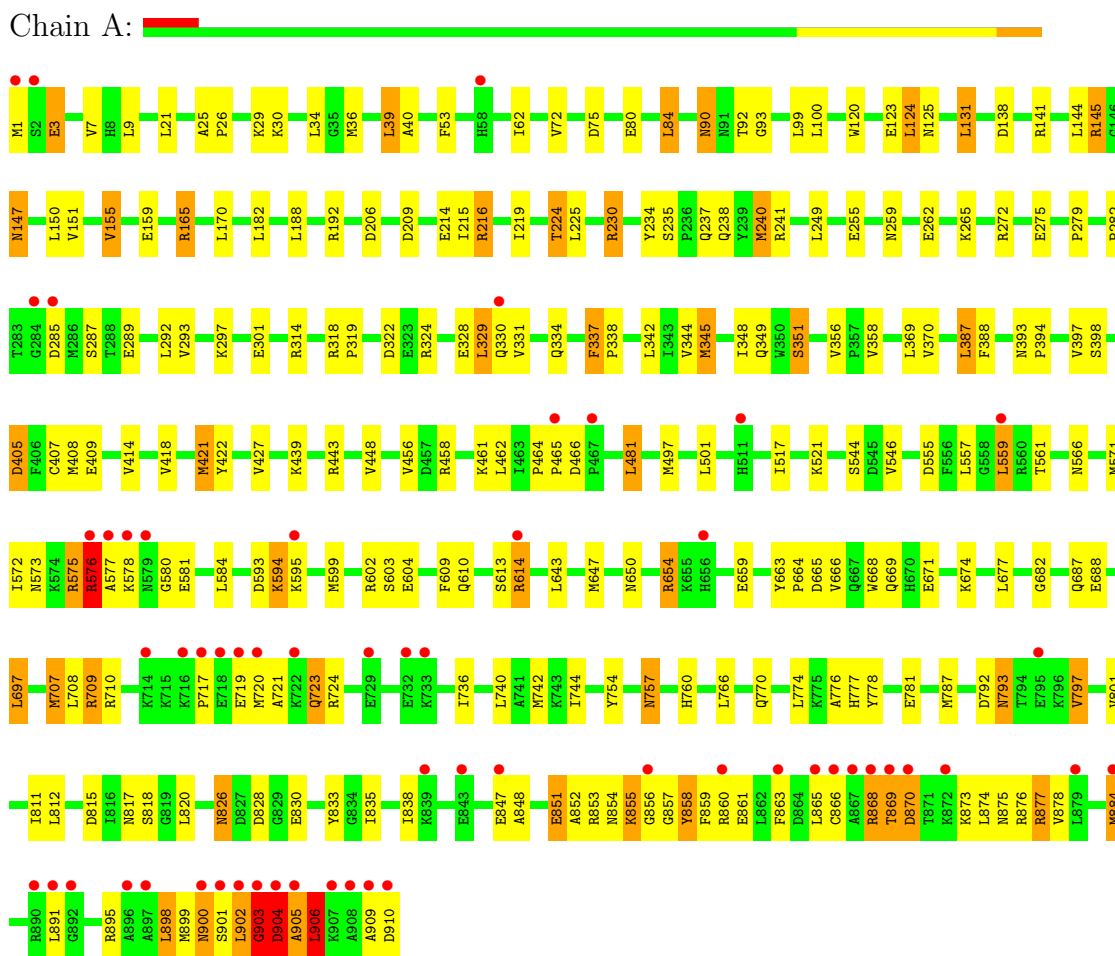
- Molecule 3 is water.

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

3 Residue-property plots

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 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 19.95 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.8 (20.00-2.30) 89.8 (19.95-2.30)	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 5.2.0019	Depositor
R, R_{free}	0.186 , 0.258 0.185 , 0.252	Depositor DCC
R_{free} test set	2021 reflections (5.27%)	DCC
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 , 50.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 40374 reflections	Xtriage
F_o, F_c correlation	0.95	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.

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	0.61	0/7381	0.72	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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	709	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	A	910	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	904	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	165	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	230	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7207	0	7162	182	0
2	A	15	0	0	0	0
3	A	399	0	0	11	0
All	All	7621	0	7162	182	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (182) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	1.16
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:HG2	1:A:614:ARG:HH11	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:903:GLY:HA3	1:A:904:ASP:CB	1.90	1.00
1:A:576:ARG:HB2	3:A:1244:HOH:O	1.61	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
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:853:ARG:HB2	1:A:859:PHE:CE1	2.19	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:216:ARG:HB2	1:A:501:LEU:HD11	1.67	0.77
1:A:863:PHE:CD1	1:A:905:ALA:HB1	2.21	0.75
1:A:418:VAL:HG12	1:A:427:VAL:CG2	2.16	0.75
1:A:599:MET:HE1	1:A:776:ALA:HB2	1.69	0.75
1:A:314:ARG:O	1:A:318:ARG:HB2	1.87	0.74
1:A:724:ARG:HD3	1:A:742:MET:HE1	1.69	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: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: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: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
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:724:ARG:CD	1:A:742:MET:HE1	2.32	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:902:LEU:H	1:A:903:GLY:CA	2.15	0.59
1:A:742:MET:HE3	1:A:742:MET:HA	1.84	0.59
1:A:576:ARG:HD2	1:A:581:GLU:O	2.03	0.59
1:A:215:ILE:HD13	1:A:497:MET:HG2	1.83	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:318:ARG:NH1	1:A:322:ASP:OD1	2.37	0.57
1:A:902:LEU:C	1:A:902:LEU:HD12	2.25	0.56
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: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:647:MET:HE1	1:A:754:TYR:HD1	1.72	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:594:LYS:HG3	1:A:595:LYS:N	2.23	0.53
1:A:289:GLU:O	1:A:293:VAL:HG23	2.08	0.53
1:A:899:MET:O	1:A:902:LEU:HB2	2.09	0.53
1:A:766:LEU:O	1:A:770:GLN:HG3	2.07	0.53
1:A:34:LEU:HD12	1:A:240:MET:CE	2.39	0.52
1:A:778:TYR:HB3	1:A:781:GLU:HG2	1.90	0.52
1:A:724:ARG:HD3	1:A:742:MET:CE	2.39	0.52
1:A:724:ARG:CD	1:A:742:MET:CE	2.88	0.51
1:A:863:PHE:HB3	3:A:1145:HOH:O	2.11	0.51
1:A:664:PRO:HD2	1:A:668:TRP:O	2.10	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:650:ASN:O	1:A:654:ARG:HG3	2.11	0.51
1:A:90:ASN:ND2	1:A:93:GLY:H	2.09	0.51
1:A:30:LYS:HG3	1:A:240:MET:HE2	1.92	0.50
1:A:868:ARG:O	1:A:869:THR:HB	2.12	0.50
1:A:25:ALA:HB3	1:A:26:PRO:HD3	1.94	0.50
1:A:877:ARG:HG2	1:A:878:VAL:N	2.27	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:742:MET:CE	1:A:742:MET:HA	2.43	0.48
1:A:707:MET:HE3	1:A:710:ARG:HD2	1.96	0.48
1:A:272:ARG:CZ	1:A:275:GLU:HB2	2.44	0.48
1:A:72:VAL:HG21	1:A:84:LEU:HB2	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:318:ARG:N	1:A:319:PRO:HD2	2.29	0.47
1:A:835:ILE:HG23	1:A:838:ILE:HD12	1.97	0.47
1:A:593:ASP:OD1	1:A:777:HIS:HE1	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:724:ARG:HH11	1:A:742:MET:HE2	1.81	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: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:724:ARG:HD2	1:A:742:MET:HE2	1.98	0.45
1:A:576:ARG:O	1:A:580:GLY:N	2.49	0.45
1:A:418:VAL:O	1:A:418:VAL:CG1	2.61	0.44
1:A:151:VAL:O	1:A:155:VAL:HG22	2.17	0.44
1:A:847:GLU:O	1:A:851:GLU:HB2	2.17	0.44
1:A:206:ASP:O	1:A:209:ASP:HB2	2.17	0.44
1:A:793:ASN:O	1:A:797:VAL:HG12	2.17	0.44
1:A:566:ASN:HB2	3:A:1002:HOH:O	2.18	0.44
1:A:145:ARG:NH1	1:A:150:LEU:HD22	2.33	0.44
1:A:724:ARG:HD2	1:A:742:MET:CE	2.48	0.43
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:757:ASN:C	1:A:757:ASN:HD22	2.22	0.43
1:A:214:GLU:OE1	1:A:230:ARG:NH2	2.51	0.43
1:A:902:LEU:CD1	1:A:902:LEU:O	2.48	0.43
1:A:708:LEU:HD13	1:A:723:GLN:CG	2.26	0.43
1:A:255:GLU:HG2	1:A:259:ASN:ND2	2.34	0.43
1:A:817:ASN:ND2	1:A:891:LEU:HD21	2.33	0.43
1:A:464:PRO:HA	1:A:465:PRO:HD3	1.90	0.43
1:A:90:ASN:C	1:A:90:ASN:HD22	2.21	0.42
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:857:GLY:N	1:A:858:TYR:HB2	2.28	0.42
1:A:421:MET:HB3	1:A:422:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:602:ARG:NH1	1:A:604:GLU:OE1	2.52	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:858:TYR:CD1	1:A:859:PHE:CD2	3.07	0.42
1:A:884:MET:HE2	1:A:895:ARG:HD3	2.01	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:826:ASN:ND2	1:A:828:ASP:HB2	2.32	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: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:858:TYR:HA	1:A:859:PHE:HA	1.90	0.41
1:A:351:SER:HB2	1:A:356:VAL:O	2.20	0.41
1:A:852:ALA:HA	1:A:855:LYS:HZ3	1.86	0.41
1:A:297:LYS:O	1:A:301:GLU:HG2	2.21	0.41
1:A:215:ILE:HD12	1:A:497:MET:CG	2.49	0.41
1:A:609:PHE:O	1:A:610:GLN:CB	2.68	0.41
1:A:324:ARG:NH2	3:A:945:HOH:O	2.54	0.41
1:A:852:ALA:O	1:A:855:LYS:HG2	2.20	0.41
1:A:898:LEU:HA	1:A:898:LEU:HD13	1.84	0.41
1:A:292:LEU:HD22	1:A:338:PRO:HB3	2.02	0.41
1:A:407[B]:CYS:HB2	1:A:409:GLU:HG2	2.02	0.41
1:A:397:VAL:HG12	3:A:989:HOH:O	2.20	0.41
1:A:90:ASN:HD21	1:A:92:THR:HB	1.86	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

5.3.1 Protein backbone ⓘ

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%)	14	11

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
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%)	677 (89%)	85 (11%)	9	9

All (85) 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	39	LEU
1	A	75	ASP
1	A	84	LEU

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Mol	Chain	Res	Type
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	147	ASN
1	A	155	VAL
1	A	188	LEU
1	A	216	ARG
1	A	224	THR
1	A	225	LEU
1	A	240	MET
1	A	249	LEU
1	A	262	GLU
1	A	265	LYS
1	A	285	ASP
1	A	287	SER
1	A	329	LEU
1	A	342	LEU
1	A	345	MET
1	A	351	SER
1	A	369	LEU
1	A	387	LEU
1	A	398	SER
1	A	405	ASP
1	A	408	MET
1	A	414	VAL
1	A	421	MET
1	A	439	LYS
1	A	443	ARG
1	A	456	VAL
1	A	481	LEU
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

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Mol	Chain	Res	Type
1	A	584	LEU
1	A	594	LYS
1	A	603	SER
1	A	613	SER
1	A	614	ARG
1	A	643	LEU
1	A	654	ARG
1	A	666	VAL
1	A	671	GLU
1	A	697	LEU
1	A	707	MET
1	A	723	GLN
1	A	757	ASN
1	A	774	LEU
1	A	792	ASP
1	A	793	ASN
1	A	797	VAL
1	A	811	ILE
1	A	820	LEU
1	A	826	ASN
1	A	851	GLU
1	A	854	ASN
1	A	855	LYS
1	A	858	TYR
1	A	860	ARG
1	A	861	GLU
1	A	868	ARG
1	A	875	ASN
1	A	876	ARG
1	A	877	ARG
1	A	884	MET
1	A	898	LEU
1	A	900	ASN
1	A	902	LEU
1	A	904	ASP
1	A	906	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	125	ASN

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Mol	Chain	Res	Type
1	A	147	ASN
1	A	237	GLN
1	A	238	GLN
1	A	644	GLN
1	A	650	ASN
1	A	723	GLN
1	A	757	ASN
1	A	777	HIS
1	A	793	ASN
1	A	826	ASN
1	A	854	ASN
1	A	875	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	911	-	4,4,4	0.16	0	6,6,6	0.32	0
2	PO4	A	912	-	4,4,4	0.25	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	A	913	-	4,4,4	0.31	0	6,6,6	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	911	-	-	0/0/0/0	0/0/0/0
2	PO4	A	912	-	-	0/0/0/0	0/0/0/0
2	PO4	A	913	-	-	0/0/0/0	0/0/0/0

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.

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	910/910 (100%)	0.16	58 (6%)	19 27	33, 41, 49, 76	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	909	ALA	10.4
1	A	1	MET	8.5
1	A	908	ALA	7.8
1	A	2	SER	7.7
1	A	902	LEU	7.5
1	A	867	ALA	6.6
1	A	863	PHE	6.6
1	A	717	PRO	5.8
1	A	718	GLU	5.7
1	A	890	ARG	4.2
1	A	905	ALA	4.1
1	A	891	LEU	4.1
1	A	903	GLY	4.1
1	A	714	LYS	4.0
1	A	576	ARG	3.9
1	A	868	ARG	3.9
1	A	872	LYS	3.9
1	A	465	PRO	3.8
1	A	716	LYS	3.7
1	A	578	LYS	3.7
1	A	577	ALA	3.6
1	A	896	ALA	3.6
1	A	467	PRO	3.5
1	A	907	LYS	3.3
1	A	860	ARG	3.3
1	A	511	HIS	3.3
1	A	904	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	897	ALA	3.2
1	A	614	ARG	3.2
1	A	869	THR	3.2
1	A	579	ASN	3.1
1	A	720[A]	MET	3.1
1	A	892	GLY	2.9
1	A	284	GLY	2.9
1	A	910	ASP	2.8
1	A	884	MET	2.8
1	A	733	LYS	2.7
1	A	839	LYS	2.7
1	A	843	GLU	2.6
1	A	865	LEU	2.6
1	A	870	ASP	2.6
1	A	719	GLU	2.5
1	A	732	GLU	2.5
1	A	856	GLY	2.5
1	A	900	ASN	2.4
1	A	595	LYS	2.4
1	A	729	GLU	2.4
1	A	879	LEU	2.4
1	A	559	LEU	2.3
1	A	58	HIS	2.3
1	A	656[A]	HIS	2.3
1	A	847	GLU	2.3
1	A	330	GLN	2.3
1	A	722	LYS	2.2
1	A	795	GLU	2.2
1	A	866	CYS	2.1
1	A	285	ASP	2.1
1	A	901	SER	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	PO4	A	913	5/5	0.32	11.53	73,75,76,76	0
2	PO4	A	912	5/5	0.24	2.51	58,59,60,61	0
2	PO4	A	911	5/5	0.12	0.54	46,47,49,49	0

6.5 Other polymers

There are no such residues in this entry.