Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:33 AM 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 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:

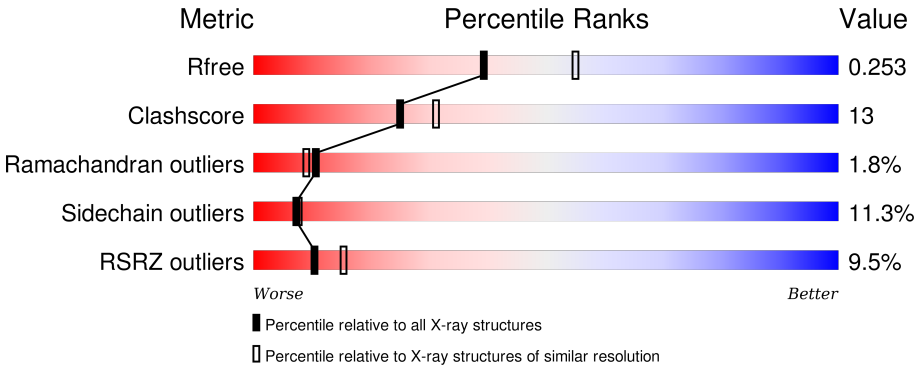
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 <=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	9% 72% 22% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	911	-	-	-	X

2 Entry composition

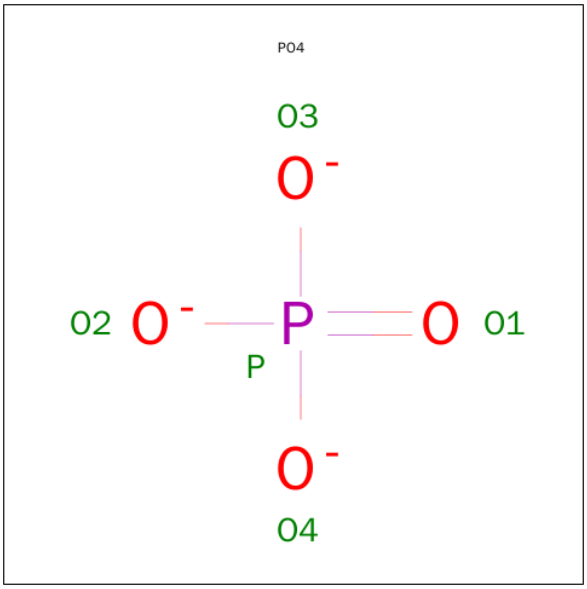
There are 3 unique types of molecules in this entry. The entry contains 7621 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: PO4) (formula: O_4P).



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.

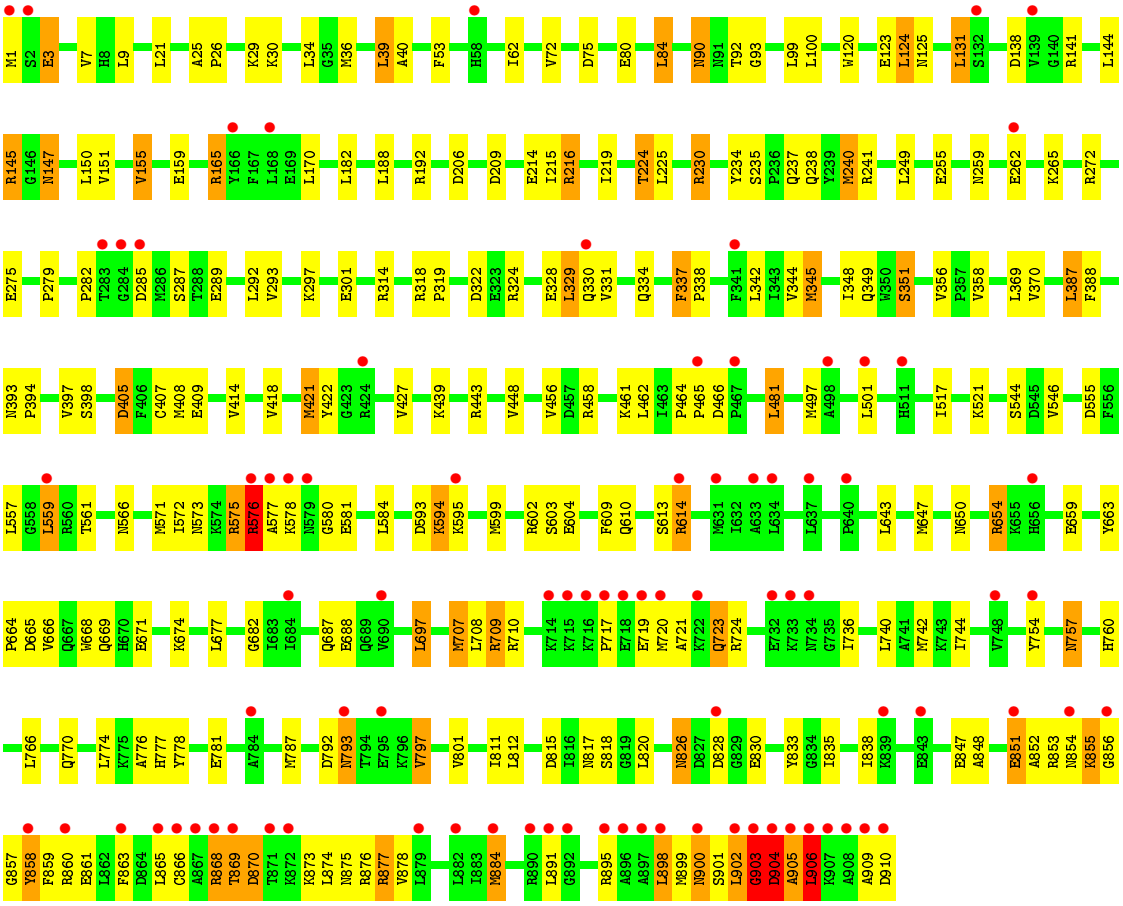
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	399	Total O 399 399	0	0

3 Residue-property plots (i)

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

Chain A:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.18 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.186 , 0.258 0.184 , 0.253	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)	0.32 , 42.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.61	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(^{o})	Ideal(^{o})
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 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	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

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 (182) 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	1.16
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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	11 10

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	762/753 (101%)	677 (89%)	85 (11%)	7 8

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 (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)

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	0.31	0	6,6,6	0.29	0
2	PO4	A	912	-	4,4,4	0.43	0	6,6,6	0.27	0
2	PO4	A	913	-	4,4,4	0.48	0	6,6,6	0.29	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.

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, 95^{th} 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%)	0.44	86 (9%) 10 15	33, 41, 49, 76	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	909	ALA	10.1
1	A	908	ALA	9.6
1	A	902	LEU	8.0
1	A	1	MET	7.9
1	A	2	SER	7.6
1	A	863	PHE	6.6
1	A	867	ALA	6.6
1	A	717	PRO	6.6
1	A	718	GLU	5.9
1	A	577	ALA	5.9
1	A	872	LYS	5.5
1	A	891	LEU	4.9
1	A	868	ARG	4.8
1	A	865	LEU	4.7
1	A	614	ARG	4.6
1	A	903	GLY	4.5
1	A	890	ARG	4.4
1	A	578	LYS	4.3
1	A	576	ARG	4.3
1	A	467	PRO	4.2
1	A	896	ALA	4.0
1	A	465	PRO	3.9
1	A	733	LYS	3.7
1	A	559	LEU	3.7
1	A	905	ALA	3.7
1	A	716	LYS	3.7
1	A	860	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	284	GLY	3.7
1	A	720[A]	MET	3.5
1	A	907	LYS	3.4
1	A	656[A]	HIS	3.4
1	A	714	LYS	3.4
1	A	511	HIS	3.4
1	A	579	ASN	3.3
1	A	283	THR	3.3
1	A	869	THR	3.2
1	A	904	ASP	3.2
1	A	879	LEU	3.1
1	A	900	ASN	3.1
1	A	285	ASP	3.0
1	A	58	HIS	3.0
1	A	719	GLU	3.0
1	A	884	MET	2.9
1	A	839	LYS	2.8
1	A	684	ILE	2.8
1	A	856	GLY	2.8
1	A	498	ALA	2.7
1	A	871	THR	2.7
1	A	501	LEU	2.7
1	A	892	GLY	2.6
1	A	895	ARG	2.6
1	A	793	ASN	2.6
1	A	854	ASN	2.5
1	A	732	GLU	2.5
1	A	634	LEU	2.5
1	A	132	SER	2.5
1	A	330	GLN	2.4
1	A	424	ARG	2.4
1	A	828	ASP	2.4
1	A	690	VAL	2.4
1	A	858	TYR	2.4
1	A	722	LYS	2.4
1	A	633	ALA	2.4
1	A	898	LEU	2.3
1	A	754	TYR	2.3
1	A	341	PHE	2.3
1	A	843	GLU	2.3
1	A	910	ASP	2.3
1	A	166	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	715	LYS	2.3
1	A	784	ALA	2.2
1	A	734	ASN	2.2
1	A	866	CYS	2.2
1	A	595	LYS	2.2
1	A	640	PRO	2.2
1	A	168	LEU	2.2
1	A	882	LEU	2.2
1	A	631	MET	2.2
1	A	637	LEU	2.2
1	A	795	GLU	2.1
1	A	139	VAL	2.1
1	A	262	GLU	2.1
1	A	748	VAL	2.1
1	A	897	ALA	2.1
1	A	906	LEU	2.0
1	A	851	GLU	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, 95^{th} 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
2	PO4	A	911	5/5	0.97	0.19	2.03	46,47,49,49	0
2	PO4	A	913	5/5	0.95	0.42	-	73,75,76,76	0
2	PO4	A	912	5/5	0.96	0.31	-	58,59,60,61	0

6.5 Other polymers (i)

There are no such residues in this entry.