Full wwPDB X-ray Structure Validation Report (i)

Oct 18, 2023 – 01:10 AM EDT

PDB ID	:	2GK7
Title	:	Structural and Functional insights into the human Upf1 helicase core
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Deposited on	:	2006-03-31
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

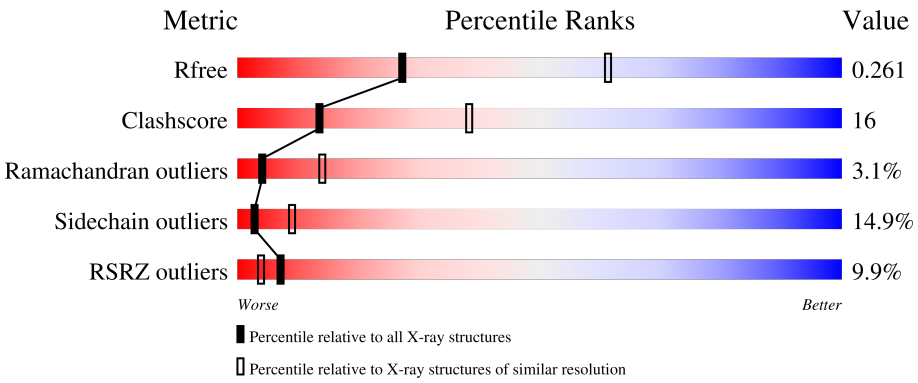
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	624	9% 60% 29% 7% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4782 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.

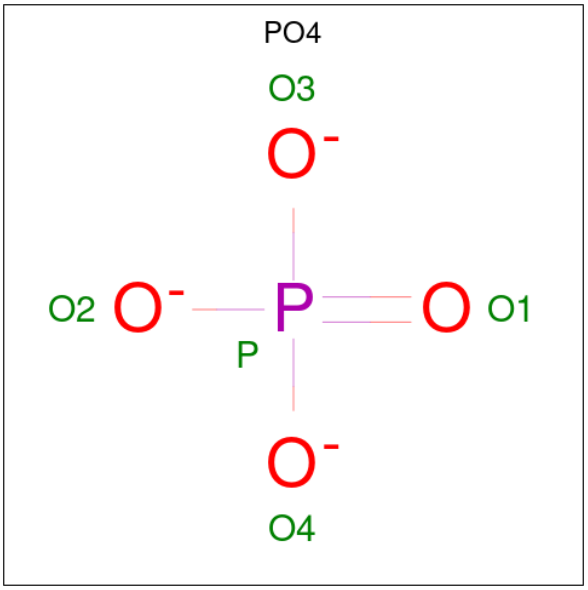
- Molecule 1 is a protein called Regulator of nonsense transcripts 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	596	4719	2994	829	873	23	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	PRO	-	cloning artifact	UNP Q92900
A	292	LEU	-	cloning artifact	UNP Q92900
A	293	GLY	-	cloning artifact	UNP Q92900
A	294	SER	-	cloning artifact	UNP Q92900

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 3 is water.

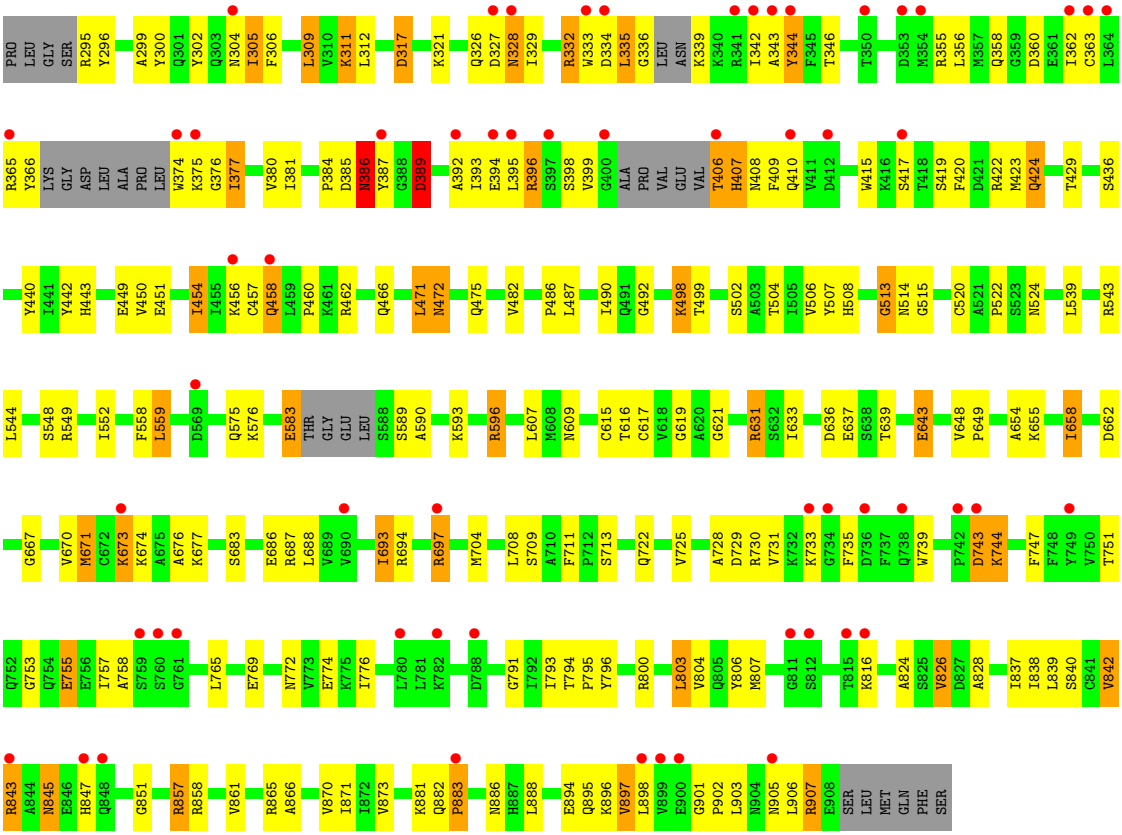
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	58	58	58	0	0

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: Regulator of nonsense transcripts 1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	195.19Å 195.19Å 45.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.82 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.80) 100.0 (19.82-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.43 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.258 , 0.298 0.254 , 0.261	Depositor DCC
R_{free} test set	1083 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	60.9	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 68.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4782	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0.52	1/4808 (0.0%)	0.65	1/6497 (0.0%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	791	GLY	C-O	-10.58	1.06	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	791	GLY	O-C-N	7.18	134.19	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	513	GLY	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	4719	0	4774	152	0
2	A	5	0	0	0	0
3	A	58	0	0	10	0
All	All	4782	0	4774	152	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 16.

All (152) 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:396:ARG:HH11	1:A:396:ARG:HG2	1.21	1.00
1:A:356:LEU:HD21	1:A:380:VAL:HG11	1.51	0.92
1:A:343:ALA:HB1	1:A:344:TYR:CD2	2.08	0.86
1:A:524:ASN:HD22	1:A:543:ARG:HH22	1.26	0.81
1:A:420:PHE:HA	1:A:423:MET:HE3	1.67	0.76
1:A:772:ASN:O	1:A:776:ILE:HG12	1.86	0.75
1:A:396:ARG:HH11	1:A:396:ARG:CG	1.97	0.75
1:A:774:GLU:HG2	1:A:806:TYR:HE2	1.52	0.74
1:A:803:LEU:O	1:A:807:MET:HG2	1.88	0.74
1:A:907:ARG:HH11	1:A:907:ARG:HG2	1.52	0.73
1:A:343:ALA:CB	1:A:344:TYR:CD2	2.71	0.73
1:A:907:ARG:HH11	1:A:907:ARG:CG	2.02	0.72
1:A:739:TRP:HZ3	1:A:871:ILE:HD11	1.55	0.72
1:A:381:ILE:HD11	1:A:394:GLU:HB2	1.70	0.71
1:A:458:GLN:HE21	1:A:458:GLN:HA	1.55	0.70
1:A:328:ASN:HB2	1:A:408:ASN:HD21	1.57	0.70
1:A:386:ASN:H	1:A:386:ASN:HD22	1.36	0.70
1:A:747:PHE:HA	1:A:897:VAL:HG21	1.75	0.69
1:A:616:THR:HB	1:A:619:GLY:H	1.58	0.69
1:A:683:SER:HB2	1:A:686:GLU:H	1.58	0.68
1:A:673:LYS:HG2	1:A:674:LYS:N	2.08	0.68
1:A:380:VAL:HA	1:A:393:ILE:HG22	1.77	0.67
1:A:671:MET:CE	1:A:671:MET:HA	2.24	0.67
1:A:774:GLU:HG2	1:A:806:TYR:CE2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:PHE:HA	1:A:897:VAL:CG2	2.24	0.66
1:A:843:ARG:NH1	1:A:845:ASN:OD1	2.29	0.66
1:A:472:ASN:ND2	1:A:475:GLN:H	1.95	0.65
1:A:482:VAL:HG13	1:A:658:ILE:HD12	1.78	0.65
1:A:492:GLY:HA3	1:A:498:LYS:HG2	1.76	0.65
1:A:335:LEU:HD23	1:A:336:GLY:H	1.61	0.65
1:A:344:TYR:CD1	1:A:392:ALA:HB2	2.32	0.64
1:A:381:ILE:HD11	1:A:394:GLU:CB	2.26	0.64
1:A:366:TYR:HB2	1:A:409:PHE:HA	1.78	0.64
1:A:472:ASN:HD22	1:A:472:ASN:C	2.00	0.64
1:A:633:ILE:HD12	1:A:654:ALA:HB2	1.79	0.64
1:A:311:LYS:HE2	1:A:424:GLN:NE2	2.13	0.64
1:A:343:ALA:HB1	1:A:344:TYR:HD2	1.62	0.63
1:A:643:GLU:OE1	1:A:687:ARG:NE	2.20	0.63
1:A:708:LEU:HD22	1:A:870:VAL:HG12	1.81	0.63
1:A:296:TYR:N	1:A:296:TYR:CD1	2.67	0.62
1:A:743:ASP:HB2	1:A:744:LYS:HD3	1.82	0.61
1:A:328:ASN:HA	1:A:409:PHE:O	2.02	0.59
1:A:861:VAL:O	1:A:865:ARG:HG2	2.02	0.59
1:A:558:PHE:CE1	1:A:559:LEU:HD13	2.38	0.59
1:A:365:ARG:HH21	1:A:375:LYS:HD3	1.66	0.59
1:A:769:GLU:HG3	1:A:873:VAL:HG12	1.85	0.58
1:A:826:VAL:HG21	1:A:858:ARG:HG3	1.83	0.58
1:A:396:ARG:HG2	1:A:396:ARG:NH1	2.01	0.58
1:A:415:TRP:CH2	1:A:417:SER:HB3	2.38	0.58
1:A:704:MET:HG3	1:A:709:SER:HB3	1.85	0.58
1:A:440:TYR:CE2	1:A:486:PRO:HG2	2.38	0.58
1:A:302:TYR:OH	1:A:643:GLU:OE2	2.22	0.57
1:A:296:TYR:H	1:A:296:TYR:HD1	1.51	0.57
1:A:334:ASP:HB2	1:A:343:ALA:HB3	1.86	0.57
1:A:902:PRO:O	1:A:903:LEU:HB2	2.06	0.56
1:A:334:ASP:CB	1:A:343:ALA:HB3	2.35	0.56
1:A:365:ARG:HB2	1:A:410:GLN:HB3	1.87	0.56
1:A:422:ARG:HD3	1:A:621:GLY:HA3	1.88	0.56
1:A:482:VAL:CG1	1:A:658:ILE:HD12	2.37	0.55
1:A:671:MET:HA	1:A:671:MET:HE2	1.89	0.55
1:A:334:ASP:HB2	1:A:343:ALA:O	2.07	0.55
1:A:631:ARG:HH11	1:A:631:ARG:HG3	1.72	0.55
1:A:317:ASP:O	1:A:321:LYS:HB2	2.07	0.54
1:A:583:GLU:OE1	1:A:583:GLU:HA	2.07	0.54
1:A:639:THR:HG21	1:A:662:ASP:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:THR:HG22	1:A:617:CYS:N	2.23	0.54
1:A:845:ASN:HD22	1:A:847:HIS:N	2.07	0.53
1:A:795:PRO:HB3	1:A:851:GLY:HA3	1.91	0.52
1:A:386:ASN:H	1:A:386:ASN:ND2	2.07	0.52
1:A:406:THR:HA	1:A:407:HIS:HB3	1.92	0.52
1:A:794:THR:HB	1:A:840:SER:HB3	1.92	0.51
1:A:755:GLU:HG2	3:A:44:HOH:O	2.09	0.51
1:A:362:ILE:CG2	1:A:363:CYS:N	2.74	0.51
1:A:558:PHE:CD1	1:A:559:LEU:HD13	2.46	0.50
1:A:305:ILE:HG13	1:A:306:PHE:N	2.25	0.50
1:A:616:THR:HG22	3:A:37:HOH:O	2.11	0.50
1:A:381:ILE:CD1	1:A:394:GLU:HB2	2.41	0.50
1:A:544:LEU:HB3	1:A:615:CYS:HB3	1.95	0.49
1:A:804:VAL:HA	3:A:30:HOH:O	2.11	0.48
1:A:374:TRP:CZ2	1:A:376:GLY:HA3	2.48	0.48
1:A:671:MET:HG3	3:A:32:HOH:O	2.13	0.48
1:A:837:ILE:HG12	1:A:866:ALA:HB2	1.94	0.48
1:A:673:LYS:HB3	1:A:673:LYS:HE2	1.42	0.48
1:A:739:TRP:CZ3	1:A:871:ILE:HD11	2.43	0.48
1:A:454:ILE:HD12	1:A:454:ILE:H	1.78	0.47
1:A:415:TRP:CZ3	1:A:417:SER:HB3	2.49	0.47
1:A:728:ALA:O	1:A:731:VAL:HG12	2.13	0.47
1:A:907:ARG:CG	1:A:907:ARG:NH1	2.67	0.47
1:A:796:TYR:OH	1:A:843:ARG:CZ	2.63	0.47
1:A:697:ARG:HG2	3:A:4:HOH:O	2.16	0.46
1:A:824:ALA:HB1	1:A:828:ALA:HB3	1.97	0.46
1:A:456:LYS:O	1:A:457:CYS:HB3	2.16	0.46
1:A:639:THR:HG21	1:A:662:ASP:H	1.80	0.46
1:A:552:ILE:HD12	1:A:552:ILE:N	2.31	0.46
1:A:362:ILE:HG22	1:A:363:CYS:N	2.31	0.46
1:A:776:ILE:HG21	1:A:871:ILE:HG21	1.96	0.46
1:A:796:TYR:HD1	1:A:842:VAL:CG2	2.29	0.46
1:A:796:TYR:CZ	1:A:843:ARG:NH2	2.84	0.46
1:A:616:THR:HG22	1:A:617:CYS:H	1.80	0.46
1:A:743:ASP:OD2	1:A:743:ASP:N	2.49	0.46
1:A:460:PRO:HG3	1:A:508:HIS:CE1	2.51	0.45
1:A:648:VAL:N	1:A:649:PRO:CD	2.79	0.45
1:A:757:ILE:HG13	1:A:758:ALA:N	2.32	0.45
1:A:648:VAL:HB	1:A:649:PRO:HD3	1.98	0.45
1:A:667:GLY:HA3	1:A:857:ARG:NH2	2.32	0.45
1:A:396:ARG:CG	1:A:396:ARG:NH1	2.66	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:MET:HA	1:A:671:MET:HE3	1.98	0.44
1:A:631:ARG:HG3	1:A:631:ARG:NH1	2.32	0.44
1:A:673:LYS:HG2	1:A:674:LYS:H	1.82	0.44
1:A:747:PHE:HB2	1:A:897:VAL:HG23	1.99	0.44
1:A:803:LEU:O	1:A:807:MET:CG	2.62	0.44
1:A:482:VAL:HG21	1:A:490:ILE:HD11	1.98	0.44
1:A:883:PRO:O	1:A:886:ASN:OD1	2.35	0.44
1:A:389:ASP:CG	1:A:800:ARG:HH22	2.21	0.44
1:A:711:PHE:CE2	1:A:888:LEU:HD23	2.53	0.44
1:A:300:TYR:O	1:A:304:ASN:CB	2.66	0.44
1:A:507:TYR:HA	1:A:539:LEU:HD11	2.00	0.44
1:A:305:ILE:O	1:A:309:LEU:HD23	2.18	0.43
1:A:332:ARG:HD2	1:A:334:ASP:OD1	2.18	0.43
1:A:443:HIS:CB	1:A:450:VAL:HG21	2.48	0.43
1:A:360:ASP:O	1:A:380:VAL:HG22	2.18	0.43
1:A:549:ARG:HH12	1:A:552:ILE:HG21	1.83	0.43
1:A:744:LYS:NZ	1:A:895:GLN:HG3	2.33	0.43
1:A:747:PHE:CE2	1:A:871:ILE:HD12	2.54	0.43
1:A:839:LEU:HB2	3:A:58:HOH:O	2.19	0.43
1:A:458:GLN:HA	1:A:458:GLN:NE2	2.29	0.43
1:A:472:ASN:HD21	1:A:475:GLN:H	1.64	0.42
1:A:502:SER:O	1:A:506:VAL:HG23	2.19	0.42
1:A:596:ARG:HG2	3:A:31:HOH:O	2.20	0.42
1:A:688:LEU:O	1:A:693:ILE:HG12	2.20	0.42
1:A:381:ILE:HG12	1:A:393:ILE:HA	2.02	0.42
1:A:522:PRO:HD2	1:A:637:GLU:HB3	2.01	0.42
1:A:299:ALA:HB2	1:A:442:TYR:HE1	1.85	0.42
1:A:471:LEU:HA	1:A:475:GLN:NE2	2.35	0.41
1:A:636:ASP:OD1	1:A:637:GLU:N	2.52	0.41
1:A:385:ASP:O	1:A:387:TYR:N	2.53	0.41
1:A:747:PHE:CB	1:A:897:VAL:HG23	2.50	0.41
1:A:358:GLN:HA	1:A:380:VAL:HG23	2.02	0.41
1:A:449:GLU:HA	3:A:36:HOH:O	2.19	0.41
1:A:520:CYS:HA	1:A:615:CYS:O	2.21	0.41
1:A:677:LYS:HA	3:A:48:HOH:O	2.20	0.41
1:A:396:ARG:HD3	1:A:396:ARG:HA	1.86	0.40
1:A:673:LYS:O	1:A:676:ALA:HB3	2.21	0.40
1:A:747:PHE:CB	1:A:897:VAL:CG2	2.98	0.40
1:A:796:TYR:HD1	1:A:842:VAL:HG21	1.86	0.40
1:A:589:SER:OG	1:A:590:ALA:N	2.53	0.40
1:A:894:GLU:C	1:A:896:LYS:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:LEU:HD21	1:A:504:THR:HG21	2.04	0.40
1:A:472:ASN:ND2	1:A:472:ASN:C	2.71	0.40
1:A:499:THR:HG23	3:A:6:HOH:O	2.20	0.40
1:A:751:THR:HG22	1:A:753:GLY:H	1.86	0.40
1:A:845:ASN:C	1:A:847:HIS:H	2.25	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	586/624 (94%)	513 (88%)	55 (9%)	18 (3%)	4 14

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	466	GLN
1	A	514	ASN
1	A	342	ILE
1	A	377	ILE
1	A	386	ASN
1	A	398	SER
1	A	513	GLY
1	A	515	GLY
1	A	898	LEU
1	A	901	GLY
1	A	389	ASP
1	A	399	VAL
1	A	906	LEU
1	A	384	PRO
1	A	733	LYS
1	A	882	GLN

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Mol	Chain	Res	Type
1	A	842	VAL
1	A	883	PRO

5.3.2 Protein sidechains (i)

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	517/540 (96%)	440 (85%)	77 (15%)	3 9

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	295	ARG
1	A	305	ILE
1	A	309	LEU
1	A	311	LYS
1	A	312	LEU
1	A	317	ASP
1	A	326	GLN
1	A	327	ASP
1	A	328	ASN
1	A	329	ILE
1	A	332	ARG
1	A	333	TRP
1	A	335	LEU
1	A	339	LYS
1	A	344	TYR
1	A	346	THR
1	A	355	ARG
1	A	377	ILE
1	A	386	ASN
1	A	389	ASP
1	A	395	LEU
1	A	396	ARG
1	A	406	THR
1	A	407	HIS

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Mol	Chain	Res	Type
1	A	419	SER
1	A	424	GLN
1	A	429	THR
1	A	436	SER
1	A	451	GLU
1	A	454	ILE
1	A	458	GLN
1	A	462	ARG
1	A	471	LEU
1	A	472	ASN
1	A	487	LEU
1	A	498	LYS
1	A	548	SER
1	A	559	LEU
1	A	575	GLN
1	A	576	LYS
1	A	583	GLU
1	A	593	LYS
1	A	596	ARG
1	A	607	LEU
1	A	609	ASN
1	A	631	ARG
1	A	643	GLU
1	A	655	LYS
1	A	658	ILE
1	A	670	VAL
1	A	671	MET
1	A	673	LYS
1	A	693	ILE
1	A	694	ARG
1	A	697	ARG
1	A	713	SER
1	A	722	GLN
1	A	725	VAL
1	A	729	ASP
1	A	730	ARG
1	A	735	PHE
1	A	743	ASP
1	A	744	LYS
1	A	755	GLU
1	A	765	LEU
1	A	793	ILE

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Mol	Chain	Res	Type
1	A	803	LEU
1	A	816	LYS
1	A	826	VAL
1	A	838	ILE
1	A	843	ARG
1	A	845	ASN
1	A	857	ARG
1	A	881	LYS
1	A	897	VAL
1	A	905	ASN
1	A	907	ARG

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

Mol	Chain	Res	Type
1	A	386	ASN
1	A	408	ASN
1	A	458	GLN
1	A	472	ASN
1	A	475	GLN
1	A	524	ASN
1	A	535	HIS
1	A	575	GLN
1	A	738	GLN
1	A	772	ASN
1	A	830	GLN
1	A	848	GLN
1	A	860	ASN
1	A	905	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	990	-	4,4,4	0.91	0	6,6,6	0.85	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	596/624 (95%)	0.62	59 (9%) 7 4	40, 66, 96, 108	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	343	ALA	7.0
1	A	905	ASN	5.2
1	A	760	SER	5.1
1	A	353	ASP	4.9
1	A	843	ARG	4.8
1	A	733	LYS	4.8
1	A	736	ASP	4.7
1	A	848	GLN	4.4
1	A	883	PRO	4.3
1	A	734	GLY	4.2
1	A	761	GLY	4.2
1	A	412	ASP	4.0
1	A	342	ILE	3.9
1	A	327	ASP	3.9
1	A	742	PRO	3.7
1	A	334	ASP	3.6
1	A	900	GLU	3.6
1	A	344	TYR	3.5
1	A	374	TRP	3.4
1	A	375	LYS	3.3
1	A	406	THR	3.2
1	A	354	MET	3.1
1	A	304	ASN	3.0
1	A	899	VAL	3.0
1	A	743	ASP	2.9
1	A	812	SER	2.9
1	A	815	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	397	SER	2.8
1	A	341	ARG	2.8
1	A	749	TYR	2.7
1	A	400	GLY	2.6
1	A	458	GLN	2.6
1	A	363	CYS	2.6
1	A	410	GLN	2.6
1	A	697	ARG	2.5
1	A	362	ILE	2.5
1	A	759	SER	2.5
1	A	811	GLY	2.5
1	A	333	TRP	2.5
1	A	788	ASP	2.4
1	A	387	TYR	2.4
1	A	816	LYS	2.4
1	A	364	LEU	2.4
1	A	782	LYS	2.4
1	A	456	LYS	2.4
1	A	673	LYS	2.3
1	A	898	LEU	2.2
1	A	417	SER	2.2
1	A	690	VAL	2.2
1	A	738	GLN	2.2
1	A	350	THR	2.2
1	A	394	GLU	2.2
1	A	569	ASP	2.1
1	A	847	HIS	2.1
1	A	392	ALA	2.1
1	A	365	ARG	2.1
1	A	395	LEU	2.0
1	A	328	ASN	2.0
1	A	780	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 monosaccharides 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(Å^2)	Q<0.9
2	PO4	A	990	5/5	0.92	0.18	61,63,64,65	0

6.5 Other polymers (i)

There are no such residues in this entry.