



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:02 PM UTC

PDB ID : 2GK7 / pdb_00002gk7
Title : Structural and Functional insights into the human Upf1 helicase core
Authors : Cheng, Z.; Muhlrاد, D.; Parker, R.; Song, H.
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 ⓘ 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

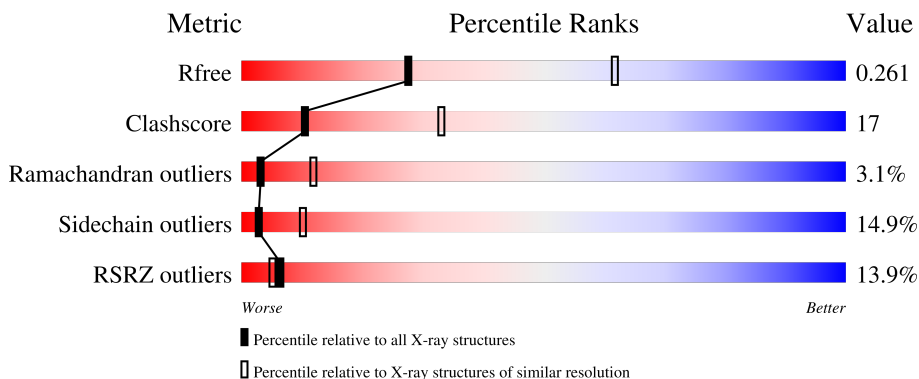
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. 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	624	13% 58% 30% 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.

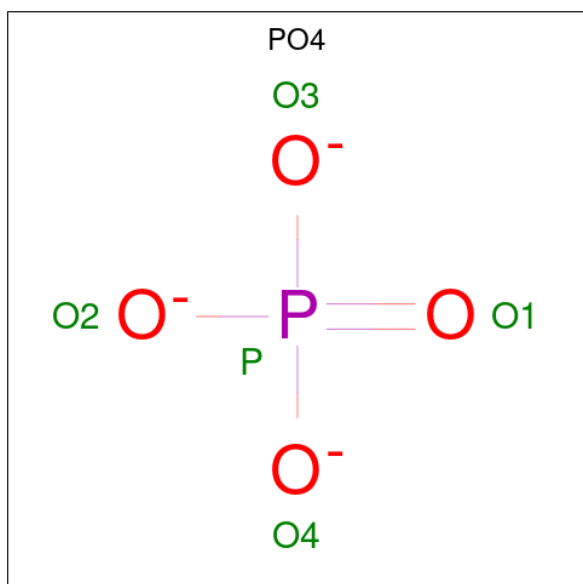
- Molecule 1 is a protein called Regulator of nonsense transcripts 1.

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 (CCD ID: PO4) (formula: O₄P).



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

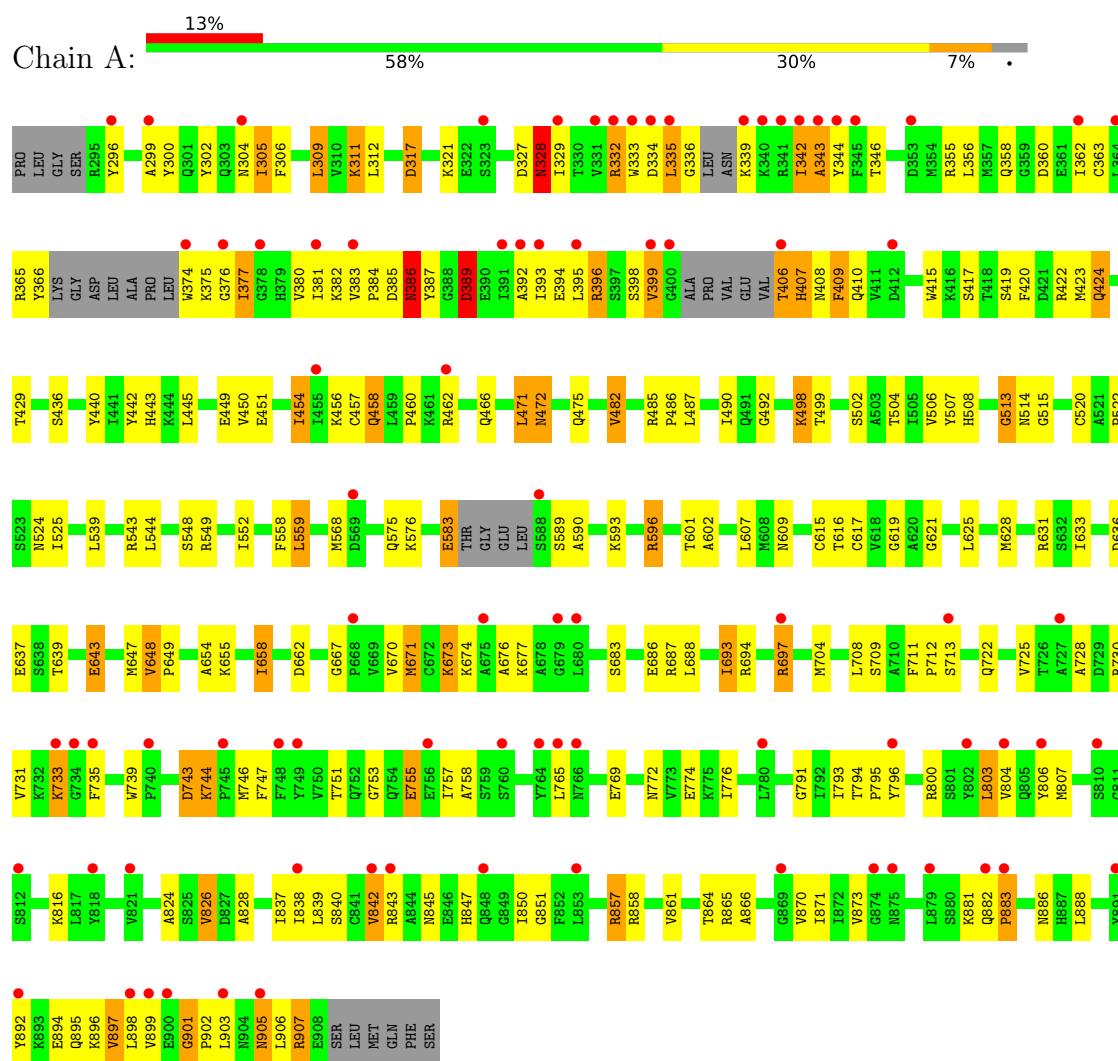
- Molecule 3 is water.

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

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



4 Data and refinement statistics

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 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.80) 99.6 (20.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.29 , 71.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	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.*

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	0.66	1/4808 (0.0%)	0.96	16/6497 (0.2%)

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	-12.74	1.06	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	791	GLY	O-C-N	8.84	134.19	122.70
1	A	850	ILE	N-CA-C	6.58	117.65	112.12
1	A	383	VAL	CA-C-N	6.56	128.04	119.84
1	A	383	VAL	C-N-CA	6.56	128.04	119.84
1	A	899	VAL	N-CA-C	6.03	117.61	108.80
1	A	901	GLY	CA-C-N	5.75	125.77	119.90
1	A	901	GLY	C-N-CA	5.75	125.77	119.90
1	A	905	ASN	N-CA-C	5.68	115.73	108.24
1	A	383	VAL	N-CA-C	5.41	114.04	107.61
1	A	648	VAL	CB-CA-C	-5.31	108.73	114.35
1	A	343	ALA	CA-C-N	5.25	131.15	121.70
1	A	343	ALA	C-N-CA	5.25	131.15	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	ARG	CA-C-N	5.14	124.64	119.19
1	A	485	ARG	C-N-CA	5.14	124.64	119.19
1	A	409	PHE	N-CA-C	5.04	117.93	109.96
1	A	328	ASN	N-CA-C	5.04	118.31	108.18

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 ⓘ

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	160	0
2	A	5	0	0	0	0
3	A	58	0	0	10	0
All	All	4782	0	4774	160	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 17.

All (160) 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:671:MET:HA	1:A:671:MET:HE2	1.54	0.88
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:445:LEU:HD13	1:A:647:MET:HE1	1.62	0.81
1:A:420:PHE:HA	1:A:423:MET:HE3	1.66	0.78
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:472:ASN:HD22	1:A:472:ASN:C	2.00	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:774:GLU:HG2	1:A:806:TYR:CE2	2.29	0.67
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:671:MET:HA	1:A:671:MET:CE	2.24	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: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:568:MET:HE3	1:A:602:ALA:HB1	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:902:PRO:O	1:A:903:LEU:HB2	2.06	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
1:A:616:THR:HG22	1:A:617:CYS:N	2.23	0.54
1:A:625:LEU:HA	1:A:628:MET:HE3	1.90	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:445:LEU:CD1	1:A:647:MET:HE1	2.37	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:746:MET:HE3	1:A:892:TYR:CZ	2.47	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:305:ILE:HG13	1:A:306:PHE:N	2.25	0.48
1:A:389:ASP:CG	1:A:800:ARG:HH22	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:744:LYS:HZ2	1:A:895:GLN:HG3	1.81	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:456:LYS:O	1:A:457:CYS:HB3	2.16	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:704:MET:HE1	1:A:864:THR:HB	1.98	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:845:ASN:C	1:A:847:HIS:H	2.25	0.45
1:A:396:ARG:CG	1:A:396:ARG:NH1	2.66	0.45
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:894:GLU:C	1:A:896:LYS:H	2.25	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:709:SER:C	1:A:712:PRO:HD2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:472:ASN:C	1:A:472:ASN:ND2	2.71	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:746:MET:HE3	1:A:892:TYR:CE2	2.56	0.40
1:A:471:LEU:HD21	1:A:504:THR:HG21	2.04	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

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	586/624 (94%)	513 (88%)	55 (9%)	18 (3%)	3	12

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
1	A	842	VAL
1	A	883	PRO

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	517/540 (96%)	440 (85%)	77 (15%)	3	10

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

Mol	Chain	Res	Type
1	A	305	ILE
1	A	309	LEU
1	A	311	LYS

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Mol	Chain	Res	Type
1	A	312	LEU
1	A	317	ASP
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	342	ILE
1	A	346	THR
1	A	355	ARG
1	A	377	ILE
1	A	382	LYS
1	A	386	ASN
1	A	389	ASP
1	A	395	LEU
1	A	396	ARG
1	A	399	VAL
1	A	406	THR
1	A	407	HIS
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	482	VAL
1	A	487	LEU
1	A	498	LYS
1	A	525	ILE
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

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Mol	Chain	Res	Type
1	A	601	THR
1	A	607	LEU
1	A	609	ASN
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	730	ARG
1	A	733	LYS
1	A	735	PHE
1	A	743	ASP
1	A	744	LYS
1	A	755	GLU
1	A	765	LEU
1	A	793	ILE
1	A	803	LEU
1	A	816	LYS
1	A	826	VAL
1	A	838	ILE
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 (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	GLN
1	A	326	GLN
1	A	386	ASN
1	A	408	ASN
1	A	458	GLN
1	A	466	GLN

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Mol	Chain	Res	Type
1	A	472	ASN
1	A	475	GLN
1	A	484	GLN
1	A	524	ASN
1	A	535	HIS
1	A	575	GLN
1	A	738	GLN
1	A	741	GLN
1	A	772	ASN
1	A	805	GLN
1	A	819	GLN
1	A	830	GLN
1	A	845	ASN
1	A	848	GLN
1	A	860	ASN
1	A	887	HIS
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 oligosaccharides 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	0.95	0	6,6,6	0.89	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, 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%)	1.08	83 (13%) 6 5	40, 66, 96, 108	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	343	ALA	7.3
1	A	843	ARG	4.6
1	A	342	ILE	4.4
1	A	334	ASP	4.3
1	A	393	ILE	4.1
1	A	898	LEU	3.7
1	A	675	ALA	3.7
1	A	353	ASP	3.6
1	A	400	GLY	3.6
1	A	412	ASP	3.6
1	A	345	PHE	3.6
1	A	697	ARG	3.5
1	A	296	TYR	3.4
1	A	344	TYR	3.3
1	A	679	GLY	3.2
1	A	842	VAL	3.2
1	A	335	LEU	3.1
1	A	395	LEU	3.1
1	A	341	ARG	3.0
1	A	333	TRP	2.9
1	A	406	THR	2.9
1	A	329	ILE	2.9
1	A	383	VAL	2.8
1	A	680	LEU	2.8
1	A	804	VAL	2.8
1	A	340	LYS	2.8
1	A	735	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	331	VAL	2.7
1	A	713	SER	2.7
1	A	796	TYR	2.7
1	A	332	ARG	2.7
1	A	780	LEU	2.7
1	A	304	ASN	2.6
1	A	812	SER	2.6
1	A	299	ALA	2.5
1	A	399	VAL	2.5
1	A	899	VAL	2.5
1	A	848	GLN	2.5
1	A	900	GLU	2.5
1	A	364	LEU	2.5
1	A	810	SER	2.5
1	A	339	LYS	2.5
1	A	588	SER	2.4
1	A	882	GLN	2.4
1	A	905	ASN	2.4
1	A	740	PRO	2.4
1	A	745	PRO	2.4
1	A	756	GLU	2.4
1	A	749	TYR	2.4
1	A	853	LEU	2.4
1	A	818	TYR	2.4
1	A	668	PRO	2.4
1	A	374	TRP	2.3
1	A	362	ILE	2.3
1	A	733	LYS	2.3
1	A	569	ASP	2.3
1	A	455	ILE	2.3
1	A	892	TYR	2.3
1	A	802	TYR	2.2
1	A	392	ALA	2.2
1	A	903	LEU	2.2
1	A	381	ILE	2.2
1	A	462	ARG	2.2
1	A	883	PRO	2.2
1	A	765	LEU	2.2
1	A	734	GLY	2.1
1	A	874	GLY	2.1
1	A	748	PHE	2.1
1	A	879	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	764	TYR	2.1
1	A	806	TYR	2.1
1	A	760	SER	2.1
1	A	766	ASN	2.1
1	A	821	VAL	2.1
1	A	378	GLY	2.1
1	A	727	ALA	2.1
1	A	838	ILE	2.1
1	A	875	ASN	2.1
1	A	869	GLY	2.1
1	A	376	GLY	2.0
1	A	391	ILE	2.0
1	A	891	TYR	2.0
1	A	323	SER	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	990	5/5	0.91	0.14	61,63,64,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.