



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:09 AM UTC

PDB ID : 6DCR / pdb_00006dcr
Title : E. coli PriA helicase winged helix domain deletion protein
Authors : Satyshur, K.A.; Windgassen, T.A.; Keck, J.L.
Deposited on : 2018-05-08
Resolution : 1.98 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

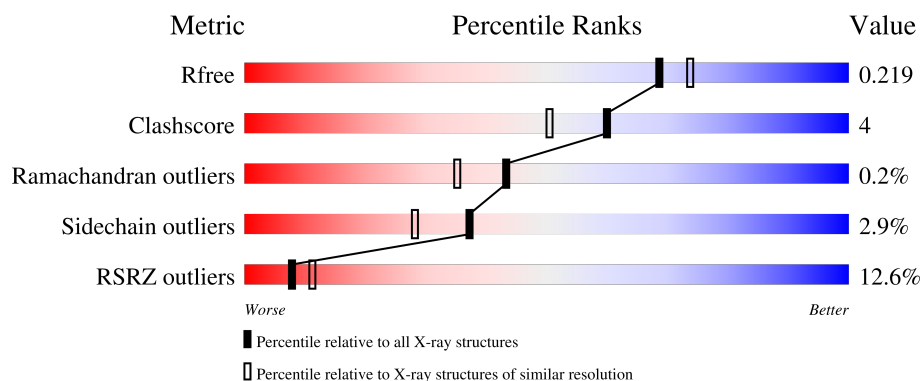
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	694	6% 84% 7% 8%
1	B	694	16% 77% 8% 14%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 19132 atoms, of which 9236 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 Primosomal protein N'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	639	Total	C	H	N	O	S	0	8	0
			9985	3188	4981	914	885	17			
1	B	600	Total	C	H	N	O	S	0	2	0
			8691	2843	4255	788	789	16			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P17888
A	-18	GLY	-	expression tag	UNP P17888
A	-17	SER	-	expression tag	UNP P17888
A	-16	SER	-	expression tag	UNP P17888
A	-15	HIS	-	expression tag	UNP P17888
A	-14	HIS	-	expression tag	UNP P17888
A	-13	HIS	-	expression tag	UNP P17888
A	-12	HIS	-	expression tag	UNP P17888
A	-11	HIS	-	expression tag	UNP P17888
A	-10	HIS	-	expression tag	UNP P17888
A	-9	SER	-	expression tag	UNP P17888
A	-8	SER	-	expression tag	UNP P17888
A	-7	GLY	-	expression tag	UNP P17888
A	-6	LEU	-	expression tag	UNP P17888
A	-5	VAL	-	expression tag	UNP P17888
A	-4	PRO	-	expression tag	UNP P17888
A	-3	ARG	-	expression tag	UNP P17888
A	-2	GLY	-	expression tag	UNP P17888
A	-1	SER	-	expression tag	UNP P17888
A	0	HIS	-	expression tag	UNP P17888
A	?	-	MET	deletion	UNP P17888
A	?	-	TRP	deletion	UNP P17888
A	?	-	TYR	deletion	UNP P17888
A	?	-	TRP	deletion	UNP P17888
A	?	-	PHE	deletion	UNP P17888

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP P17888
A	?	-	THR	deletion	UNP P17888
A	?	-	GLU	deletion	UNP P17888
A	?	-	GLN	deletion	UNP P17888
A	?	-	GLY	deletion	UNP P17888
A	?	-	GLN	deletion	UNP P17888
A	?	-	ALA	deletion	UNP P17888
A	?	-	VAL	deletion	UNP P17888
A	?	-	ASP	deletion	UNP P17888
A	?	-	LEU	deletion	UNP P17888
A	?	-	ASN	deletion	UNP P17888
A	?	-	SER	deletion	UNP P17888
A	?	-	LEU	deletion	UNP P17888
A	?	-	LYS	deletion	UNP P17888
A	?	-	ARG	deletion	UNP P17888
A	?	-	SER	deletion	UNP P17888
A	?	-	PRO	deletion	UNP P17888
A	?	-	LYS	deletion	UNP P17888
A	?	-	GLN	deletion	UNP P17888
A	?	-	GLN	deletion	UNP P17888
A	?	-	GLN	deletion	UNP P17888
A	?	-	ALA	deletion	UNP P17888
A	?	-	LEU	deletion	UNP P17888
A	?	-	ALA	deletion	UNP P17888
A	?	-	ALA	deletion	UNP P17888
A	?	-	LEU	deletion	UNP P17888
A	?	-	ARG	deletion	UNP P17888
A	?	-	GLN	deletion	UNP P17888
A	?	-	GLY	deletion	UNP P17888
A	?	-	LYS	deletion	UNP P17888
A	?	-	ILE	deletion	UNP P17888
A	?	-	TRP	deletion	UNP P17888
A	?	-	ARG	deletion	UNP P17888
A	?	-	ASP	deletion	UNP P17888
A	?	-	GLN	deletion	UNP P17888
A	?	-	VAL	deletion	UNP P17888
A	?	-	ALA	deletion	UNP P17888
A	?	-	THR	deletion	UNP P17888
A	?	-	LEU	deletion	UNP P17888
A	?	-	GLU	deletion	UNP P17888
A	?	-	PHE	deletion	UNP P17888
A	?	-	ASN	deletion	UNP P17888

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP P17888
A	?	-	ALA	deletion	UNP P17888
A	?	-	ALA	deletion	UNP P17888
A	?	-	LEU	deletion	UNP P17888
A	?	-	GLN	deletion	UNP P17888
A	?	-	ALA	deletion	UNP P17888
A	?	-	LEU	deletion	UNP P17888
A	?	-	ARG	deletion	UNP P17888
A	?	-	LYS	deletion	UNP P17888
A	?	-	LYS	deletion	UNP P17888
A	?	-	GLY	deletion	UNP P17888
A	173	ASP	LEU	linker	UNP P17888
A	174	ILE	CYS	linker	UNP P17888
B	-19	MET	-	expression tag	UNP P17888
B	-18	GLY	-	expression tag	UNP P17888
B	-17	SER	-	expression tag	UNP P17888
B	-16	SER	-	expression tag	UNP P17888
B	-15	HIS	-	expression tag	UNP P17888
B	-14	HIS	-	expression tag	UNP P17888
B	-13	HIS	-	expression tag	UNP P17888
B	-12	HIS	-	expression tag	UNP P17888
B	-11	HIS	-	expression tag	UNP P17888
B	-10	HIS	-	expression tag	UNP P17888
B	-9	SER	-	expression tag	UNP P17888
B	-8	SER	-	expression tag	UNP P17888
B	-7	GLY	-	expression tag	UNP P17888
B	-6	LEU	-	expression tag	UNP P17888
B	-5	VAL	-	expression tag	UNP P17888
B	-4	PRO	-	expression tag	UNP P17888
B	-3	ARG	-	expression tag	UNP P17888
B	-2	GLY	-	expression tag	UNP P17888
B	-1	SER	-	expression tag	UNP P17888
B	0	HIS	-	expression tag	UNP P17888
B	?	-	MET	deletion	UNP P17888
B	?	-	TRP	deletion	UNP P17888
B	?	-	TYR	deletion	UNP P17888
B	?	-	TRP	deletion	UNP P17888
B	?	-	PHE	deletion	UNP P17888
B	?	-	ALA	deletion	UNP P17888
B	?	-	THR	deletion	UNP P17888
B	?	-	GLU	deletion	UNP P17888
B	?	-	GLN	deletion	UNP P17888

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLY	deletion	UNP P17888
B	?	-	GLN	deletion	UNP P17888
B	?	-	ALA	deletion	UNP P17888
B	?	-	VAL	deletion	UNP P17888
B	?	-	ASP	deletion	UNP P17888
B	?	-	LEU	deletion	UNP P17888
B	?	-	ASN	deletion	UNP P17888
B	?	-	SER	deletion	UNP P17888
B	?	-	LEU	deletion	UNP P17888
B	?	-	LYS	deletion	UNP P17888
B	?	-	ARG	deletion	UNP P17888
B	?	-	SER	deletion	UNP P17888
B	?	-	PRO	deletion	UNP P17888
B	?	-	LYS	deletion	UNP P17888
B	?	-	GLN	deletion	UNP P17888
B	?	-	GLN	deletion	UNP P17888
B	?	-	GLN	deletion	UNP P17888
B	?	-	ALA	deletion	UNP P17888
B	?	-	LEU	deletion	UNP P17888
B	?	-	ALA	deletion	UNP P17888
B	?	-	ALA	deletion	UNP P17888
B	?	-	LEU	deletion	UNP P17888
B	?	-	ARG	deletion	UNP P17888
B	?	-	GLN	deletion	UNP P17888
B	?	-	GLY	deletion	UNP P17888
B	?	-	LYS	deletion	UNP P17888
B	?	-	ILE	deletion	UNP P17888
B	?	-	TRP	deletion	UNP P17888
B	?	-	ARG	deletion	UNP P17888
B	?	-	ASP	deletion	UNP P17888
B	?	-	GLN	deletion	UNP P17888
B	?	-	VAL	deletion	UNP P17888
B	?	-	ALA	deletion	UNP P17888
B	?	-	THR	deletion	UNP P17888
B	?	-	LEU	deletion	UNP P17888
B	?	-	GLU	deletion	UNP P17888
B	?	-	PHE	deletion	UNP P17888
B	?	-	ASN	deletion	UNP P17888
B	?	-	ASP	deletion	UNP P17888
B	?	-	ALA	deletion	UNP P17888
B	?	-	ALA	deletion	UNP P17888
B	?	-	LEU	deletion	UNP P17888

Continued on next page...

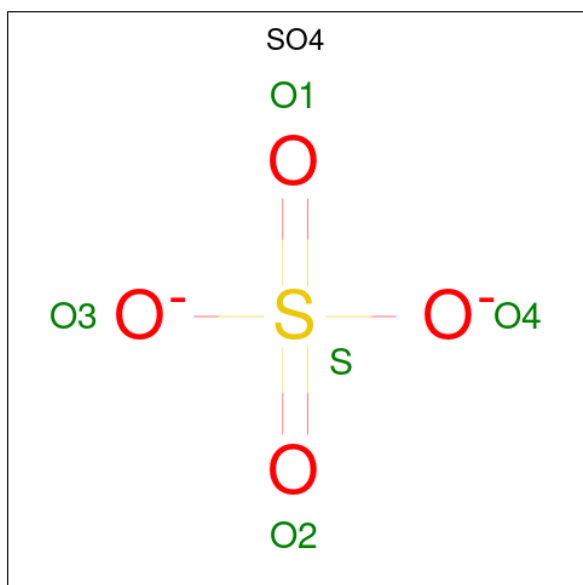
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLN	deletion	UNP P17888
B	?	-	ALA	deletion	UNP P17888
B	?	-	LEU	deletion	UNP P17888
B	?	-	ARG	deletion	UNP P17888
B	?	-	LYS	deletion	UNP P17888
B	?	-	LYS	deletion	UNP P17888
B	?	-	GLY	deletion	UNP P17888
B	173	ASP	LEU	linker	UNP P17888
B	174	ILE	CYS	linker	UNP P17888

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

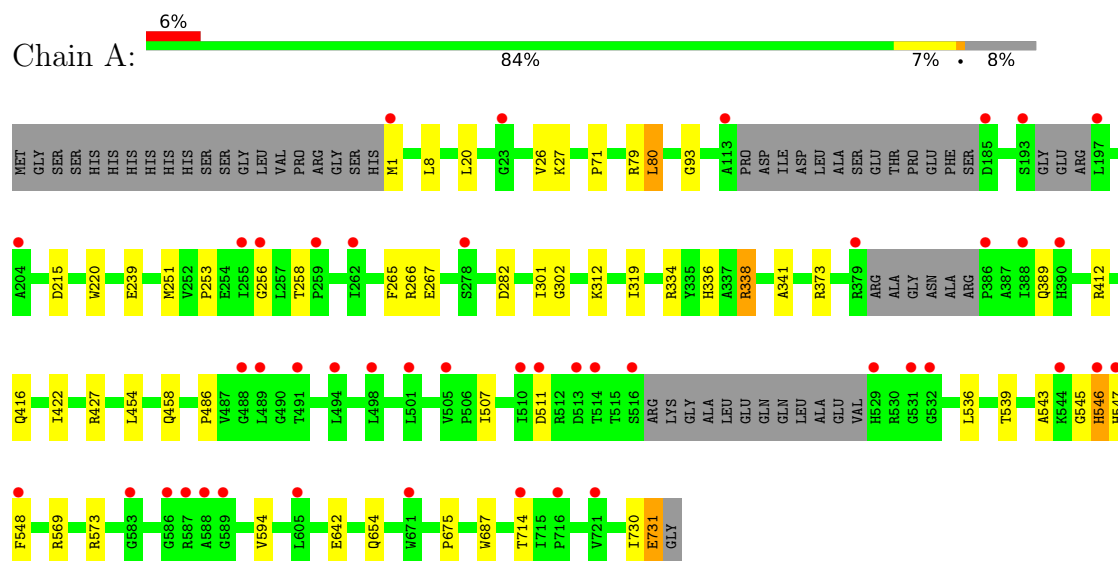
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	337	Total	O	0	0
			337	337		
4	B	75	Total	O	0	0
			75	75		

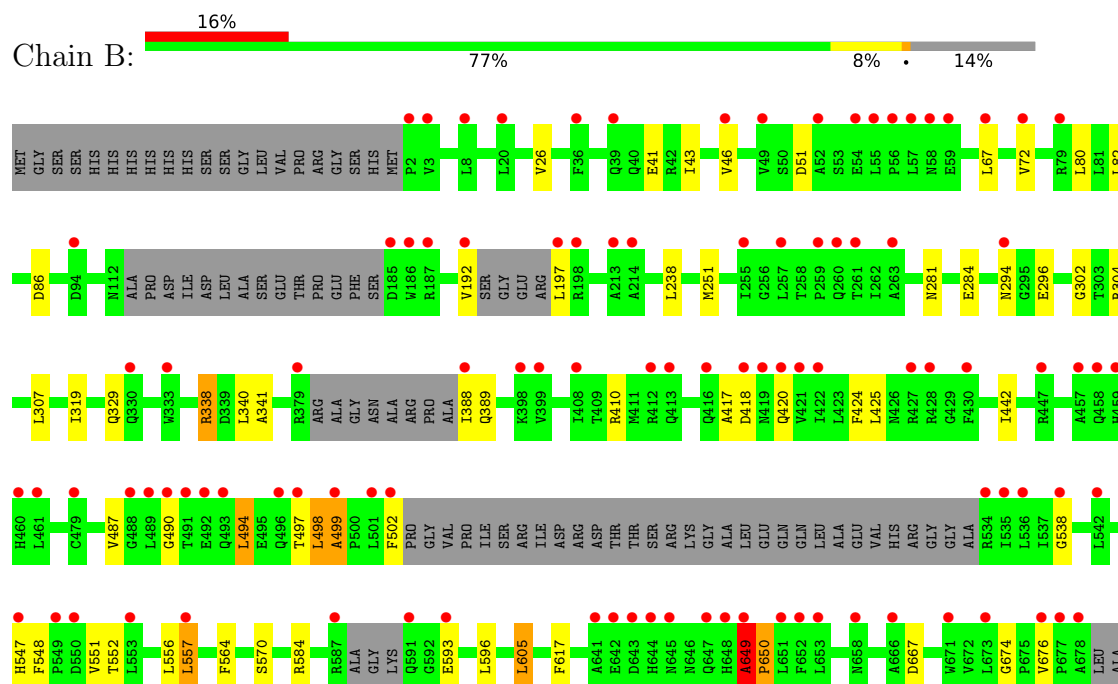
3 Residue-property plots

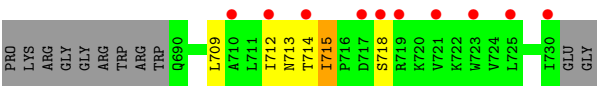
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Primosomal protein N¹



• Molecule 1: Primosomal protein N¹





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.13Å 56.51Å 195.86Å 90.00° 97.67° 90.00°	Depositor
Resolution (Å)	48.83 – 1.98 48.83 – 1.98	Depositor EDS
% Data completeness (in resolution range)	96.8 (48.83-1.98) 96.8 (48.83-1.98)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 1.98Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.186 , 0.215 0.190 , 0.219	Depositor DCC
R_{free} test set	5085 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 74.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19132	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: ZN, SO4

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	0.65	2/5148 (0.0%)	0.68	1/7019 (0.0%)
1	B	0.45	0/4544	0.61	4/6221 (0.1%)
All	All	0.56	2/9692 (0.0%)	0.65	5/13240 (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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	PRO	C-O	-6.62	1.15	1.23
1	A	239	GLU	C-O	-6.32	1.16	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	499	ALA	O-C-N	6.83	124.98	120.27
1	B	649	ALA	CA-C-N	-6.74	112.83	119.64
1	B	649	ALA	C-N-CA	-6.74	112.83	119.64
1	A	730	ILE	N-CA-C	-6.16	106.73	112.83
1	B	650	PRO	CA-N-CD	-5.02	104.97	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	338	ARG	Sidechain

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	5004	4981	4970	39	0
1	B	4436	4255	4247	42	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	25	0	0	2	0
3	B	15	0	0	0	0
4	A	337	0	0	5	0
4	B	75	0	0	0	0
All	All	9896	9236	9217	81	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 4.

All (81) 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:B:499:ALA:O	1:B:502:PHE:O	1.55	1.22
1:A:427:ARG:HA	1:A:539:THR:HG21	1.47	0.92
1:B:712:ILE:O	1:B:715:ILE:HB	1.70	0.90
1:A:427:ARG:HA	1:A:539:THR:CG2	2.06	0.86
1:A:511:ASP:OD2	1:A:539:THR:HB	1.82	0.79
1:B:494:LEU:HA	1:B:497:THR:OG1	1.85	0.77
1:A:220:TRP:CH2	1:A:373:ARG:HD2	2.29	0.68
1:B:494:LEU:O	1:B:497:THR:OG1	2.13	0.67
1:A:220:TRP:CZ3	1:A:373:ARG:HD2	2.33	0.64
1:B:713:ASN:O	1:B:715:ILE:N	2.32	0.62
1:B:715:ILE:O	1:B:715:ILE:HG22	2.00	0.60
1:B:51:ASP:OD1	1:B:51:ASP:N	2.35	0.59
1:A:539:THR:HG22	1:A:539:THR:O	2.04	0.58
1:A:543:ALA:HB3	1:A:546:HIS:HB2	1.85	0.58
1:B:715:ILE:HG22	1:B:718:SER:HB3	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:ARG:NH2	3:A:804:SO4:O4	2.37	0.57
1:A:373:ARG:NH1	4:A:906:HOH:O	2.37	0.57
1:B:494:LEU:CA	1:B:497:THR:OG1	2.53	0.56
1:B:547:HIS:HA	1:B:584:ARG:HH22	1.71	0.56
1:B:72:VAL:O	1:B:72:VAL:HG12	2.05	0.55
1:B:547:HIS:CG	1:B:548:PHE:N	2.74	0.55
1:A:215:ASP:HB2	4:A:931:HOH:O	2.08	0.54
1:B:425:LEU:HD23	1:B:490:GLY:HA2	1.90	0.53
1:A:511:ASP:OD2	1:A:539:THR:CB	2.56	0.52
1:B:294[B]:ASN:ND2	1:B:296:GLU:OE2	2.44	0.51
1:B:547:HIS:CG	1:B:548:PHE:H	2.30	0.49
1:B:494:LEU:C	1:B:497:THR:OG1	2.56	0.49
1:A:319:ILE:HD11	1:A:341:ALA:CB	2.42	0.49
1:A:282:ASP:OD1	4:A:901:HOH:O	2.20	0.49
1:B:649:ALA:H	1:B:650:PRO:CD	2.25	0.49
1:B:649:ALA:N	1:B:650:PRO:CD	2.76	0.48
1:A:427:ARG:HG2	1:A:539:THR:HG22	1.96	0.48
1:B:605:LEU:HD22	1:B:617:PHE:CD1	2.49	0.48
1:A:253:PRO:O	1:A:256:GLY:N	2.47	0.47
1:B:304:ARG:NH1	1:B:329:GLN:OE1	2.47	0.47
1:A:422:ILE:HG12	1:A:536:LEU:HB2	1.96	0.47
1:B:499:ALA:O	1:B:502:PHE:C	2.49	0.47
1:B:494:LEU:O	1:B:498:LEU:N	2.47	0.47
1:A:389:GLN:HA	1:A:594:VAL:O	2.15	0.47
1:A:412:ARG:O	1:A:416:GLN:HG2	2.15	0.46
1:B:557:LEU:N	1:B:557:LEU:HD13	2.31	0.46
1:A:334:ARG:NH2	3:A:805:SO4:O1	2.45	0.46
1:A:458:GLN:OE1	1:A:458:GLN:N	2.49	0.45
1:B:43:ILE:HD12	1:B:67:LEU:HD11	1.99	0.45
1:A:258:THR:HG21	1:A:545:GLY:HA3	1.99	0.45
1:A:319:ILE:HD11	1:A:341:ALA:HB3	1.98	0.45
1:B:420:GLN:O	1:B:551:VAL:HA	2.17	0.45
1:B:307:LEU:HD21	1:B:340:LEU:CB	2.47	0.45
1:A:80:LEU:C	1:A:80:LEU:HD23	2.41	0.45
1:B:388:ILE:HG23	1:B:593:GLU:HA	1.99	0.45
1:A:427:ARG:CA	1:A:539:THR:CG2	2.88	0.45
1:A:548:PHE:N	1:A:548:PHE:CD1	2.85	0.44
1:B:556:LEU:HD12	1:B:596:LEU:HG	1.99	0.44
1:B:26:VAL:HG21	1:B:46:VAL:HG21	1.98	0.44
1:A:569[A]:ARG:HG2	1:A:569[A]:ARG:HH11	1.82	0.44
1:A:454:LEU:HD23	1:A:486:PRO:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LEU:C	1:B:80:LEU:HD23	2.43	0.44
1:A:654:GLN:HG3	1:A:675:PRO:HG2	1.99	0.44
1:A:336:HIS:CE1	1:A:338:ARG:HB3	2.53	0.43
1:A:251:MET:HA	1:A:302:GLY:O	2.18	0.43
1:B:281:ASN:OD1	1:B:284:GLU:HG3	2.18	0.43
1:A:266:ARG:HH11	1:A:266:ARG:HG2	1.84	0.43
1:A:8:LEU:O	1:A:93:GLY:HA3	2.19	0.42
1:B:307:LEU:HD21	1:B:340:LEU:HB3	2.01	0.42
1:B:319:ILE:HD11	1:B:341:ALA:CB	2.49	0.42
1:B:424:PHE:C	1:B:425:LEU:HD12	2.44	0.42
1:B:442:ILE:HD13	1:B:564:PHE:CD1	2.54	0.42
1:A:569[B]:ARG:NE	1:A:731:GLU:HB3	2.34	0.42
1:B:715:ILE:O	1:B:715:ILE:CG2	2.68	0.42
1:A:20:LEU:HD11	1:A:26:VAL:HG12	2.00	0.42
1:A:79:ARG:HD3	4:A:1028:HOH:O	2.19	0.42
1:B:251:MET:HA	1:B:302:GLY:O	2.19	0.41
1:A:265:PHE:CD2	1:A:301:ILE:HD11	2.55	0.41
1:B:674:GLY:HA2	1:B:676:VAL:HG13	2.02	0.41
1:A:642:GLU:HA	1:A:687:TRP:O	2.21	0.41
1:A:312:LYS:NZ	4:A:921:HOH:O	2.54	0.41
1:B:605:LEU:HD23	1:B:605:LEU:HA	1.84	0.41
1:A:569[A]:ARG:HG2	1:A:569[A]:ARG:NH1	2.35	0.41
1:B:424:PHE:HA	1:B:538:GLY:O	2.21	0.41
1:B:417:ALA:O	1:B:418:ASP:C	2.64	0.40
1:B:667:ASP:OD1	1:B:667:ASP:C	2.65	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	637/694 (92%)	615 (96%)	22 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	588/694 (85%)	564 (96%)	22 (4%)	2 (0%)	36	27
All	All	1225/1388 (88%)	1179 (96%)	44 (4%)	2 (0%)	43	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	714	THR
1	B	649	ALA

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	528/579 (91%)	518 (98%)	10 (2%)	50	44
1	B	436/579 (75%)	418 (96%)	18 (4%)	27	16
All	All	964/1158 (83%)	936 (97%)	28 (3%)	37	28

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	27	LYS
1	A	80	LEU
1	A	267	GLU
1	A	338	ARG
1	A	507	ILE
1	A	546	HIS
1	A	547	HIS
1	A	714	THR
1	A	731	GLU
1	B	41	GLU
1	B	82	LEU
1	B	86	ASP
1	B	192	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	197	LEU
1	B	238	LEU
1	B	338	ARG
1	B	389	GLN
1	B	410	ARG
1	B	487	VAL
1	B	494	LEU
1	B	498	LEU
1	B	552	THR
1	B	557	LEU
1	B	570	SER
1	B	605	LEU
1	B	709	LEU
1	B	715	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	456	GLN
1	A	493	GLN
1	A	529	HIS
1	A	713	ASN
1	B	189	ASN
1	B	368	GLN
1	B	390	HIS
1	B	426	ASN
1	B	603	HIS

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](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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	$\# Z > 2$
3	SO4	A	807	-	4,4,4	0.43	0	6,6,6	0.07	0
3	SO4	B	803	-	4,4,4	0.43	0	6,6,6	0.08	0
3	SO4	B	804	-	4,4,4	0.25	0	6,6,6	0.08	0
3	SO4	B	805	-	4,4,4	0.28	0	6,6,6	0.31	0
3	SO4	A	804	-	4,4,4	0.27	0	6,6,6	0.44	0
3	SO4	A	805	-	4,4,4	0.20	0	6,6,6	0.19	0
3	SO4	A	803	-	4,4,4	0.45	0	6,6,6	1.07	0
3	SO4	A	806	-	4,4,4	0.23	0	6,6,6	0.08	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	804	SO4	1	0
3	A	805	SO4	1	0

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	639/694 (92%)	0.48	45 (7%) 22 30	20, 60, 127, 185	6 (0%)
1	B	600/694 (86%)	1.16	111 (18%) 3 4	43, 94, 154, 186	1 (0%)
All	All	1239/1388 (89%)	0.81	156 (12%) 8 11	20, 79, 147, 186	7 (0%)

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	PRO	7.2
1	B	587	ARG	5.6
1	B	58	ASN	5.6
1	B	55	LEU	5.4
1	B	649	ALA	5.3
1	B	57	LEU	4.9
1	B	502	PHE	4.9
1	A	513	ASP	4.7
1	A	588	ALA	4.7
1	B	412	ARG	4.4
1	A	379	ARG	4.3
1	B	422	ILE	4.3
1	B	535	ILE	4.2
1	B	651	LEU	4.2
1	B	459	HIS	4.2
1	A	197	LEU	4.1
1	A	501	LEU	4.1
1	B	643	ASP	4.0
1	A	586	GLY	3.9
1	B	399	VAL	3.9
1	B	379	ARG	3.9
1	B	550	ASP	3.9
1	A	113	ALA	3.8
1	B	79	ARG	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	430	PHE	3.7
1	B	714	THR	3.7
1	B	185	ASP	3.7
1	A	583	GLY	3.7
1	A	494	LEU	3.6
1	B	197	LEU	3.6
1	B	647	GLN	3.6
1	B	257	LEU	3.6
1	B	641	ALA	3.5
1	B	458	GLN	3.5
1	B	648	HIS	3.5
1	B	645	ASN	3.5
1	B	408	ILE	3.5
1	B	488	GLY	3.3
1	B	501	LEU	3.3
1	A	386	PRO	3.3
1	B	421	VAL	3.3
1	B	52	ALA	3.3
1	B	536	LEU	3.3
1	B	678	ALA	3.2
1	B	676	VAL	3.2
1	B	557	LEU	3.2
1	A	587	ARG	3.2
1	B	333	TRP	3.1
1	B	263	ALA	3.1
1	B	490	GLY	3.1
1	B	534	ARG	3.1
1	B	489	LEU	3.1
1	B	717	ASP	3.1
1	B	591	GLN	3.1
1	B	457	ALA	3.1
1	A	547	HIS	3.1
1	B	460	HIS	3.1
1	B	260	GLN	3.1
1	A	255	ILE	3.0
1	B	712	ILE	3.0
1	B	213	ALA	3.0
1	B	725	LEU	3.0
1	A	505	VAL	3.0
1	B	491	THR	3.0
1	B	259	PRO	3.0
1	B	418	ASP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	666	ALA	2.9
1	A	514	THR	2.9
1	B	644	HIS	2.9
1	B	3	VAL	2.8
1	B	72	VAL	2.8
1	B	54	GLU	2.8
1	B	36	PHE	2.8
1	A	714	THR	2.8
1	A	529	HIS	2.8
1	B	673	LEU	2.8
1	B	723	TRP	2.8
1	B	192	VAL	2.8
1	B	416	GLN	2.7
1	B	420	GLN	2.7
1	A	716	PRO	2.7
1	B	496	GLN	2.7
1	A	548	PHE	2.7
1	B	255	ILE	2.7
1	B	671	TRP	2.7
1	B	493	GLN	2.7
1	A	193	SER	2.7
1	B	94	ASP	2.6
1	B	39	GLN	2.6
1	A	531	GLY	2.6
1	B	730	ILE	2.6
1	A	1	MET	2.6
1	A	671	TRP	2.6
1	A	388	ILE	2.6
1	B	710	ALA	2.6
1	B	330	GLN	2.5
1	B	497	THR	2.5
1	A	259	PRO	2.5
1	B	427	ARG	2.5
1	B	547	HIS	2.5
1	B	413	GLN	2.5
1	B	549	PRO	2.5
1	B	187	ARG	2.5
1	A	546	HIS	2.5
1	A	262	ILE	2.5
1	A	511	ASP	2.5
1	B	56	PRO	2.5
1	B	553	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	388	ILE	2.4
1	B	677	PRO	2.4
1	B	294[A]	ASN	2.4
1	A	488	GLY	2.4
1	A	510	ILE	2.4
1	B	59	GLU	2.4
1	B	419	ASN	2.4
1	A	23	GLY	2.4
1	A	532	GLY	2.4
1	A	589	GLY	2.4
1	B	447	ARG	2.3
1	B	46	VAL	2.3
1	B	479	CYS	2.3
1	B	461	LEU	2.3
1	B	542	LEU	2.3
1	B	398	LYS	2.3
1	A	185	ASP	2.3
1	B	492	GLU	2.3
1	A	721	VAL	2.3
1	B	652	PHE	2.2
1	A	278	SER	2.2
1	B	653	LEU	2.2
1	B	718	SER	2.2
1	A	390	HIS	2.2
1	B	721	VAL	2.2
1	A	491	THR	2.2
1	A	544	LYS	2.2
1	B	658	ASN	2.2
1	B	593	GLU	2.2
1	A	489	LEU	2.2
1	B	8	LEU	2.2
1	B	67	LEU	2.2
1	B	198	ARG	2.2
1	B	428	ARG	2.2
1	B	719	ARG	2.2
1	B	261	THR	2.1
1	B	186	TRP	2.1
1	B	538	GLY	2.1
1	A	498	LEU	2.1
1	B	214	ALA	2.1
1	A	516	SER	2.1
1	B	642	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	256	GLY	2.1
1	B	49	VAL	2.1
1	A	605	LEU	2.0
1	B	20	LEU	2.0
1	A	204	ALA	2.0
1	B	499	ALA	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(Å ²)	Q<0.9
3	SO4	B	803	5/5	0.51	0.13	54,54,58,90	0
3	SO4	A	806	5/5	0.66	0.22	177,179,180,186	0
3	SO4	A	807	5/5	0.67	0.14	56,57,59,88	0
3	SO4	B	804	5/5	0.79	0.20	141,144,145,151	0
3	SO4	A	805	5/5	0.89	0.13	113,115,119,123	0
3	SO4	A	804	5/5	0.94	0.09	74,85,89,94	0
3	SO4	B	805	5/5	0.94	0.08	67,68,84,87	0
3	SO4	A	803	5/5	0.96	0.08	48,51,62,66	0
2	ZN	A	801	1/1	0.98	0.07	65,65,65,65	0
2	ZN	A	802	1/1	0.98	0.09	64,64,64,64	0
2	ZN	B	801	1/1	0.98	0.07	76,76,76,76	0
2	ZN	B	802	1/1	0.98	0.05	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.