



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:47 am BST

PDB ID : 6DCR
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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

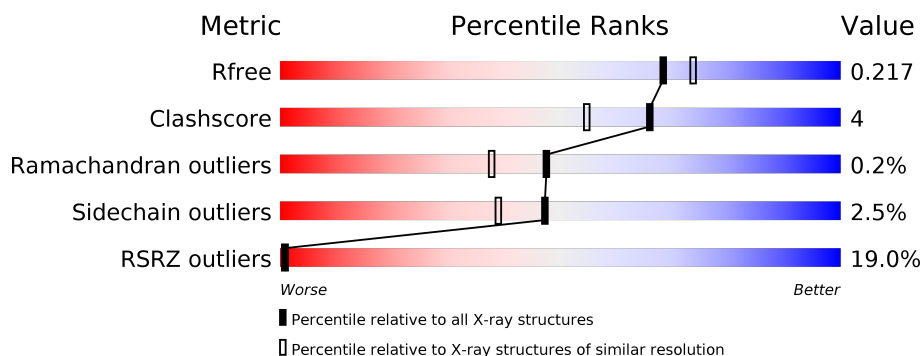
1 Overall quality at a glance

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}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 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	<div> <div>14%</div> <div>85%</div> <div>7%</div> <div>8%</div> </div>
1	B	694	<div> <div>20%</div> <div>77%</div> <div>8%</div> <div>14%</div> </div>

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
3	SO4	A	806	-	-	-	X

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

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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

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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

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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

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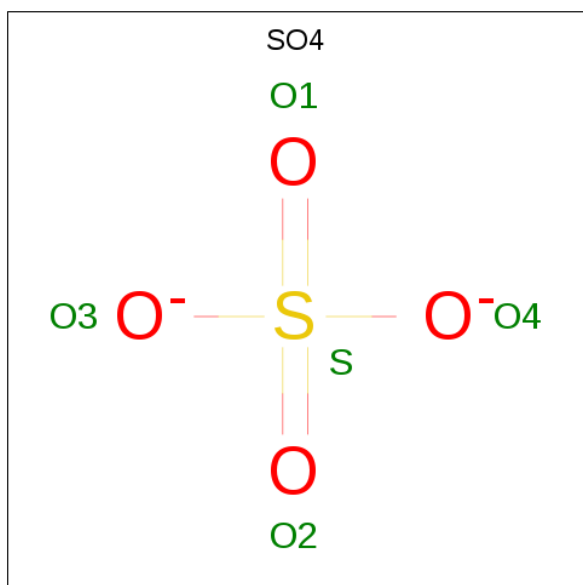
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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLN	deletion	UNP P17888
B	?	-	ALA	deletion	UNP P17888
B	?	-	LEU	deletion	UNP P17888
B	?	-	ARG	deletion	UNP P17888
B	?	-	LYS	deletion	UNP P17888
B	?	-	LYS	deletion	UNP P17888
B	?	-	GLY	deletion	UNP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

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is SULFATE ION (three-letter code: 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		

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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		

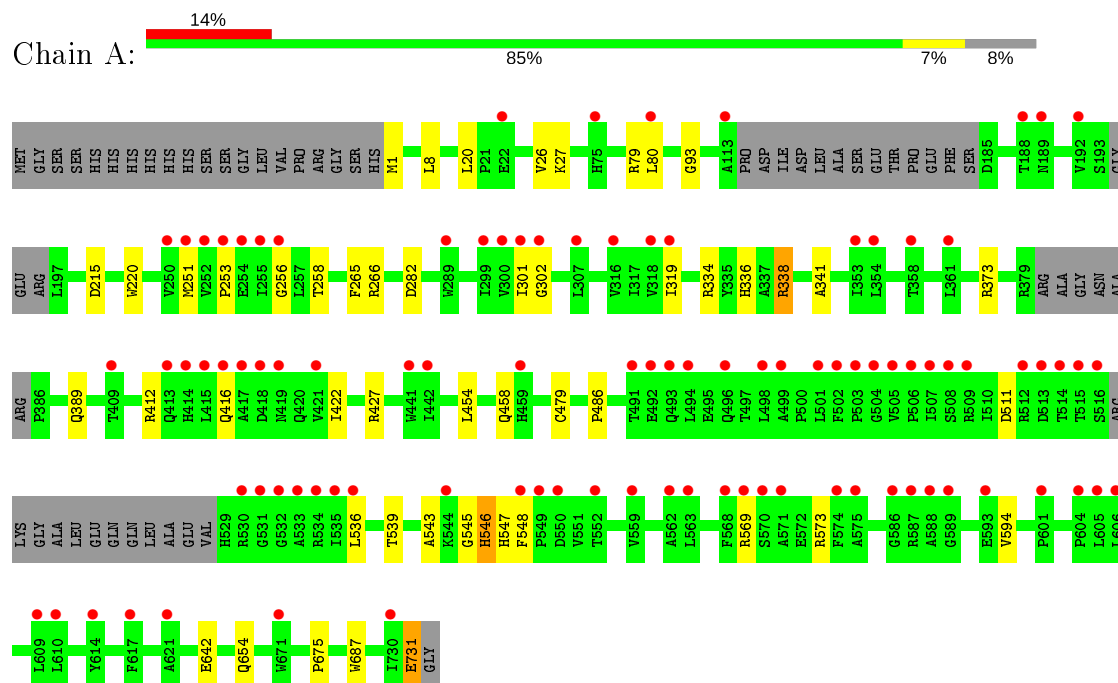
- Molecule 4 is water.

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

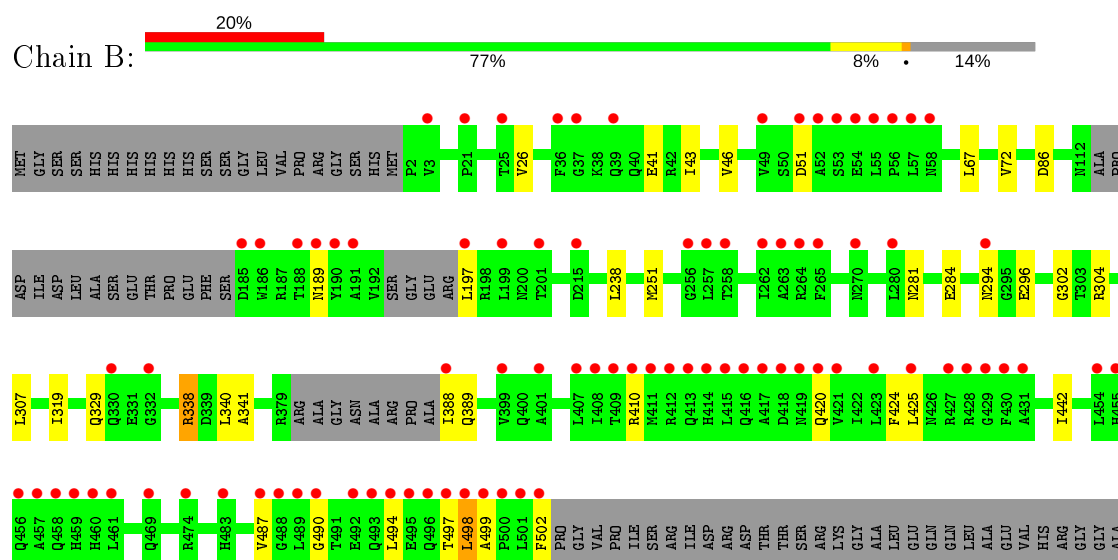
3 Residue-property plots

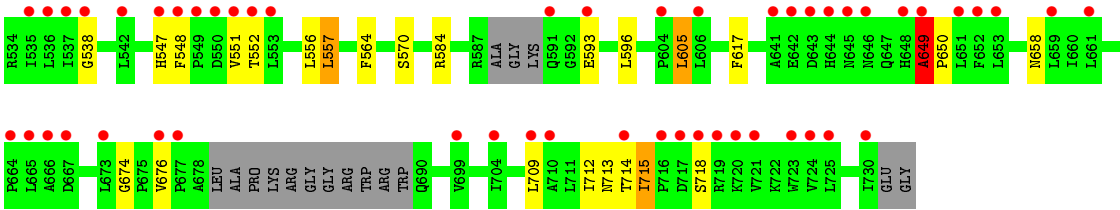
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



• Molecule 1: Primosomal protein N'





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 0.187 , 0.217	Depositor DCC
R_{free} test set	5085 reflections (4.99%)	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 , 72.0	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 [i](#)

5.1 Standard geometry [i](#)

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	0/5148	0.70	0/7019
1	B	0.43	0/4544	0.59	1/6221 (0.0%)
All	All	0.56	0/9692	0.65	1/13240 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	649	ALA	C-N-CD	6.40	141.83	128.40

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 [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	5004	4981	4970	38	0
1	B	4436	4255	4247	37	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	4	0
4	B	75	0	0	0	0
All	All	9896	9236	9217	75	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 (75) 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:HG22	1:B:715:ILE:O	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
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:CG	1:B:548:PHE:N	2.74	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:HD13	1:B:557:LEU:N	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:319:ILE:HD11	1:A:341:ALA:HB3	1.98	0.45
1:A:258:THR:HG21	1:A:545:GLY:HA3	1.99	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: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:B:494:LEU:C	1:B:497:THR:OG1	2.56	0.45
1:A:548:PHE:CD1	1:A:548:PHE:N	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
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:319:ILE:HD11	1:B:341:ALA:CB	2.49	0.42
1:B:307:LEU:HD21	1:B:340:LEU:HB3	2.01	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:CG2	1:B:715:ILE:O	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:80:LEU:HD23	1:A:80:LEU:C	2.41	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	637/694 (92%)	615 (96%)	22 (4%)	0	100	100
1	B	588/694 (85%)	564 (96%)	22 (4%)	2 (0%)	41	29
All	All	1225/1388 (88%)	1179 (96%)	44 (4%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

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

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	528/579 (91%)	521 (99%)	7 (1%)	69	64
1	B	436/579 (75%)	419 (96%)	17 (4%)	32	19
All	All	964/1158 (83%)	940 (98%)	24 (2%)	47	39

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	27	LYS
1	A	338	ARG
1	A	479	CYS
1	A	546	HIS
1	A	547	HIS
1	A	731	GLU
1	B	41	GLU
1	B	86	ASP
1	B	189	ASN
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	498	LEU
1	B	552	THR
1	B	557	LEU
1	B	570	SER
1	B	605	LEU
1	B	658	ASN
1	B	709	LEU
1	B	715	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	713	ASN
1	B	40	GLN

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](#)

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	B	805	-	4,4,4	0.19	0	6,6,6	0.33	0
3	SO4	A	803	-	4,4,4	0.36	0	6,6,6	1.19	1 (16%)
3	SO4	A	804	-	4,4,4	0.17	0	6,6,6	0.47	0
3	SO4	A	806	-	4,4,4	0.16	0	6,6,6	0.05	0
3	SO4	B	803	-	4,4,4	0.32	0	6,6,6	0.05	0
3	SO4	A	805	-	4,4,4	0.12	0	6,6,6	0.18	0
3	SO4	B	804	-	4,4,4	0.18	0	6,6,6	0.12	0
3	SO4	A	807	-	4,4,4	0.32	0	6,6,6	0.05	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	803	SO4	O4-S-O3	2.36	119.12	109.06

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%)	1.05	97 (15%) 2 2	31, 55, 115, 171	0
1	B	600/694 (86%)	1.38	139 (23%) 0 0	55, 86, 141, 172	0
All	All	1239/1388 (89%)	1.21	236 (19%) 1 1	31, 72, 134, 172	0

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	489	LEU	10.2
1	B	499	ALA	8.8
1	B	641	ALA	7.8
1	B	419	ASN	7.6
1	A	513	ASP	7.4
1	B	421	VAL	7.4
1	B	723	TRP	7.3
1	A	586	GLY	7.2
1	B	488	GLY	7.2
1	B	501	LEU	7.1
1	B	55	LEU	7.1
1	B	644	HIS	7.0
1	B	498	LEU	6.8
1	B	495	GLU	6.6
1	B	52	ALA	6.5
1	A	496	GLN	6.3
1	B	185	ASP	6.3
1	B	537	ILE	6.2
1	A	507	ILE	6.1
1	B	412	ARG	6.1
1	B	415	LEU	6.1
1	B	717	ASP	6.1
1	B	388	ILE	6.0
1	B	536	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
1	B	54	GLU	5.9
1	B	407	LEU	5.8
1	B	538	GLY	5.8
1	B	494	LEU	5.7
1	B	665	LEU	5.7
1	B	553	LEU	5.6
1	B	502	PHE	5.6
1	B	408	ILE	5.5
1	B	417	ALA	5.5
1	B	643	ASP	5.4
1	B	676	VAL	5.4
1	B	418	ASP	5.4
1	A	492	GLU	5.4
1	B	591	GLN	5.4
1	B	257	LEU	5.3
1	B	414	HIS	5.2
1	A	588	ALA	5.2
1	B	399	VAL	5.2
1	B	497	THR	5.1
1	A	499	ALA	5.1
1	B	430	PHE	5.1
1	A	533	ALA	5.0
1	B	719	ARG	5.0
1	B	57	LEU	5.0
1	B	552	THR	5.0
1	A	516	SER	5.0
1	B	51	ASP	4.9
1	B	413	GLN	4.9
1	B	718	SER	4.9
1	B	457	ALA	4.8
1	B	724	VAL	4.8
1	A	415	LEU	4.8
1	B	411	MET	4.8
1	A	589	GLY	4.8
1	B	454	LEU	4.8
1	A	505	VAL	4.6
1	A	417	ALA	4.6
1	B	699	VAL	4.6
1	B	648	HIS	4.6
1	B	593	GLU	4.6
1	B	666	ALA	4.5
1	A	532	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	514	THR	4.4
1	B	721	VAL	4.4
1	A	515	THR	4.4
1	B	646	ASN	4.4
1	B	188	THR	4.3
1	A	192	VAL	4.2
1	B	493	GLN	4.2
1	A	508	SER	4.2
1	B	190	TYR	4.2
1	B	197	LEU	4.2
1	B	258	THR	4.2
1	A	498	LEU	4.1
1	A	494	LEU	4.1
1	A	512	ARG	4.1
1	B	549	PRO	4.0
1	B	428	ARG	4.0
1	B	191	ALA	4.0
1	B	496	GLN	4.0
1	B	189	ASN	3.9
1	B	21	PRO	3.9
1	B	535	ILE	3.9
1	A	416	GLN	3.8
1	A	418	ASP	3.8
1	B	262	ILE	3.8
1	B	36	PHE	3.7
1	B	459	HIS	3.7
1	A	502	PHE	3.7
1	B	25	THR	3.7
1	B	199	LEU	3.7
1	B	551	VAL	3.7
1	A	413	GLN	3.7
1	B	201	THR	3.6
1	B	677	PRO	3.6
1	B	653	LEU	3.6
1	B	720	LYS	3.6
1	B	652	PHE	3.5
1	A	536	LEU	3.5
1	B	661	LEU	3.5
1	A	506	PRO	3.5
1	B	186	TRP	3.5
1	A	419	ASN	3.4
1	B	710	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	730	ILE	3.3
1	A	255	ILE	3.3
1	B	410	ARG	3.3
1	B	416	GLN	3.2
1	B	409	THR	3.2
1	B	332	GLY	3.2
1	B	487	VAL	3.2
1	B	270	ASN	3.2
1	B	492	GLU	3.1
1	B	49	VAL	3.1
1	B	53	SER	3.1
1	A	550	ASP	3.1
1	B	264	ARG	3.1
1	B	483	HIS	3.0
1	A	188	THR	3.0
1	B	423	LEU	3.0
1	A	587	ARG	3.0
1	B	401	ALA	3.0
1	B	716	PRO	3.0
1	A	568	PHE	2.9
1	B	725	LEU	2.9
1	B	427	ARG	2.9
1	A	535	ILE	2.9
1	B	265	PHE	2.9
1	A	610	LEU	2.9
1	B	500	PRO	2.9
1	B	263	ALA	2.8
1	A	491	THR	2.7
1	A	319	ILE	2.7
1	A	503	PRO	2.7
1	A	414	HIS	2.7
1	A	409	THR	2.7
1	A	552	THR	2.7
1	A	493	GLN	2.6
1	A	504	GLY	2.6
1	B	429	GLY	2.6
1	A	421	VAL	2.6
1	B	490	GLY	2.6
1	B	542	LEU	2.6
1	B	461	LEU	2.6
1	A	254	GLU	2.6
1	A	459	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	575	ALA	2.6
1	A	671	TRP	2.6
1	A	113	ALA	2.5
1	A	534	ARG	2.5
1	A	189	ASN	2.5
1	B	474	ARG	2.5
1	A	301	ILE	2.5
1	B	548	PHE	2.5
1	A	531	GLY	2.5
1	B	256	GLY	2.5
1	B	547	HIS	2.5
1	A	442	ILE	2.5
1	B	645	ASN	2.5
1	A	562	ALA	2.5
1	B	704	ILE	2.4
1	A	300	VAL	2.4
1	B	58	ASN	2.4
1	A	501	LEU	2.4
1	B	642	GLU	2.4
1	B	550	ASP	2.4
1	A	574	PHE	2.4
1	A	353	ILE	2.4
1	A	569[A]	ARG	2.4
1	A	302	GLY	2.4
1	B	456	GLN	2.4
1	A	361	LEU	2.4
1	B	280	LEU	2.4
1	A	606	LEU	2.3
1	B	425	LEU	2.3
1	B	649	ALA	2.3
1	A	22	GLU	2.3
1	A	593	GLU	2.3
1	A	605	LEU	2.3
1	B	469	GLN	2.3
1	B	673	LEU	2.3
1	A	614	TYR	2.3
1	B	667	ASP	2.3
1	A	252	VAL	2.3
1	A	299	ILE	2.3
1	B	294[A]	ASN	2.3
1	A	571[A]	ALA	2.3
1	A	354	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	458	GLN	2.3
1	B	714	THR	2.3
1	A	548	PHE	2.3
1	A	617	PHE	2.3
1	A	250	VAL	2.3
1	A	601	PRO	2.3
1	A	621	ALA	2.3
1	B	330	GLN	2.3
1	A	609	LEU	2.3
1	A	358	THR	2.2
1	B	39	GLN	2.2
1	B	420	GLN	2.2
1	A	604	PRO	2.2
1	B	215	ASP	2.2
1	A	75[A]	HIS	2.2
1	A	544	LYS	2.2
1	B	3	VAL	2.2
1	A	251	MET	2.1
1	A	441	TRP	2.1
1	A	318	VAL	2.1
1	B	37	GLY	2.1
1	B	651	LEU	2.1
1	A	570[A]	SER	2.1
1	A	549	PRO	2.1
1	A	730	ILE	2.1
1	A	307	LEU	2.1
1	A	563	LEU	2.1
1	B	659	LEU	2.1
1	A	509	ARG	2.1
1	B	460	HIS	2.1
1	A	253	PRO	2.1
1	A	559	VAL	2.1
1	B	709	LEU	2.1
1	B	604	PRO	2.1
1	B	56	PRO	2.1
1	B	606	LEU	2.1
1	A	256	GLY	2.1
1	B	455	HIS	2.0
1	A	316	VAL	2.0
1	B	431	ALA	2.0
1	B	664	PRO	2.0
1	A	289	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	80	LEU	2.0
1	A	530	ARG	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. 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	A	806	5/5	0.64	0.65	177,179,180,186	0
3	SO4	B	803	5/5	0.80	0.34	54,54,58,90	0
3	SO4	A	805	5/5	0.91	0.15	113,115,119,123	0
3	SO4	B	804	5/5	0.92	0.23	141,144,145,151	0
3	SO4	A	807	5/5	0.93	0.42	56,57,59,88	0
3	SO4	B	805	5/5	0.95	0.10	67,68,84,87	0
3	SO4	A	804	5/5	0.97	0.15	74,85,89,94	0
3	SO4	A	803	5/5	0.97	0.22	48,51,62,66	0
2	ZN	A	802	1/1	0.97	0.23	64,64,64,64	0
2	ZN	B	802	1/1	0.98	0.10	66,66,66,66	0
2	ZN	B	801	1/1	0.98	0.06	76,76,76,76	0
2	ZN	A	801	1/1	0.99	0.22	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.