



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:38 PM UTC

PDB ID : 5JWR / pdb_00005jwr
Title : Crystal structure of foldswitch-stabilized KaiB in complex with the N-terminal CI domain of KaiC and a dimer of KaiA C-terminal domains from *Thermosynechococcus elongatus*
Authors : Tseng, R.; Goularte, N.F.; Chavan, A.; Luu, J.; Chang, Y.G.; Heilser, J.; Tripathi, S.; LiWang, A.; Partch, C.L.
Deposited on : 2016-05-12
Resolution : 2.61 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

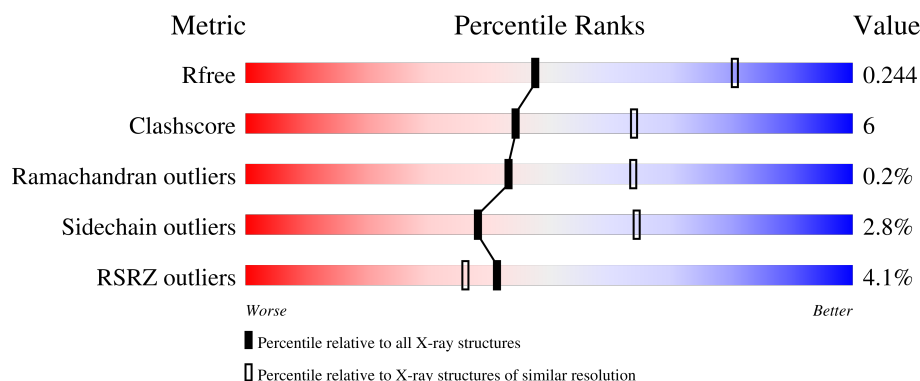
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	247	2% 82% 11% 6%
1	C	247	7% 70% 19% 11%
2	B	99	4% 74% 16% 10%
2	D	99	2% 66% 19% 12%

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Mol	Chain	Length	Quality of chain
3	E	145	% 78% 13% 9%
3	F	145	2% 77% 16% 8%
3	G	145	3% 74% 17% • 8%
3	H	145	7% 78% 12% •• 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9528 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 Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1825	1167	310	345	3			
1	C	221	Total	C	N	O	S	0	0	0
			1735	1109	293	330	3			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	ASP	-	expression tag	UNP Q79V60
A	10	TYR	-	expression tag	UNP Q79V60
A	11	LYS	-	expression tag	UNP Q79V60
A	12	ASP	-	expression tag	UNP Q79V60
A	13	ASP	-	expression tag	UNP Q79V60
A	14	ASP	-	expression tag	UNP Q79V60
A	15	ASP	-	expression tag	UNP Q79V60
A	16	LYS	-	expression tag	UNP Q79V60
A	41	ALA	ARG	engineered mutation	UNP Q79V60
A	173	ALA	LYS	engineered mutation	UNP Q79V60
A	248	ASP	-	expression tag	UNP Q79V60
A	249	TYR	-	expression tag	UNP Q79V60
A	250	LYS	-	expression tag	UNP Q79V60
A	251	ASP	-	expression tag	UNP Q79V60
A	252	ASP	-	expression tag	UNP Q79V60
A	253	ASP	-	expression tag	UNP Q79V60
A	254	ASP	-	expression tag	UNP Q79V60
A	255	LYS	-	expression tag	UNP Q79V60
C	9	ASP	-	expression tag	UNP Q79V60
C	10	TYR	-	expression tag	UNP Q79V60
C	11	LYS	-	expression tag	UNP Q79V60
C	12	ASP	-	expression tag	UNP Q79V60
C	13	ASP	-	expression tag	UNP Q79V60
C	14	ASP	-	expression tag	UNP Q79V60
C	15	ASP	-	expression tag	UNP Q79V60

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Chain	Residue	Modelled	Actual	Comment	Reference
C	16	LYS	-	expression tag	UNP Q79V60
C	41	ALA	ARG	engineered mutation	UNP Q79V60
C	173	ALA	LYS	engineered mutation	UNP Q79V60
C	248	ASP	-	expression tag	UNP Q79V60
C	249	TYR	-	expression tag	UNP Q79V60
C	250	LYS	-	expression tag	UNP Q79V60
C	251	ASP	-	expression tag	UNP Q79V60
C	252	ASP	-	expression tag	UNP Q79V60
C	253	ASP	-	expression tag	UNP Q79V60
C	254	ASP	-	expression tag	UNP Q79V60
C	255	LYS	-	expression tag	UNP Q79V60

- Molecule 2 is a protein called Circadian clock protein KaiB.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	89	Total	C	N	O	0	0	0
			691	449	121	121			
2	D	87	Total	C	N	O	0	0	0
			678	440	119	119			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	ALA	TYR	engineered mutation	UNP Q79V61
B	89	ALA	GLY	engineered mutation	UNP Q79V61
B	91	ARG	ASP	engineered mutation	UNP Q79V61
B	94	ALA	TYR	engineered mutation	UNP Q79V61
D	8	ALA	TYR	engineered mutation	UNP Q79V61
D	89	ALA	GLY	engineered mutation	UNP Q79V61
D	91	ARG	ASP	engineered mutation	UNP Q79V61
D	94	ALA	TYR	engineered mutation	UNP Q79V61

- Molecule 3 is a protein called Circadian clock protein KaiA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	132	Total	C	N	O	0	0	0
			1113	713	195	202			
3	F	134	Total	C	N	O	0	0	0
			1129	723	197	206			
3	G	133	Total	C	N	O	0	0	0
			1120	718	196	203			

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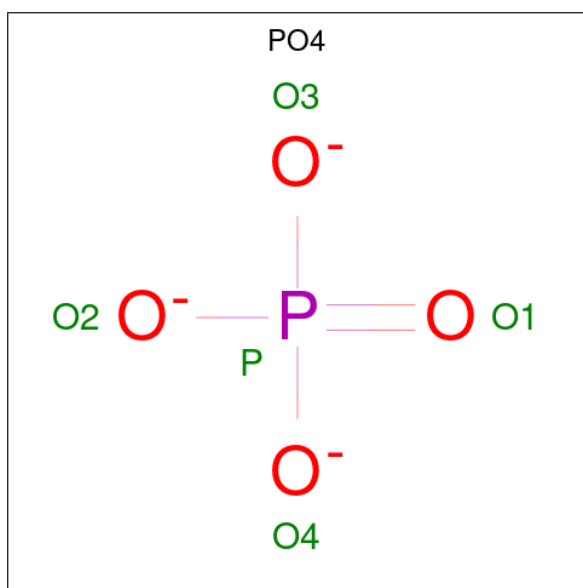
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	133	Total	C	N	O	S	0	0	0
			1121	719	196	203	3			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	139	ASP	-	expression tag	UNP Q79V62
E	140	TYR	-	expression tag	UNP Q79V62
E	141	LYS	-	expression tag	UNP Q79V62
E	142	ASP	-	expression tag	UNP Q79V62
E	143	ASP	-	expression tag	UNP Q79V62
E	144	ASP	-	expression tag	UNP Q79V62
E	145	ASP	-	expression tag	UNP Q79V62
E	146	LYS	-	expression tag	UNP Q79V62
E	272	SER	CYS	engineered mutation	UNP Q79V62
F	139	ASP	-	expression tag	UNP Q79V62
F	140	TYR	-	expression tag	UNP Q79V62
F	141	LYS	-	expression tag	UNP Q79V62
F	142	ASP	-	expression tag	UNP Q79V62
F	143	ASP	-	expression tag	UNP Q79V62
F	144	ASP	-	expression tag	UNP Q79V62
F	145	ASP	-	expression tag	UNP Q79V62
F	146	LYS	-	expression tag	UNP Q79V62
F	272	SER	CYS	engineered mutation	UNP Q79V62
G	139	ASP	-	expression tag	UNP Q79V62
G	140	TYR	-	expression tag	UNP Q79V62
G	141	LYS	-	expression tag	UNP Q79V62
G	142	ASP	-	expression tag	UNP Q79V62
G	143	ASP	-	expression tag	UNP Q79V62
G	144	ASP	-	expression tag	UNP Q79V62
G	145	ASP	-	expression tag	UNP Q79V62
G	146	LYS	-	expression tag	UNP Q79V62
G	272	SER	CYS	engineered mutation	UNP Q79V62
H	139	ASP	-	expression tag	UNP Q79V62
H	140	TYR	-	expression tag	UNP Q79V62
H	141	LYS	-	expression tag	UNP Q79V62
H	142	ASP	-	expression tag	UNP Q79V62
H	143	ASP	-	expression tag	UNP Q79V62
H	144	ASP	-	expression tag	UNP Q79V62
H	145	ASP	-	expression tag	UNP Q79V62
H	146	LYS	-	expression tag	UNP Q79V62
H	272	SER	CYS	engineered mutation	UNP Q79V62

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

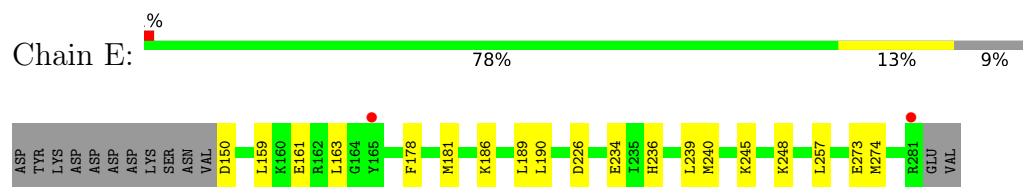


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		

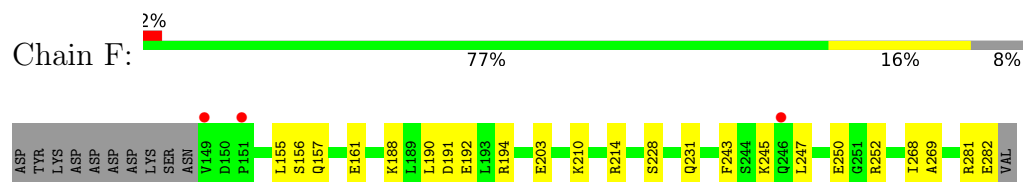
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O	0	0
			26	26		
5	B	5	Total	O	0	0
			5	5		
5	C	10	Total	O	0	0
			10	10		
5	D	7	Total	O	0	0
			7	7		
5	E	17	Total	O	0	0
			17	17		
5	F	10	Total	O	0	0
			10	10		
5	G	15	Total	O	0	0
			15	15		
5	H	16	Total	O	0	0
			16	16		

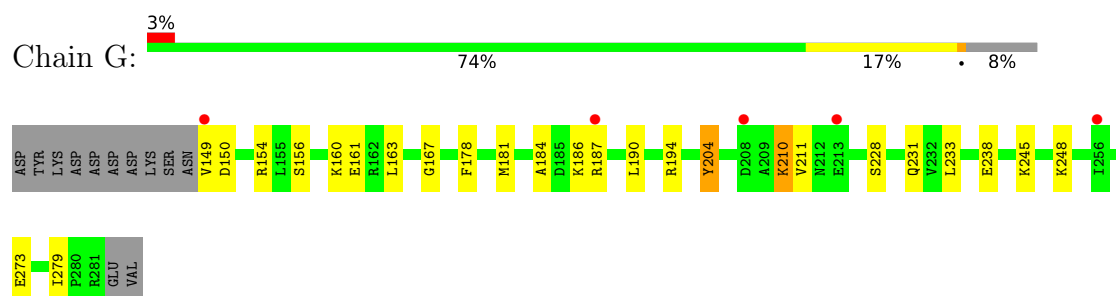
● Molecule 3: Circadian clock protein KaiA



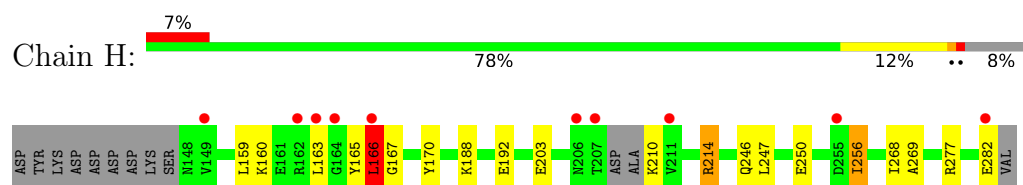
● Molecule 3: Circadian clock protein KaiA



● Molecule 3: Circadian clock protein KaiA



● Molecule 3: Circadian clock protein KaiA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.59Å 79.11Å 80.84Å 107.27° 90.71° 111.20°	Depositor
Resolution (Å)	44.84 – 2.61 44.84 – 2.61	Depositor EDS
% Data completeness (in resolution range)	95.5 (44.84-2.61) 95.5 (44.84-2.61)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.12 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.185 , 0.242 0.194 , 0.244	Depositor DCC
R_{free} test set	2324 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9528	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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	0.32	0/1858	0.74	0/2513
1	C	0.35	0/1765	0.79	0/2388
2	B	0.33	0/699	0.80	0/948
2	D	0.32	0/686	0.91	1/930 (0.1%)
3	E	0.36	0/1133	0.84	0/1521
3	F	0.33	0/1149	0.80	1/1543 (0.1%)
3	G	0.31	0/1140	0.81	1/1531 (0.1%)
3	H	0.32	0/1140	0.82	2/1529 (0.1%)
All	All	0.33	0/9570	0.80	5/12903 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	38	GLY	N-CA-C	-12.38	98.73	111.85
3	H	166	LEU	N-CA-C	5.96	118.67	111.40
3	H	165	TYR	N-CA-C	5.87	120.16	112.89
3	F	155	LEU	N-CA-C	-5.46	105.41	111.36
3	G	204	TYR	N-CA-C	5.26	117.01	111.28

There are no chirality outliers.

There are no planarity outliers.

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	1825	0	1823	21	0
1	C	1735	0	1735	30	0
2	B	691	0	771	8	0
2	D	678	0	755	12	0
3	E	1113	0	1132	13	0
3	F	1129	0	1147	13	0
3	G	1120	0	1141	15	0
3	H	1121	0	1139	10	0
4	A	5	0	0	0	0
4	C	5	0	0	0	0
5	A	26	0	0	1	0
5	B	5	0	0	0	0
5	C	10	0	0	0	0
5	D	7	0	0	0	0
5	E	17	0	0	1	0
5	F	10	0	0	0	0
5	G	15	0	0	0	0
5	H	16	0	0	0	0
All	All	9528	0	9643	114	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 6.

The worst 5 of 114 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)
3:E:234:GLU:OE2	3:F:156:SER:OG	1.95	0.83
2:B:71:PRO:O	2:B:91:ARG:NH2	2.16	0.78
3:E:181:MET:HE3	3:E:186:LYS:HA	1.66	0.78
3:H:167:GLY:O	3:H:277:ARG:NH2	2.17	0.78
1:C:201:VAL:O	1:C:203:ASP:N	2.16	0.76

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	227/247 (92%)	218 (96%)	9 (4%)	0	100	100
1	C	217/247 (88%)	207 (95%)	8 (4%)	2 (1%)	14	28
2	B	87/99 (88%)	87 (100%)	0	0	100	100
2	D	85/99 (86%)	85 (100%)	0	0	100	100
3	E	130/145 (90%)	129 (99%)	1 (1%)	0	100	100
3	F	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
3	G	131/145 (90%)	129 (98%)	2 (2%)	0	100	100
3	H	129/145 (89%)	128 (99%)	1 (1%)	0	100	100
All	All	1138/1272 (90%)	1114 (98%)	22 (2%)	2 (0%)	43	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	202	SER
1	C	215	GLU

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	197/212 (93%)	192 (98%)	5 (2%)	42	68
1	C	188/212 (89%)	181 (96%)	7 (4%)	30	55
2	B	77/85 (91%)	74 (96%)	3 (4%)	28	53
2	D	76/85 (89%)	72 (95%)	4 (5%)	20	41
3	E	123/136 (90%)	121 (98%)	2 (2%)	55	78
3	F	125/136 (92%)	124 (99%)	1 (1%)	73	87
3	G	124/136 (91%)	122 (98%)	2 (2%)	55	78
3	H	124/136 (91%)	119 (96%)	5 (4%)	28	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1034/1138 (91%)	1005 (97%)	29 (3%)	38 64

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	217	ARG
3	H	256	ILE
2	D	37	LYS
3	H	166	LEU
2	D	18	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	153	HIS
3	H	157	GLN
3	H	212	ASN
1	C	174	GLN
1	A	174	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PO4	C	301	-	4,4,4	0.95	0	6,6,6	0.51	0
4	PO4	A	301	-	4,4,4	0.98	0	6,6,6	0.47	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	231/247 (93%)	0.16	4 (1%) 69 65	33, 62, 104, 148	0
1	C	221/247 (89%)	0.53	17 (7%) 19 15	34, 73, 132, 189	0
2	B	89/99 (89%)	0.17	4 (4%) 38 33	30, 58, 105, 127	0
2	D	87/99 (87%)	0.16	2 (2%) 61 56	30, 57, 103, 119	0
3	E	132/145 (91%)	0.21	2 (1%) 72 68	36, 57, 110, 149	0
3	F	134/145 (92%)	0.14	3 (2%) 62 57	33, 56, 100, 136	0
3	G	133/145 (91%)	0.20	5 (3%) 44 39	32, 56, 113, 143	0
3	H	133/145 (91%)	0.36	10 (7%) 20 16	33, 59, 108, 148	0
All	All	1160/1272 (91%)	0.26	47 (4%) 41 36	30, 61, 110, 189	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	18	GLU	7.3
1	C	19	VAL	6.8
1	C	197	VAL	4.8
3	F	246	GLN	4.3
2	B	94	ALA	4.2

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
4	PO4	C	301	5/5	0.95	0.07	50,60,66,79	0
4	PO4	A	301	5/5	0.97	0.07	37,54,59,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.