WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

May 24, 2020 – 12:51 am BST

PDB ID	:	5JWR
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

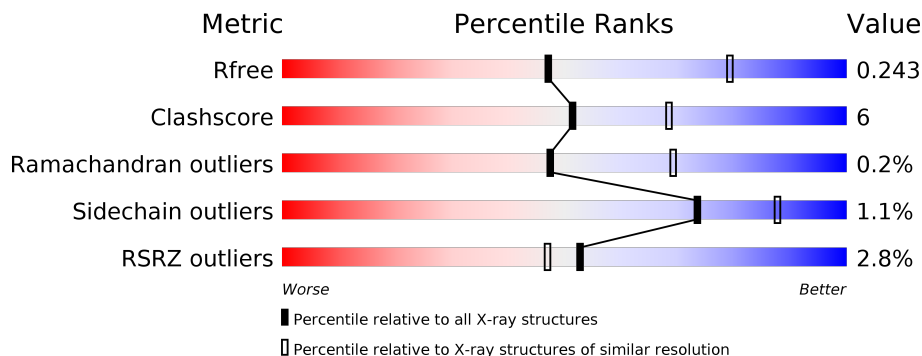|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 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	Percentile Ranks	Value
Rfree		0.243
Clashscore		6
Ramachandran outliers		0.2%
Sidechain outliers		1.1%
RSRZ outliers		2.8%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (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 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 <=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	% 83% 11% 6%
1	C	247	5% 71% 18% 11%
2	B	99	3% 77% 13% 10%
2	D	99	3% 67% 17% • 12%
3	E	145	3% 81% 10% 9%
3	F	145	2% 78% 14% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	145	77% 15% 8%
3	H	145	3% 80% 11% · 8%

2 Entry composition (i)

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

Continued on next page...

Continued from previous page...

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 691	C 449	N 121	O 121	0	0	0
2	D	87	Total 678	C 440	N 119	O 119	0	0	0

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 1113	C 713	N 195	O 202	S 3	0	0	0
3	F	134	Total 1129	C 723	N 197	O 206	S 3	0	0	0
3	G	133	Total 1120	C 718	N 196	O 203	S 3	0	0	0

Continued on next page...

Continued from previous page...

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

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 (three-letter code: PO4) (formula: O_4P).
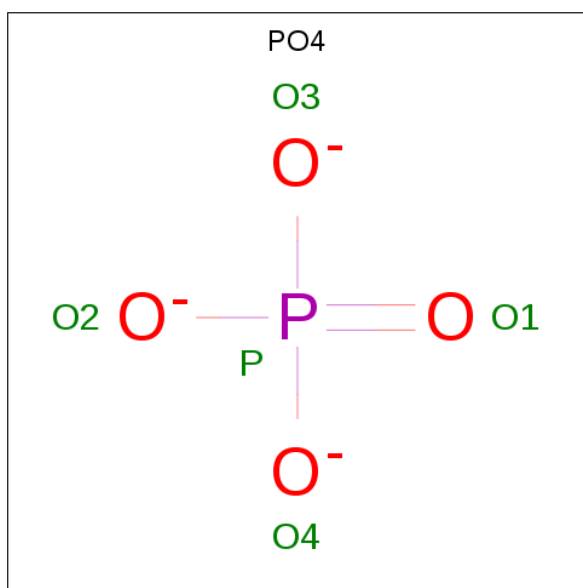
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total O P 5 4 1		0	0
4	C	1	Total O P 5 4 1		0	0

- Molecule 5 is water.

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

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: Circadian clock protein kinase KaiC
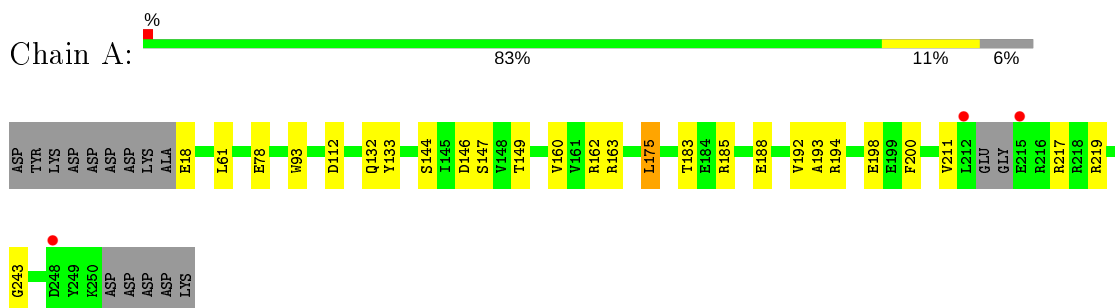
- Molecule 1: Circadian clock protein kinase KaiC
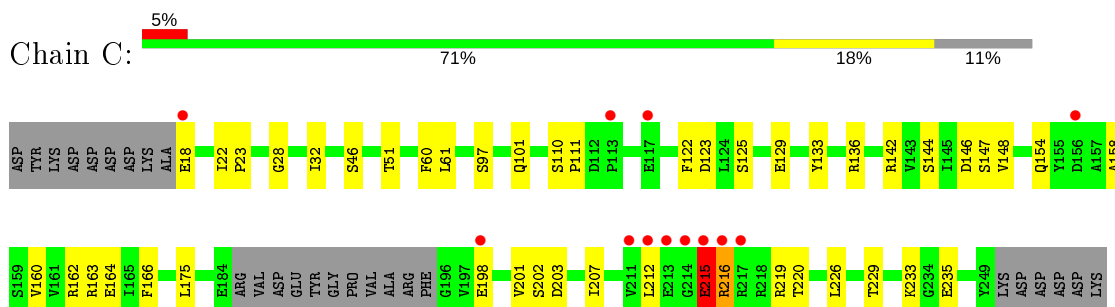
- Molecule 2: Circadian clock protein KaiB

- Molecule 2: Circadian clock protein KaiB

- Molecule 3: Circadian clock protein KaiA
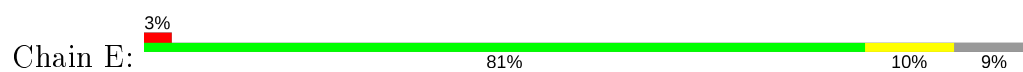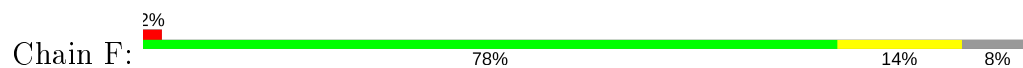
Chain E:

• Molecule 3: Circadian clock protein KaiA

Chain F:

• Molecule 3: Circadian clock protein KaiA

Chain G:

• Molecule 3: Circadian clock protein KaiA

Chain H:
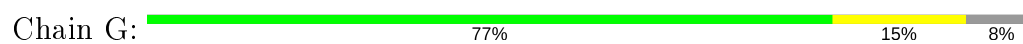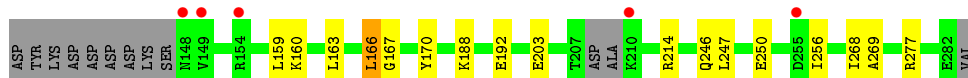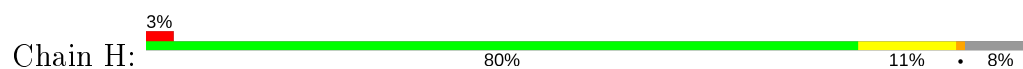
4   Data and refinement statistics (i)

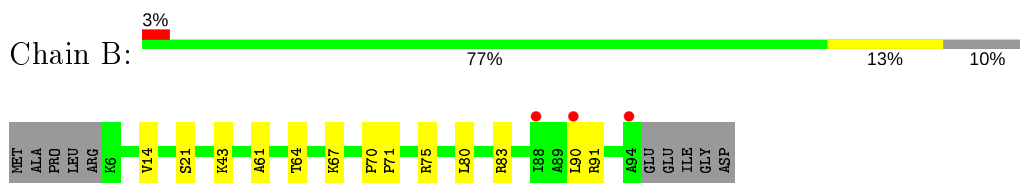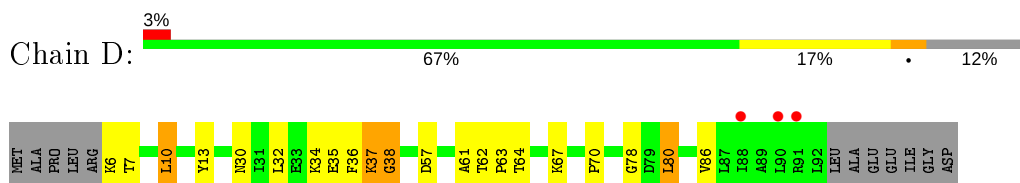| Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	74.59Å 79.11Å 80.84Å 107.27° 90.71° 111.20°	Depositor
Resolution (Å)	44.84 – 2.61 44.84 – 2.61	Depositor EDS
% Data completeness (in resolution range)	95.5 (44.84-2.61) 95.5 (44.84-2.61)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	5.12 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.185 , 0.242 0.192 , 0.243	Depositor DCC
R_{free} test set	2324 reflections (4.91%)	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)	0.33 , 59.9	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	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.*

---

[1] Intensities estimated from amplitudes.
[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.26	0/1858	0.46	0/2513
1	C	0.29	0/1765	0.51	1/2388 (0.0%)
2	B	0.24	0/699	0.47	0/948
2	D	0.24	0/686	0.55	2/930 (0.2%)
3	E	0.28	0/1133	0.55	0/1521
3	F	0.25	0/1149	0.50	0/1543
3	G	0.25	0/1140	0.46	0/1531
3	H	0.25	0/1140	0.50	0/1529
All	All	0.26	0/9570	0.50	3/12903 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	38	GLY	N-CA-C	-5.75	98.73	113.10
2	D	10	LEU	CA-CB-CG	5.24	127.35	115.30
1	C	212	LEU	CA-CB-CG	5.11	127.06	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1825	0	1823	21	0
1	C	1735	0	1735	30	0
2	B	691	0	771	7	0
2	D	678	0	755	12	0
3	E	1113	0	1132	9	0
3	F	1129	0	1147	13	0
3	G	1120	0	1141	13	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	107	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.

All (107) 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: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
3:G:194:ARG:NH1	3:G:238:GLU:OE1	2.23	0.71
3:E:163:LEU:HD22	3:E:273:GLU:HG2	1.73	0.68
2:D:6:LYS:N	2:D:7:THR:HA	2.08	0.68
3:G:149:VAL:HG23	3:G:150:ASP:H	1.62	0.64
1:A:160:VAL:HG23	1:A:163:ARG:HH21	1.62	0.64
1:A:193:ALA:N	1:A:198:GLU:OE1	2.30	0.63
3:F:210:LYS:O	3:F:214:ARG:NH1	2.32	0.63
3:E:236:HIS:O	3:E:240:MET:HG2	1.99	0.60
2:D:67:LYS:NZ	2:D:70:PRO:O	2.29	0.60
1:C:233:LYS:H	1:C:233:LYS:HD2	1.65	0.60
3:G:163:LEU:HD22	3:G:273:GLU:HG2	1.85	0.59
2:B:83:ARG:HH11	2:B:83:ARG:HG3	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:VAL:HG23	1:A:163:ARG:NH2	2.19	0.58
3:G:184:ALA:HA	3:G:187:ARG:HH21	1.68	0.57
2:D:37:LYS:HG3	2:D:38:GLY:N	2.19	0.57
1:A:183:THR:HG21	1:A:193:ALA:HB1	1.87	0.57
1:A:18:GLU:N	5:A:402:HOH:O	2.38	0.57
1:C:198:GLU:N	1:C:198:GLU:OE1	2.35	0.57
1:A:192:VAL:HB	1:A:198:GLU:HG2	1.86	0.56
3:H:246:GLN:NE2	3:H:250:GLU:OE2	2.33	0.56
3:F:191:ASP:OD1	3:F:194:ARG:NH1	2.39	0.56
3:H:188:LYS:NZ	3:H:192:GLU:OE2	2.39	0.55
2:D:61:ALA:O	2:D:64:THR:OG1	2.18	0.55
1:C:160:VAL:HG23	1:C:163:ARG:HH21	1.71	0.55
3:H:203:GLU:OE2	3:H:214:ARG:NH2	2.34	0.54
3:G:233:LEU:HD22	3:H:159:LEU:HD12	1.90	0.53
1:C:233:LYS:N	1:C:233:LYS:HD2	2.24	0.53
3:F:157:GLN:NE2	3:F:161:GLU:OE2	2.40	0.52
3:G:190:LEU:O	3:G:194:ARG:HG3	2.10	0.52
3:G:204:TYR:HA	3:G:211:VAL:HG11	1.92	0.51
1:A:112:ASP:OD2	2:B:75:ARG:NH2	2.43	0.51
3:H:188:LYS:O	3:H:192:GLU:HG3	2.11	0.51
1:C:51:THR:HA	1:C:219:ARG:HH12	1.77	0.50
1:A:188:GLU:HG3	1:A:211:VAL:HG12	1.93	0.49
1:A:93:TRP:HH2	1:A:243:GLY:HA2	1.77	0.49
3:E:245:LYS:O	3:E:248:LYS:HG2	2.13	0.49
1:C:46:SER:HB3	1:C:207:ILE:HD13	1.96	0.48
1:A:185:ARG:NH2	1:A:188:GLU:O	2.46	0.48
3:F:250:GLU:OE1	3:F:252:ARG:NH2	2.47	0.48
2:D:13:TYR:OH	2:D:57:ASP:OD2	2.23	0.47
3:H:247:LEU:HD11	3:H:256:ILE:HD11	1.95	0.47
1:A:132:GLN:HG3	1:A:175:LEU:HD21	1.95	0.47
1:C:215:GLU:HB2	1:C:216:ARG:HG3	1.95	0.47
3:G:228:SER:OG	3:G:231:GLN:HG3	2.14	0.47
2:B:67:LYS:HD2	2:B:70:PRO:HD2	1.97	0.47
3:F:190:LEU:O	3:F:194:ARG:HG3	2.15	0.47
1:C:146:ASP:HA	1:C:147:SER:HA	1.59	0.47
1:A:61:LEU:HD11	1:A:144:SER:HB2	1.97	0.47
1:C:28:GLY:O	1:C:32:ILE:HG12	2.15	0.46
1:C:133:TYR:OH	3:G:161:GLU:OE1	2.32	0.46
2:D:37:LYS:HG3	2:D:38:GLY:H	1.81	0.46
1:C:220:THR:HG21	1:C:235:GLU:OE1	2.16	0.45
1:C:111:PRO:HD3	1:C:154:GLN:HE22	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:160:LYS:O	3:H:163:LEU:HB2	2.16	0.45
1:A:149:THR:HG21	1:A:194:ARG:HB3	1.98	0.45
1:A:133:TYR:OH	3:E:161:GLU:OE2	2.35	0.45
3:F:188:LYS:O	3:F:192:GLU:HG3	2.16	0.45
1:C:125:SER:O	1:C:129:GLU:HG2	2.16	0.45
1:A:185:ARG:HD3	1:A:192:VAL:O	2.17	0.44
1:C:97:SER:O	1:C:101:GLN:HG3	2.17	0.44
2:D:34:LYS:HE3	2:D:35:GLU:HG3	1.99	0.44
1:C:162:ARG:HG2	1:C:166:PHE:CE1	2.52	0.44
2:D:63:PRO:HG2	2:D:78:GLY:O	2.17	0.44
3:G:245:LYS:O	3:G:248:LYS:HG2	2.17	0.44
1:A:146:ASP:HA	1:A:147:SER:HA	1.63	0.44
1:C:158:ALA:O	1:C:162:ARG:HB2	2.18	0.44
3:G:156:SER:O	3:G:160:LYS:HG3	2.16	0.44
3:F:243:PHE:O	3:F:247:LEU:HD13	2.17	0.44
1:A:78:GLU:OE1	1:A:78:GLU:HA	2.17	0.44
1:C:110:SER:HB2	1:C:111:PRO:HD2	1.99	0.43
2:B:61:ALA:O	2:B:64:THR:OG1	2.28	0.43
2:D:80:LEU:HG	2:D:86:VAL:HG21	2.00	0.43
1:A:18:GLU:OE2	1:C:136:ARG:NH1	2.52	0.42
1:A:217:ARG:HD2	1:A:219:ARG:NE	2.34	0.42
1:C:123:ASP:OD1	2:D:62:THR:OG1	2.35	0.42
2:D:30:ASN:O	2:D:34:LYS:HE2	2.19	0.42
2:B:14:VAL:HB	2:B:21:SER:HB3	2.02	0.42
2:B:43:LYS:HE3	2:B:43:LYS:HB2	1.67	0.42
1:C:162:ARG:HG2	1:C:166:PHE:CZ	2.54	0.42
1:C:60:PHE:CZ	1:C:142:ARG:HD3	2.55	0.42
3:E:159:LEU:O	3:E:163:LEU:HB2	2.19	0.42
3:F:245:LYS:HE3	3:F:245:LYS:HB2	1.79	0.42
3:G:210:LYS:HE2	3:G:210:LYS:HB2	1.82	0.42
3:E:226:ASP:OD2	3:F:281:ARG:NH1	2.53	0.42
1:A:162:ARG:HG2	1:A:200:PHE:CD2	2.55	0.41
1:C:18:GLU:O	1:C:229:THR:HB	2.21	0.41
2:D:32:LEU:HA	2:D:36:PHE:HB3	2.02	0.41
1:A:149:THR:HG23	1:A:183:THR:HG23	2.02	0.41
1:C:148:VAL:HG13	1:C:198:GLU:OE2	2.21	0.41
1:C:61:LEU:HD11	1:C:144:SER:HB2	2.02	0.41
1:C:215:GLU:HB2	1:C:216:ARG:CG	2.49	0.41
3:E:150:ASP:N	5:E:304:HOH:O	2.53	0.41
3:F:268:ILE:HG13	3:F:269:ALA:N	2.35	0.41
3:H:166:LEU:O	3:H:170:TYR:OH	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:268:ILE:HG13	3:H:269:ALA:N	2.36	0.41
1:C:122:PHE:O	1:C:160:VAL:HG21	2.21	0.41
1:C:160:VAL:O	1:C:164:GLU:HG2	2.21	0.41
3:E:178:PHE:HD1	3:E:189:LEU:HD23	1.86	0.41
1:C:22:ILE:HD12	1:C:23:PRO:HD2	2.02	0.41
1:C:226:LEU:HD12	1:C:226:LEU:HA	1.96	0.40
3:G:167:GLY:HA3	3:G:279:ILE:HD11	2.02	0.40
3:F:203:GLU:OE2	3:F:214:ARG:NH1	2.54	0.40
3:F:228:SER:OG	3:F:231:GLN:HG3	2.21	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	227/247 (92%)	218 (96%)	9 (4%)	0	100	100
1	C	217/247 (88%)	207 (95%)	8 (4%)	2 (1%)	17	33
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%)	47	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	202	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	215	GLU

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	197/212 (93%)	196 (100%)	1 (0%)	88	95
1	C	188/212 (89%)	185 (98%)	3 (2%)	62	81
2	B	77/85 (91%)	75 (97%)	2 (3%)	46	70
2	D	76/85 (89%)	73 (96%)	3 (4%)	32	56
3	E	123/136 (90%)	122 (99%)	1 (1%)	81	92
3	F	125/136 (92%)	125 (100%)	0	100	100
3	G	124/136 (91%)	124 (100%)	0	100	100
3	H	124/136 (91%)	123 (99%)	1 (1%)	81	92
All	All	1034/1138 (91%)	1023 (99%)	11 (1%)	73	88

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	LEU
2	B	80	LEU
2	B	90	LEU
1	C	175	LEU
1	C	215	GLU
1	C	216	ARG
2	D	10	LEU
2	D	37	LYS
2	D	80	LEU
3	E	190	LEU
3	H	166	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	154	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)

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	A	301	-	4,4,4	0.94	0	6,6,6	0.44	0
4	PO4	C	301	-	4,4,4	0.91	0	6,6,6	0.48	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%)	-0.44	3 (1%)	77	73	33, 62, 104, 148	0
1	C	221/247 (89%)	-0.11	12 (5%)	25	20	34, 73, 132, 189	0
2	B	89/99 (89%)	-0.10	3 (3%)	45	38	30, 58, 105, 127	0
2	D	87/99 (87%)	-0.20	3 (3%)	45	38	30, 57, 103, 119	0
3	E	132/145 (91%)	-0.18	4 (3%)	50	44	36, 57, 110, 149	0
3	F	134/145 (92%)	-0.30	3 (2%)	62	57	33, 56, 100, 136	0
3	G	133/145 (91%)	-0.25	0	100	100	32, 56, 113, 143	0
3	H	133/145 (91%)	-0.20	5 (3%)	40	34	33, 59, 108, 148	0
All	All	1160/1272 (91%)	-0.24	33 (2%)	53	47	30, 61, 110, 189	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	148	ASN	7.3
1	C	212	LEU	6.2
1	C	216	ARG	5.1
1	C	215	GLU	4.8
1	C	18	GLU	4.7
1	C	214	GLY	4.2
2	B	94	ALA	4.2
1	C	213	GLU	4.0
3	H	149	VAL	3.8
2	D	88	ILE	3.3
3	E	281	ARG	3.2
3	H	154	ARG	3.1
1	C	156	ASP	2.9
3	H	255	ASP	2.8
1	C	117	GLU	2.8
2	D	90	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	91	ARG	2.6
1	C	211	VAL	2.6
3	F	246	GLN	2.6
2	B	90	LEU	2.5
3	H	210	LYS	2.3
1	A	215	GLU	2.3
1	A	248	ASP	2.3
3	F	249	LEU	2.2
3	F	154	ARG	2.2
3	E	255	ASP	2.2
2	B	88	ILE	2.1
3	E	165	TYR	2.1
1	C	217	ARG	2.1
1	C	198	GLU	2.1
1	A	212	LEU	2.0
3	E	252	ARG	2.0
1	C	113	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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(Å²)	Q<0.9
4	PO4	A	301	5/5	0.98	0.15	37,54,59,61	0
4	PO4	C	301	5/5	0.98	0.13	50,60,66,79	0

6.5 Other polymers ⓘ

There are no such residues in this entry.