



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:33 PM GMT

PDB ID : 4TLB  
Title : Crystal structure of N-terminal C1 domain of KaiC  
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Deposited on : 2014-05-29  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

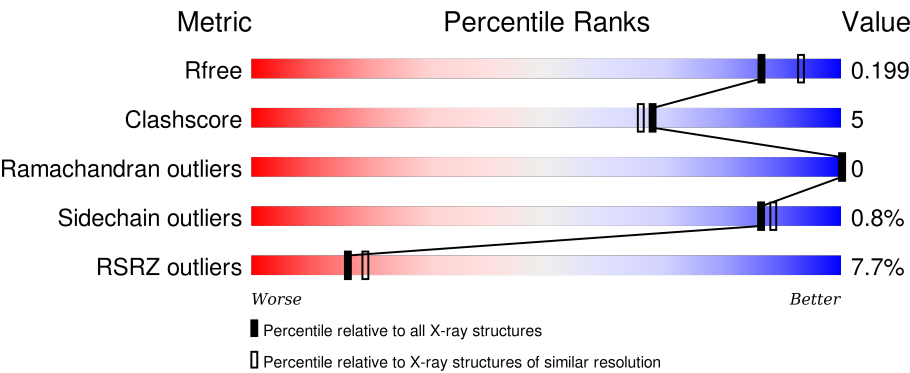
# 1 Overall quality at a glance i

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 <sub>free</sub>	91344	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	253	<div><div>9%</div><div><div></div><div>76%</div><div>13%</div><div>11%</div></div></div>
1	B	253	<div><div>4%</div><div><div></div><div>76%</div><div>11%</div><div>12%</div></div></div>
1	C	253	<div><div>7%</div><div><div></div><div>82%</div><div>7%</div><div>11%</div></div></div>
1	D	253	<div><div>6%</div><div><div></div><div>81%</div><div>9%</div><div>10%</div></div></div>
1	E	253	<div><div>9%</div><div><div></div><div>77%</div><div>11%</div><div>10%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	253	<div> <div>5%</div> <div>81%</div> <div>6%</div> <div>13%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12055 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	224	Total	C	N	O	S	0	5	0
			1803	1153	311	335	4			
1	B	222	Total	C	N	O	S	0	7	0
			1799	1155	309	329	6			
1	C	225	Total	C	N	O	S	0	6	0
			1828	1168	318	338	4			
1	D	228	Total	C	N	O	S	0	9	0
			1847	1181	317	345	4			
1	E	227	Total	C	N	O	S	0	10	0
			1855	1190	318	343	4			
1	F	220	Total	C	N	O	S	0	3	0
			1760	1127	303	326	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	146	PRO	SER	engineered mutation	UNP Q79PF4
B	146	PRO	SER	engineered mutation	UNP Q79PF4
C	146	PRO	SER	engineered mutation	UNP Q79PF4
D	146	PRO	SER	engineered mutation	UNP Q79PF4
E	146	PRO	SER	engineered mutation	UNP Q79PF4
F	146	PRO	SER	engineered mutation	UNP Q79PF4

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

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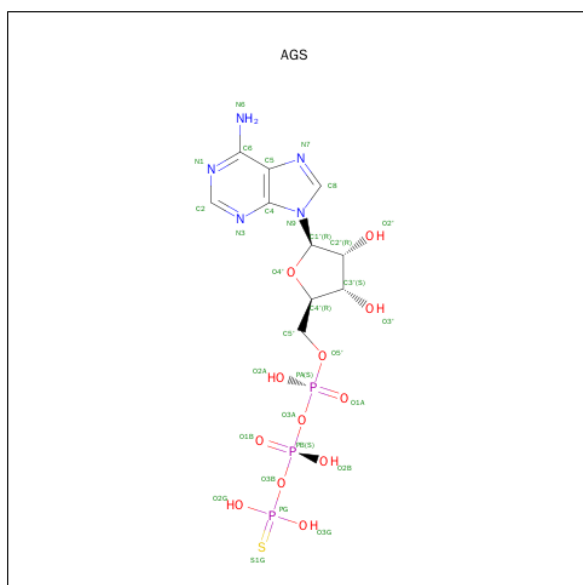
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
4	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
4	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
4	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
4	E	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
4	F	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0

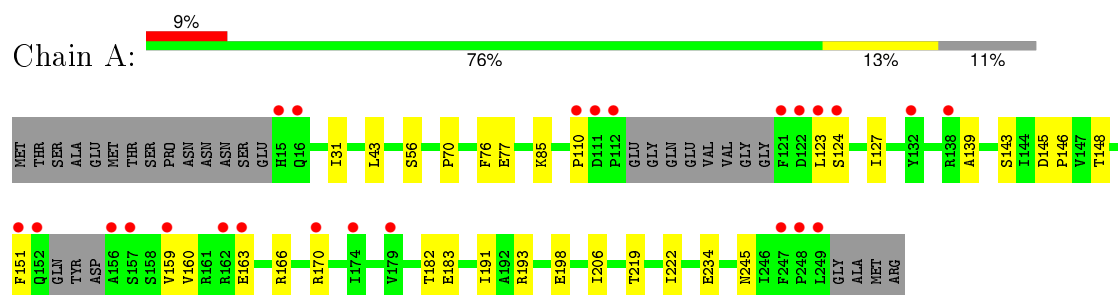
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	126	Total 126	O 126	0	0
5	B	183	Total 183	O 183	0	0
5	C	160	Total 160	O 160	0	0
5	D	171	Total 171	O 171	0	0
5	E	163	Total 163	O 163	0	0
5	F	162	Total 162	O 162	0	0

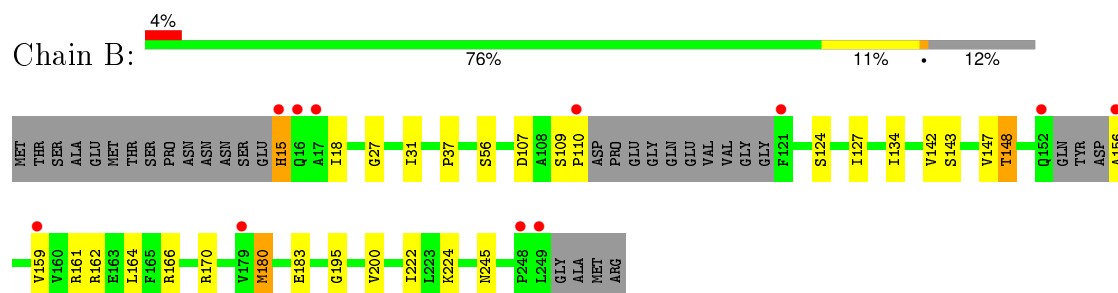
### 3 Residue-property plots [i](#)

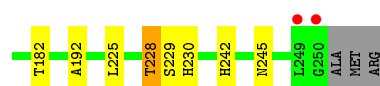
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

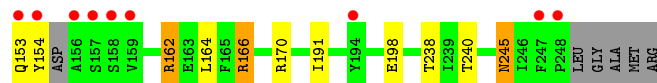
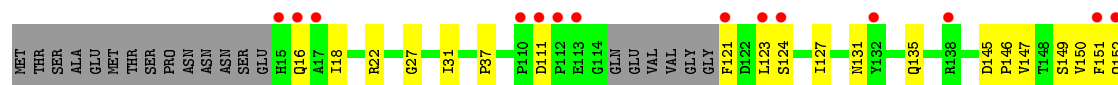
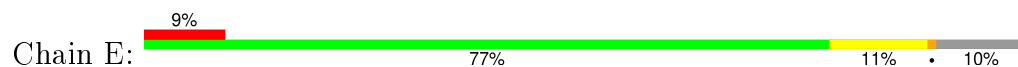


- Molecule 1: Circadian clock protein kinase KaiC

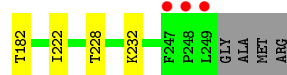
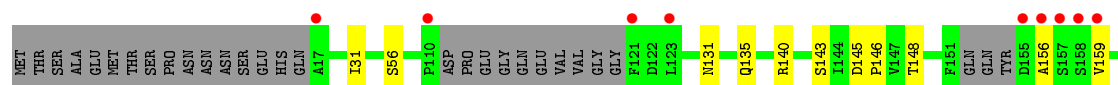
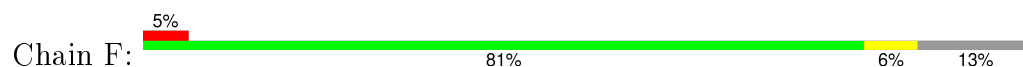




- Molecule 1: Circadian clock protein kinase KaiC



- Molecule 1: Circadian clock protein kinase KaiC





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.06Å 133.56Å 150.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.43 – 1.98 29.43 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.43-1.98) 99.6 (29.43-1.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	13.76 (at 1.98Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.163 , 0.199 0.163 , 0.199	Depositor DCC
$R_{free}$ test set	5614 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.8	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 112078 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12055	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, AGS, CL

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	0.37	0/1850	0.53	0/2496
1	B	0.42	0/1851	0.56	0/2495
1	C	0.42	0/1872	0.57	0/2524
1	D	0.41	0/1907	0.56	0/2574
1	E	0.44	0/1919	0.57	1/2590 (0.0%)
1	F	0.45	0/1799	0.58	0/2427
All	All	0.42	0/11198	0.56	1/15106 (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	E	166	ARG	NE-CZ-NH1	-5.89	117.35	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	15	HIS	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1803	0	1832	20	0
1	B	1799	0	1848	22	0
1	C	1828	0	1854	11	0
1	D	1847	0	1881	20	0
1	E	1855	0	1891	28	0
1	F	1760	0	1793	10	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	31	0	12	1	0
4	B	31	0	12	0	0
4	C	31	0	12	0	0
4	D	31	0	12	0	0
4	E	31	0	12	0	0
4	F	31	0	12	0	0
5	A	126	0	0	2	0
5	B	183	0	0	1	0
5	C	160	0	0	1	0
5	D	171	0	0	2	0
5	E	163	0	0	1	0
5	F	162	0	0	3	0
All	All	12055	0	11171	105	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 5.

All (105) 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:E:162:ARG:HH12	1:E:166:ARG:HH12	1.33	0.76
1:E:123:LEU:HD23	1:E:166:ARG:HE	1.49	0.76
1:C:128:GLU:OE2	1:C:170:ARG:NH2	2.19	0.75
1:A:127:ILE:HG21	1:A:170:ARG:HD3	1.67	0.75
1:B:124:SER:HB3	1:B:166:ARG:HH22	1.52	0.74
1:E:162:ARG:HH12	1:E:166:ARG:NH1	1.87	0.72
1:E:162:ARG:HG2	1:E:162:ARG:HH11	1.54	0.72
1:E:238:THR:OG1	1:E:245[B]:ASN:OD1	2.08	0.71
1:A:193:ARG:NH1	1:B:195:GLY:O	2.28	0.66
1:B:164:LEU:HD11	1:B:180[B]:MET:HE1	1.77	0.66
1:B:110:PRO:HG2	1:C:165:PHE:CE2	2.30	0.66
1:E:22:ARG:NH2	5:E:543:HOH:O	2.28	0.66
1:C:163:GLU:OE2	1:C:166:ARG:NH2	2.30	0.65
1:E:127:ILE:HD13	1:E:170:ARG:HD3	1.79	0.63
1:E:162:ARG:NH1	1:E:166:ARG:HH12	1.96	0.62
1:A:77:GLU:OE2	1:B:161:ARG:NH2	2.31	0.62
1:D:151:PHE:HZ	1:D:164[B]:LEU:HG	1.63	0.62
1:E:162:ARG:HH12	1:E:166:ARG:NH2	1.98	0.61
1:E:162:ARG:NH1	1:E:166:ARG:HH22	1.98	0.61
1:D:16:GLN:HB2	1:D:228[B]:THR:HG23	1.83	0.61
1:E:162:ARG:HG2	1:E:162:ARG:NH1	2.15	0.61
1:A:76:PHE:O	1:A:110:PRO:HD3	2.01	0.60
1:E:162:ARG:HH12	1:E:166:ARG:HH22	1.49	0.60
1:E:162:ARG:HH12	1:E:166:ARG:CZ	2.16	0.57
4:A:303:AGS:O3G	1:B:224:LYS:NZ	2.36	0.56
1:C:152:GLN:HA	1:C:194:TYR:OH	2.05	0.56
1:D:182[B]:THR:HG21	1:D:192:ALA:HB1	1.87	0.56
1:B:18:ILE:HD12	1:B:37:PRO:HB3	1.88	0.56
1:E:123:LEU:HD23	1:E:166:ARG:NE	2.21	0.55
1:E:240:THR:HG23	1:E:245[B]:ASN:HD21	1.70	0.55
1:D:12:ASN:ND2	5:D:401:HOH:O	2.38	0.55
1:B:148:THR:HG21	1:B:183:GLU:H	1.72	0.54
1:E:153:GLN:HG3	1:E:154:TYR:CD2	2.42	0.54
1:E:121:PHE:CE2	1:E:150:VAL:HG13	2.43	0.54
1:D:25:ILE:O	5:D:560:HOH:O	2.18	0.54
1:D:16:GLN:OE1	1:D:228[B]:THR:HG21	2.09	0.53
1:A:85:LYS:HE3	1:B:18:ILE:HG22	1.90	0.52
1:F:56[A]:SER:HB2	1:F:143:SER:HB3	1.92	0.52
1:E:16:GLN:HA	1:E:16:GLN:NE2	2.25	0.52
1:B:127:ILE:CG2	1:B:170:ARG:HG2	2.39	0.52
1:A:148:THR:HG21	1:A:183:GLU:H	1.75	0.52
1:F:228[B]:THR:HG23	5:F:544:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191[B]:ILE:HG21	1:E:198:GLU:HB3	1.91	0.51
1:A:124:SER:OG	1:A:166:ARG:NH2	2.44	0.51
1:A:245:ASN:HB2	5:A:474:HOH:O	2.10	0.50
1:D:151:PHE:CZ	1:D:164[B]:LEU:HG	2.45	0.50
1:F:232:LYS:NZ	5:F:533:HOH:O	2.40	0.49
1:B:107:ASP:OD1	1:B:109:SER:HB2	2.12	0.49
1:F:140:ARG:NH1	5:F:549:HOH:O	2.45	0.49
1:B:156:ALA:O	1:B:159:VAL:HG12	2.13	0.49
1:D:76:PHE:O	1:D:110:PRO:HD3	2.13	0.48
1:E:131:ASN:O	1:E:135:GLN:HG2	2.14	0.48
1:D:56[A]:SER:HB2	1:D:143:SER:HB3	1.96	0.47
1:E:27:GLY:O	1:E:31[B]:ILE:HG12	2.14	0.47
1:B:56[A]:SER:HB2	1:B:143:SER:HB3	1.97	0.47
1:D:225[B]:LEU:HD23	1:D:230:HIS:HB3	1.97	0.47
1:D:225[B]:LEU:HD11	1:D:228[B]:THR:HB	1.97	0.47
1:D:12:ASN:OD1	1:D:16:GLN:NE2	2.48	0.47
1:F:31:ILE:HG22	1:F:222:ILE:HD12	1.96	0.47
1:B:27:GLY:O	1:B:31[B]:ILE:HG12	2.15	0.47
1:B:159:VAL:HG23	1:B:162:ARG:NH2	2.30	0.47
1:F:148:THR:HG23	1:F:182:THR:HG22	1.96	0.47
1:B:127:ILE:HG23	1:B:170:ARG:HG2	1.96	0.46
1:C:127:ILE:CG2	1:C:170:ARG:HG2	2.45	0.46
1:C:128:GLU:CD	1:C:170:ARG:HH22	2.18	0.46
1:D:228[B]:THR:HG22	1:D:229:SER:N	2.30	0.46
1:A:70:PRO:HB2	1:A:139:ALA:HA	1.99	0.45
1:A:123:LEU:O	1:A:127:ILE:HG13	2.17	0.45
1:A:77:GLU:OE1	1:B:200:VAL:HG12	2.16	0.44
1:F:156:ALA:HB3	1:F:159:VAL:HG12	1.99	0.44
1:D:121:PHE:HE2	1:D:126:LEU:HD22	1.83	0.44
1:A:31:ILE:HG22	1:A:222:ILE:HD12	2.00	0.43
1:E:124:SER:HA	1:E:127:ILE:HD12	2.00	0.43
1:E:149:SER:HA	1:E:152:GLN:HB2	2.00	0.43
1:C:161:ARG:HG3	1:C:200:VAL:HG11	2.00	0.43
1:A:191:ILE:HG23	1:A:206[B]:ILE:HD11	2.00	0.43
1:E:121:PHE:N	1:E:153:GLN:HE22	2.17	0.43
1:C:110:PRO:HG2	1:D:165:PHE:CE2	2.53	0.43
1:E:151:PHE:CZ	1:E:164:LEU:HD13	2.54	0.43
1:F:145:ASP:HA	1:F:146:PRO:HA	1.82	0.43
1:A:198:GLU:OE2	5:A:522:HOH:O	2.21	0.43
1:D:76:PHE:O	1:D:109:SER:HA	2.19	0.42
1:D:148:THR:OG1	1:D:182[B]:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56[B]:SER:HB3	1:F:143:SER:HB3	2.01	0.42
1:C:145:ASP:HA	1:C:146:PRO:HA	1.84	0.42
1:A:56[A]:SER:HB2	1:A:143:SER:HB3	2.02	0.42
1:A:151:PHE:HB3	1:A:160:VAL:HG22	2.02	0.42
1:B:245:ASN:HB2	5:B:406:HOH:O	2.19	0.41
1:D:123:LEU:HD23	1:D:127:ILE:HG13	2.02	0.41
1:B:134:ILE:HD11	1:B:142:VAL:HG21	2.02	0.41
1:E:18:ILE:HG12	1:E:37:PRO:HB3	2.02	0.41
1:A:145:ASP:HA	1:A:146:PRO:HA	1.84	0.41
1:A:159:VAL:O	1:A:163:GLU:HG2	2.20	0.41
1:F:131:ASN:O	1:F:135:GLN:HG2	2.19	0.41
1:C:76:PHE:HE2	1:C:144:ILE:HG23	1.86	0.41
1:E:166:ARG:HB2	1:E:166:ARG:NH1	2.36	0.41
1:E:145:ASP:HA	1:E:146:PRO:HA	1.85	0.41
1:B:56[B]:SER:HB3	1:B:143:SER:HB3	2.01	0.41
1:B:31[A]:ILE:HG22	1:B:222:ILE:HD12	2.03	0.41
1:D:242[B]:HIS:ND1	1:D:245:ASN:OD1	2.53	0.41
1:A:219:THR:HB	1:A:234:GLU:HB3	2.02	0.41
1:A:43:LEU:HD11	1:A:182:THR:CG2	2.51	0.41
1:B:147:VAL:HG11	1:B:180[B]:MET:HE3	2.03	0.40
1:D:164[B]:LEU:HA	1:D:164[B]:LEU:HD23	1.95	0.40
1:C:102:LYS:HE2	5:C:501:HOH:O	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	223/253 (88%)	218 (98%)	5 (2%)	0	100	100
1	B	223/253 (88%)	215 (96%)	8 (4%)	0	100	100
1	C	225/253 (89%)	219 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	231/253 (91%)	224 (97%)	7 (3%)	0	100	100
1	E	231/253 (91%)	226 (98%)	5 (2%)	0	100	100
1	F	217/253 (86%)	212 (98%)	5 (2%)	0	100	100
All	All	1350/1518 (89%)	1314 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	199/217 (92%)	199 (100%)	0	100	100
1	B	199/217 (92%)	195 (98%)	4 (2%)	63	63
1	C	200/217 (92%)	199 (100%)	1 (0%)	92	93
1	D	206/217 (95%)	204 (99%)	2 (1%)	82	84
1	E	206/217 (95%)	201 (98%)	5 (2%)	57	55
1	F	193/217 (89%)	193 (100%)	0	100	100
All	All	1203/1302 (92%)	1191 (99%)	12 (1%)	86	84

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	15	HIS
1	B	148	THR
1	B	180[A]	MET
1	B	180[B]	MET
1	C	153	GLN
1	D	228[A]	THR
1	D	228[B]	THR
1	E	111	ASP
1	E	147	VAL
1	E	162	ARG

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Mol	Chain	Res	Type
1	E	245[A]	ASN
1	E	245[B]	ASN

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

Mol	Chain	Res	Type
1	E	16	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 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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	$\# Z  > 2$
4	AGS	A	303	2	26,33,33	0.76	1 (3%)	24,52,52	0.71	0
4	AGS	B	303	2	26,33,33	0.79	0	24,52,52	0.73	0
4	AGS	C	303	2	26,33,33	0.77	1 (3%)	24,52,52	0.75	0
4	AGS	D	303	2	26,33,33	0.80	1 (3%)	24,52,52	0.82	1 (4%)
4	AGS	E	303	2	26,33,33	0.59	0	24,52,52	0.75	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	AGS	F	301	2	26,33,33	0.74	0	24,52,52	0.52	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AGS	A	303	2	-	0/17/38/38	0/3/3/3
4	AGS	B	303	2	-	0/17/38/38	0/3/3/3
4	AGS	C	303	2	-	0/17/38/38	0/3/3/3
4	AGS	D	303	2	-	0/17/38/38	0/3/3/3
4	AGS	E	303	2	-	0/17/38/38	0/3/3/3
4	AGS	F	301	2	-	0/17/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	303	AGS	PG-S1G	2.16	1.94	1.90
4	A	303	AGS	PG-S1G	2.19	1.94	1.90
4	D	303	AGS	PG-S1G	2.53	1.95	1.90

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	303	AGS	O2B-PB-O3B	2.42	115.62	105.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	303	AGS	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	224/253 (88%)	0.51	24 (10%) 8 10	13, 31, 65, 99	0
1	B	222/253 (87%)	0.16	11 (4%) 32 36	12, 22, 51, 99	0
1	C	225/253 (88%)	0.15	17 (7%) 17 20	11, 22, 55, 99	0
1	D	228/253 (90%)	0.25	16 (7%) 19 23	10, 21, 54, 109	0
1	E	227/253 (89%)	0.27	23 (10%) 9 11	9, 22, 63, 118	0
1	F	220/253 (86%)	0.17	12 (5%) 29 33	9, 22, 54, 94	0
All	All	1346/1518 (88%)	0.25	103 (7%) 16 19	9, 23, 60, 118	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	250	GLY	16.3
1	E	15	HIS	9.4
1	E	154	TYR	8.6
1	F	110	PRO	8.0
1	E	151	PHE	7.8
1	A	249	LEU	7.6
1	D	12	ASN	6.4
1	D	249	LEU	6.1
1	B	121	PHE	5.7
1	F	121	PHE	5.7
1	A	132	TYR	5.5
1	C	247	PHE	5.4
1	D	121	PHE	5.4
1	B	15	HIS	5.3
1	A	121	PHE	5.3
1	A	15	HIS	5.0
1	A	111	ASP	5.0
1	C	249	LEU	5.0
1	A	112	PRO	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	152	GLN	4.8
1	E	121	PHE	4.7
1	B	16	GLN	4.7
1	C	156	ALA	4.6
1	B	152	GLN	4.5
1	B	248	PRO	4.4
1	E	16	GLN	4.3
1	C	250	GLY	4.2
1	D	110	PRO	4.2
1	E	153	GLN	4.1
1	C	151	PHE	4.1
1	E	156	ALA	4.0
1	A	123	LEU	4.0
1	F	156	ALA	3.9
1	E	247	PHE	3.9
1	C	153	GLN	3.9
1	F	249	LEU	3.8
1	F	158	SER	3.7
1	E	112	PRO	3.7
1	C	121	PHE	3.7
1	A	159	VAL	3.7
1	E	152	GLN	3.6
1	D	112	PRO	3.6
1	B	159	VAL	3.6
1	A	248	PRO	3.5
1	D	123	LEU	3.4
1	D	122	ASP	3.3
1	F	155	ASP	3.3
1	D	156	ALA	3.3
1	B	110	PRO	3.2
1	D	155	ASP	3.1
1	E	111	ASP	3.1
1	E	132	TYR	3.1
1	F	248	PRO	3.1
1	B	249	LEU	3.1
1	F	159	VAL	3.0
1	A	110	PRO	3.0
1	A	162	ARG	2.9
1	D	56[A]	SER	2.9
1	E	124	SER	2.9
1	E	159	VAL	2.9
1	E	110	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	152	GLN	2.8
1	B	17	ALA	2.8
1	A	156	ALA	2.8
1	F	247	PHE	2.7
1	E	17	ALA	2.7
1	A	174	ILE	2.7
1	A	138	ARG	2.7
1	E	123	LEU	2.7
1	C	122	ASP	2.6
1	D	111	ASP	2.6
1	A	157	SER	2.6
1	F	157	SER	2.6
1	E	248	PRO	2.6
1	C	173	GLN	2.5
1	B	156	ALA	2.5
1	A	16	GLN	2.5
1	E	158	SER	2.5
1	A	151	PHE	2.5
1	D	55	PHE	2.4
1	A	122	ASP	2.4
1	C	162	ARG	2.4
1	E	113	GLU	2.4
1	C	16	GLN	2.3
1	A	179	VAL	2.3
1	A	163	GLU	2.3
1	C	132[A]	TYR	2.3
1	E	157	SER	2.3
1	A	170	ARG	2.3
1	A	124	SER	2.3
1	E	194	TYR	2.2
1	D	162	ARG	2.2
1	E	138	ARG	2.2
1	C	99	ASP	2.1
1	A	247	PHE	2.1
1	D	132	TYR	2.1
1	B	179	VAL	2.1
1	C	150	VAL	2.1
1	C	179	VAL	2.1
1	C	15	HIS	2.0
1	D	158	SER	2.0
1	F	17	ALA	2.0
1	F	123	LEU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	AGS	B	303	31/31	0.98	0.10	-0.42	12,15,22,23	0
4	AGS	F	301	31/31	0.98	0.09	-0.43	12,15,24,31	0
4	AGS	E	303	31/31	0.97	0.10	-0.54	9,14,20,24	0
4	AGS	D	303	31/31	0.98	0.09	-0.82	10,15,23,24	0
4	AGS	A	303	31/31	0.98	0.09	-0.82	15,20,28,28	0
4	AGS	C	303	31/31	0.99	0.07	-1.19	11,14,18,20	0
3	CL	A	302	1/1	1.00	0.03	-	20,20,20,20	0
3	CL	F	303	1/1	0.99	0.03	-	17,17,17,17	0
2	MG	F	302	1/1	0.99	0.11	-	16,16,16,16	0
2	MG	B	301	1/1	0.99	0.12	-	14,14,14,14	0
2	MG	D	301	1/1	0.98	0.11	-	19,19,19,19	0
3	CL	E	302	1/1	0.99	0.06	-	16,16,16,16	0
3	CL	C	302	1/1	1.00	0.03	-	16,16,16,16	0
2	MG	A	301	1/1	0.98	0.09	-	20,20,20,20	0
3	CL	D	302	1/1	0.99	0.03	-	14,14,14,14	0
2	MG	C	301	1/1	0.99	0.04	-	16,16,16,16	0
3	CL	B	302	1/1	1.00	0.06	-	20,20,20,20	0
2	MG	E	301	1/1	0.98	0.04	-	16,16,16,16	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.