Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 07:44 PM GMT

PDB ID	:	4TLC
Title	:	Crystal structure of N-terminal C1 domain of KaiC
Authors	:	Abe, J.; Hiyama, T.B.; Mukaiyama, A.; Son, S.; Akiyama, S.
Deposited on	:	2014-05-29
Resolution	:	2.09 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

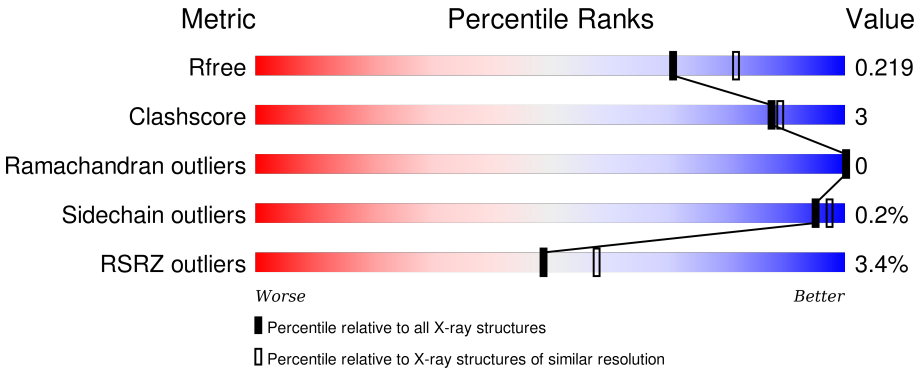
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.09 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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. 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	253	5% 83% 7% 10%
1	B	253	3% 86% 11%
1	C	253	2% 81% 8% 11%
1	D	253	2% 84% 12%
1	E	253	4% 83% 7% 10%

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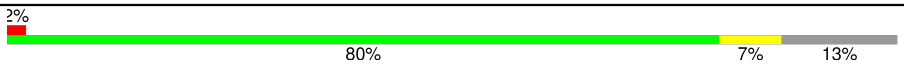
Mol	Chain	Length	Quality of chain
1	F	253	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11822 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	227	Total	C	N	O	S	0	0	0
			1806	1150	315	337	4			
1	B	226	Total	C	N	O	S	0	1	0
			1800	1146	315	335	4			
1	C	225	Total	C	N	O	S	0	1	0
			1797	1144	314	335	4			
1	D	223	Total	C	N	O	S	0	4	0
			1799	1143	315	337	4			
1	E	228	Total	C	N	O	S	0	3	0
			1836	1169	319	344	4			
1	F	219	Total	C	N	O	S	0	1	0
			1742	1110	304	324	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	146	GLY	SER	engineered mutation	UNP Q79PF4
B	146	GLY	SER	engineered mutation	UNP Q79PF4
C	146	GLY	SER	engineered mutation	UNP Q79PF4
D	146	GLY	SER	engineered mutation	UNP Q79PF4
E	146	GLY	SER	engineered mutation	UNP Q79PF4
F	146	GLY	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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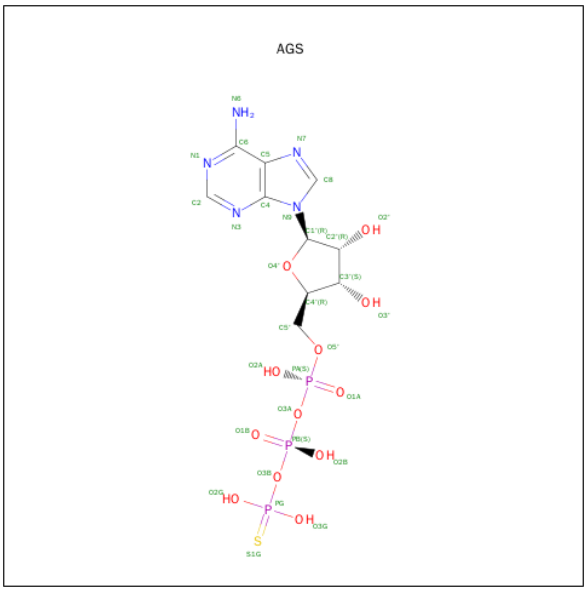
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

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

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

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



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

- Molecule 5 is water.

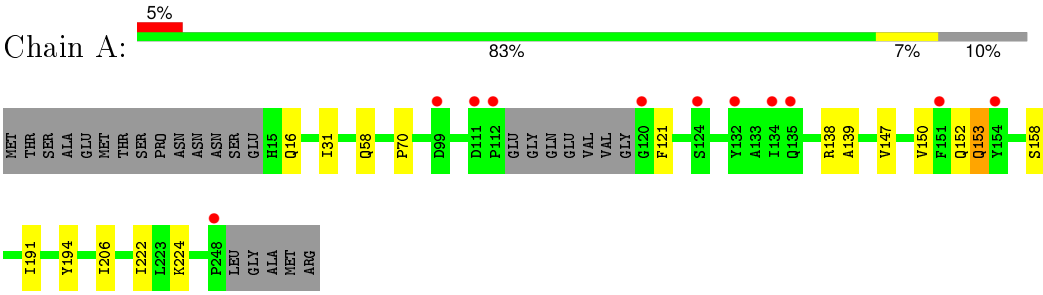
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	112	Total	O	0	0
			112	112		
5	B	161	Total	O	0	0
			161	161		
5	C	156	Total	O	0	0
			156	156		
5	D	154	Total	O	0	0
			154	154		
5	E	138	Total	O	0	0
			138	138		
5	F	123	Total	O	0	0
			123	123		

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.

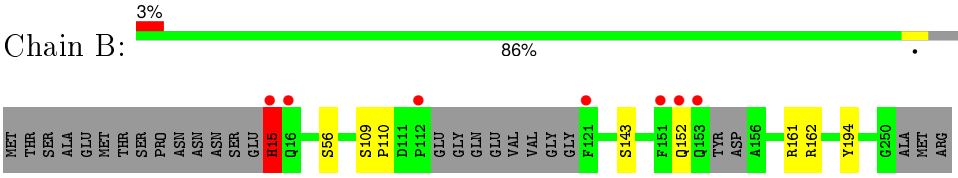
- Molecule 1: Circadian clock protein kinase KaiC

Chain A:



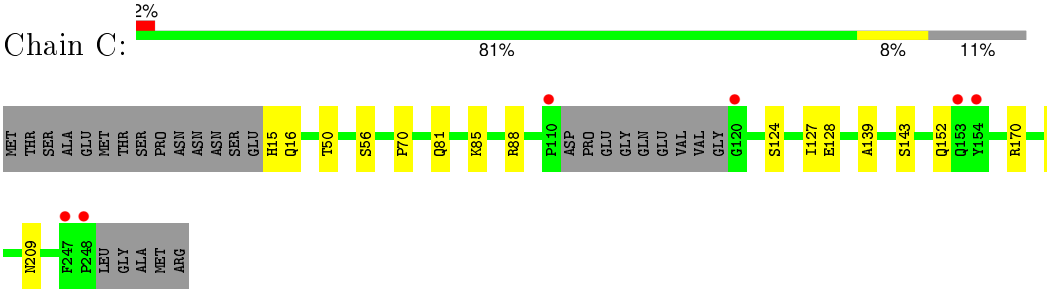
- Molecule 1: Circadian clock protein kinase KaiC

Chain B:



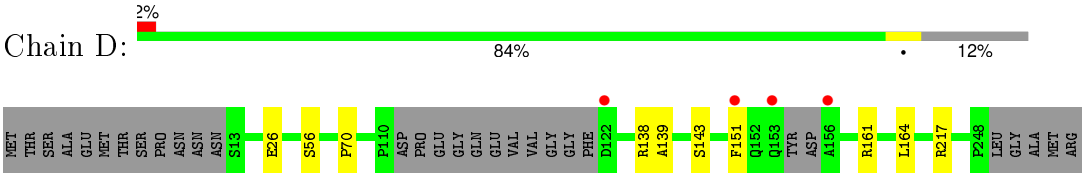
- Molecule 1: Circadian clock protein kinase KaiC

Chain C:



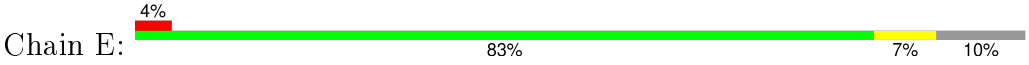
- Molecule 1: Circadian clock protein kinase KaiC

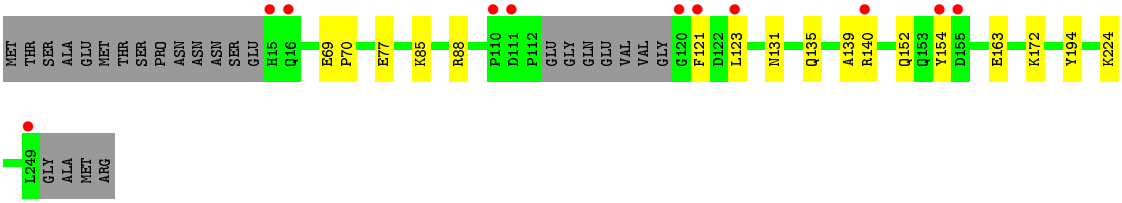
Chain D:



- Molecule 1: Circadian clock protein kinase KaiC

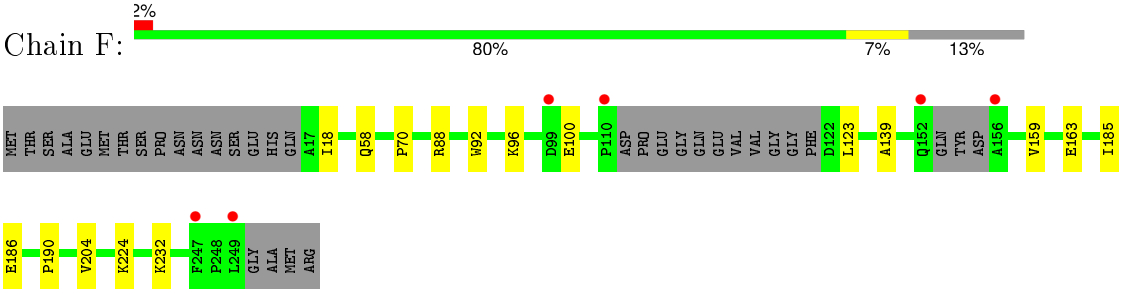
Chain E:





- Molecule 1: Circadian clock protein kinase KaiC

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.88Å 133.38Å 149.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.30 – 2.09 42.30 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.1 (42.30-2.09) 99.1 (42.30-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.39 (at 2.08Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.174 , 0.219 0.174 , 0.219	Depositor DCC
R_{free} test set	4716 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 94355 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11822	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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, 0.375 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	0.24	0/1839	0.46	0/2481
1	B	0.25	0/1831	0.49	2/2468 (0.1%)
1	C	0.24	0/1829	0.43	0/2466
1	D	0.25	0/1828	0.44	0/2463
1	E	0.24	0/1869	0.46	0/2522
1	F	0.24	0/1770	0.44	0/2385
All	All	0.24	0/10966	0.45	2/14785 (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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	15	HIS	CB-CA-C	-8.23	93.95	110.40
1	B	15	HIS	N-CA-CB	5.76	120.97	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	153	GLN	Peptide
1	B	15	HIS	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	1806	0	1812	13	0
1	B	1800	0	1813	7	0
1	C	1797	0	1805	12	0
1	D	1799	0	1814	6	0
1	E	1836	0	1840	12	0
1	F	1742	0	1767	12	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	0	0
4	B	31	0	12	0	0
4	C	31	0	12	0	0
4	D	31	0	12	1	0
4	E	31	0	12	0	0
4	F	31	0	12	1	0
5	A	112	0	0	1	0
5	B	161	0	0	0	0
5	C	156	0	0	0	0
5	D	154	0	0	1	0
5	E	138	0	0	2	0
5	F	123	0	0	2	0
All	All	11822	0	10923	57	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 3.

All (57) 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:88:ARG:NH1	5:E:401:HOH:O	2.16	0.79
1:E:121:PHE:HE2	1:E:123:LEU:HD23	1.51	0.76
1:C:128:GLU:OE2	1:C:170:ARG:NH2	2.21	0.72
1:E:121:PHE:CE2	1:E:123:LEU:HD23	2.31	0.66
1:C:152:GLN:OE1	1:D:161:ARG:NH1	2.24	0.66
1:E:77:GLU:OE1	5:E:501:HOH:O	2.13	0.66
1:A:16:GLN:OE1	1:F:88:ARG:HD3	1.98	0.64
1:B:15:HIS:O	1:B:15:HIS:CG	2.48	0.64
1:F:190:PRO:O	5:F:514:HOH:O	2.15	0.60
1:E:69:GLU:HB3	1:E:140:ARG:HB2	1.84	0.59
1:F:232:LYS:NZ	5:F:508:HOH:O	2.37	0.57
1:C:15:HIS:CG	1:C:16:GLN:H	2.23	0.56
1:C:152:GLN:HA	1:C:194:TYR:OH	2.07	0.55
1:F:70:PRO:HB2	1:F:139:ALA:HA	1.88	0.54
1:E:154:TYR:CE2	1:E:163:GLU:HG3	2.44	0.53
1:D:26:GLU:OE1	1:D:26:GLU:HA	2.08	0.53
1:E:131:ASN:O	1:E:135:GLN:HG2	2.10	0.52
1:A:153:GLN:HE22	1:B:162:ARG:NH2	2.08	0.52
1:A:147:VAL:O	1:A:150:VAL:HG22	2.11	0.51
1:B:56[A]:SER:HB2	1:B:143:SER:HB3	1.94	0.49
1:A:191:ILE:HD12	1:A:206:ILE:HD11	1.94	0.49
1:F:123:LEU:HD22	1:F:163:GLU:HB3	1.94	0.49
1:C:185:ILE:HG13	1:C:186:GLU:HG3	1.94	0.48
1:A:152:GLN:HA	1:A:194:TYR:OH	2.14	0.48
1:E:85:LYS:HE2	1:F:18:ILE:HG12	1.96	0.48
1:F:58:GLN:HG2	1:F:92:TRP:CH2	2.49	0.48
4:D:303:AGS:O3G	1:E:224:LYS:NZ	2.46	0.46
1:A:224:LYS:NZ	4:F:303:AGS:O3G	2.39	0.46
1:A:70:PRO:HB2	1:A:139:ALA:HA	1.97	0.46
1:F:185:ILE:HG13	1:F:186:GLU:HG3	1.98	0.46
1:E:152:GLN:HA	1:E:194:TYR:OH	2.15	0.45
1:C:85:LYS:HA	1:C:88:ARG:HH21	1.80	0.45
1:E:70:PRO:HB2	1:E:139:ALA:HA	1.97	0.45
1:B:56[B]:SER:HB3	1:B:143:SER:HB3	1.98	0.45
1:D:70:PRO:HB2	1:D:139:ALA:HA	1.99	0.44
1:C:15:HIS:ND1	1:C:16:GLN:N	2.65	0.44
1:D:56[A]:SER:HB2	1:D:143:SER:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:GLN:OE1	1:B:161:ARG:NH1	2.47	0.44
1:A:31:ILE:HG22	1:A:222:ILE:HD12	2.00	0.43
1:C:56[A]:SER:HB2	1:C:143:SER:HB3	2.01	0.43
1:D:151:PHE:CZ	1:D:164[A]:LEU:HG	2.54	0.42
1:F:204:VAL:HG23	1:F:224:LYS:HE2	2.02	0.42
1:C:124:SER:O	1:C:127:ILE:HG22	2.20	0.42
1:A:138:ARG:HA	1:A:138:ARG:HD2	1.65	0.42
1:F:123:LEU:HA	1:F:123:LEU:HD12	1.89	0.42
1:C:127:ILE:HA	1:C:127:ILE:HD12	1.93	0.42
1:F:96:LYS:HE2	1:F:100:GLU:OE2	2.19	0.42
1:D:217:ARG:HD2	5:D:418:HOH:O	2.20	0.42
1:C:50:THR:HG22	1:C:209:ASN:HB2	2.02	0.42
1:C:70:PRO:HB2	1:C:139:ALA:HA	2.02	0.42
1:A:121:PHE:CE1	1:A:150:VAL:HB	2.55	0.41
1:A:58:GLN:NE2	5:A:498:HOH:O	2.48	0.41
1:F:159:VAL:O	1:F:163:GLU:HG2	2.20	0.41
1:E:172:LYS:HB2	1:E:172:LYS:HE3	1.93	0.41
1:B:109:SER:HA	1:B:110:PRO:HD3	1.88	0.40
1:B:152:GLN:HA	1:B:194:TYR:OH	2.21	0.40
1:A:158:SER:O	1:A:162:ARG: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	223/253 (88%)	218 (98%)	5 (2%)	0	100	100
1	B	221/253 (87%)	215 (97%)	6 (3%)	0	100	100
1	C	222/253 (88%)	218 (98%)	4 (2%)	0	100	100
1	D	221/253 (87%)	216 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	227/253 (90%)	218 (96%)	9 (4%)	0	100	100
1	F	214/253 (85%)	205 (96%)	9 (4%)	0	100	100
All	All	1328/1518 (88%)	1290 (97%)	38 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	195/216 (90%)	195 (100%)	0	100	100
1	B	195/216 (90%)	195 (100%)	0	100	100
1	C	194/216 (90%)	193 (100%)	1 (0%)	92	95
1	D	196/216 (91%)	195 (100%)	1 (0%)	92	95
1	E	199/216 (92%)	199 (100%)	0	100	100
1	F	189/216 (88%)	189 (100%)	0	100	100
All	All	1168/1296 (90%)	1166 (100%)	2 (0%)	95	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	81	GLN
1	D	138	ARG

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

Mol	Chain	Res	Type
1	A	153	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 carbohydrates in this entry.

5.6 Ligand geometry

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	0.73	1 (3%)	24,52,52	0.49	0
4	AGS	B	303	2	26,33,33	0.77	1 (3%)	24,52,52	0.42	0
4	AGS	C	303	2	26,33,33	0.71	1 (3%)	24,52,52	0.49	0
4	AGS	D	303	2	26,33,33	0.73	1 (3%)	24,52,52	0.50	0
4	AGS	E	303	2	26,33,33	0.70	1 (3%)	24,52,52	0.46	0
4	AGS	F	303	2	26,33,33	0.69	1 (3%)	24,52,52	0.51	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	303	2	-	0/17/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	303	AGS	PG-S1G	2.27	1.94	1.90
4	E	303	AGS	PG-S1G	2.32	1.94	1.90
4	C	303	AGS	PG-S1G	2.40	1.95	1.90
4	D	303	AGS	PG-S1G	2.54	1.95	1.90
4	A	303	AGS	PG-S1G	2.55	1.95	1.90
4	B	303	AGS	PG-S1G	2.74	1.95	1.90

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	303	AGS	1	0
4	F	303	AGS	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, 95^{th} 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	227/253 (89%)	0.13	12 (5%) 30 39	18, 36, 77, 114	0
1	B	226/253 (89%)	-0.33	7 (3%) 52 61	17, 28, 63, 114	0
1	C	225/253 (88%)	-0.42	6 (2%) 58 65	16, 29, 56, 85	0
1	D	223/253 (88%)	-0.18	4 (1%) 71 76	16, 29, 60, 103	0
1	E	228/253 (90%)	-0.15	11 (4%) 34 43	15, 30, 76, 101	0
1	F	219/253 (86%)	-0.32	6 (2%) 58 65	15, 31, 61, 108	0
All	All	1348/1518 (88%)	-0.21	46 (3%) 49 58	15, 30, 67, 114	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	15	HIS	6.3
1	A	120	GLY	5.7
1	F	249	LEU	5.1
1	D	122	ASP	4.9
1	D	151	PHE	4.9
1	A	132	TYR	4.8
1	B	152	GLN	4.7
1	E	120	GLY	4.4
1	D	153	GLN	4.2
1	A	248	PRO	4.0
1	F	110	PRO	3.9
1	A	151	PHE	3.9
1	A	112	PRO	3.8
1	C	120	GLY	3.7
1	E	16	GLN	3.7
1	B	151	PHE	3.5
1	B	153	GLN	3.5
1	E	249	LEU	3.4
1	E	110	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	154	TYR	3.2
1	F	99	ASP	3.0
1	A	154	TYR	3.0
1	D	156	ALA	2.9
1	E	15	HIS	2.9
1	A	124	SER	2.9
1	C	247	PHE	2.7
1	E	140	ARG	2.7
1	E	154	TYR	2.7
1	A	99	ASP	2.6
1	B	121	PHE	2.6
1	C	153	GLN	2.5
1	E	111	ASP	2.4
1	A	135	GLN	2.4
1	E	121	PHE	2.3
1	C	248	PRO	2.3
1	F	156	ALA	2.3
1	F	247	PHE	2.3
1	F	152	GLN	2.2
1	A	111	ASP	2.1
1	A	170	ARG	2.1
1	B	112	PRO	2.1
1	E	123	LEU	2.1
1	A	134	ILE	2.0
1	C	110	PRO	2.0
1	B	16	GLN	2.0
1	E	155	ASP	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^{th} 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^2)	Q<0.9
4	AGS	B	303	31/31	0.98	0.08	-0.38	16,21,26,28	0
4	AGS	A	303	31/31	0.98	0.09	-0.44	19,26,33,59	0
4	AGS	E	303	31/31	0.97	0.08	-0.46	15,20,28,33	0
4	AGS	D	303	31/31	0.98	0.09	-0.67	16,20,26,32	0
4	AGS	F	303	31/31	0.98	0.07	-0.95	17,24,36,44	0
4	AGS	C	303	31/31	0.98	0.07	-1.39	16,21,29,30	0
3	CL	C	302	1/1	1.00	0.03	-	24,24,24,24	0
2	MG	D	301	1/1	0.98	0.04	-	22,22,22,22	0
3	CL	A	302	1/1	1.00	0.03	-	25,25,25,25	0
2	MG	F	301	1/1	0.97	0.03	-	23,23,23,23	0
3	CL	E	302	1/1	1.00	0.04	-	23,23,23,23	0
2	MG	B	301	1/1	0.95	0.05	-	24,24,24,24	0
3	CL	F	302	1/1	0.99	0.05	-	22,22,22,22	0
2	MG	C	301	1/1	0.95	0.04	-	21,21,21,21	0
3	CL	D	302	1/1	1.00	0.07	-	21,21,21,21	0
2	MG	E	301	1/1	0.96	0.06	-	23,23,23,23	0
2	MG	A	301	1/1	0.98	0.04	-	27,27,27,27	0
3	CL	B	302	1/1	1.00	0.04	-	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.