W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 07:48 PM GMT

PDB ID	:	4TL9
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	:	1.82 Å(reported)

The following versions of software and data (see references (i)) 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 1.82 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		0.217
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		0.5%
RSRZ outliers		7.8%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
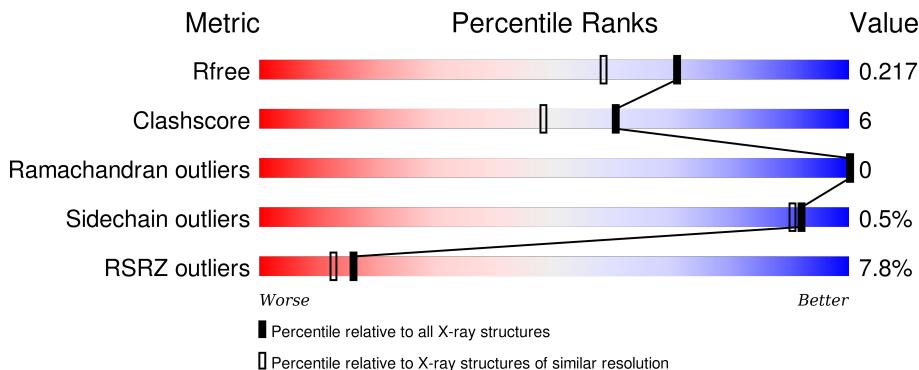
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	5422 (1.84-1.80)
Clashscore	102246	6347 (1.84-1.80)
Ramachandran outliers	100387	6276 (1.84-1.80)
Sidechain outliers	100360	6276 (1.84-1.80)
RSRZ outliers	91569	5439 (1.84-1.80)

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	10% / 74% / 13% / 13%
1	B	253	4% / 76% / 10% / 14%
1	C	253	6% / 76% / 11% / 12%
1	D	253	4% / 77% / 10% / 13%
1	E	253	10% / 76% / 10% / 14%
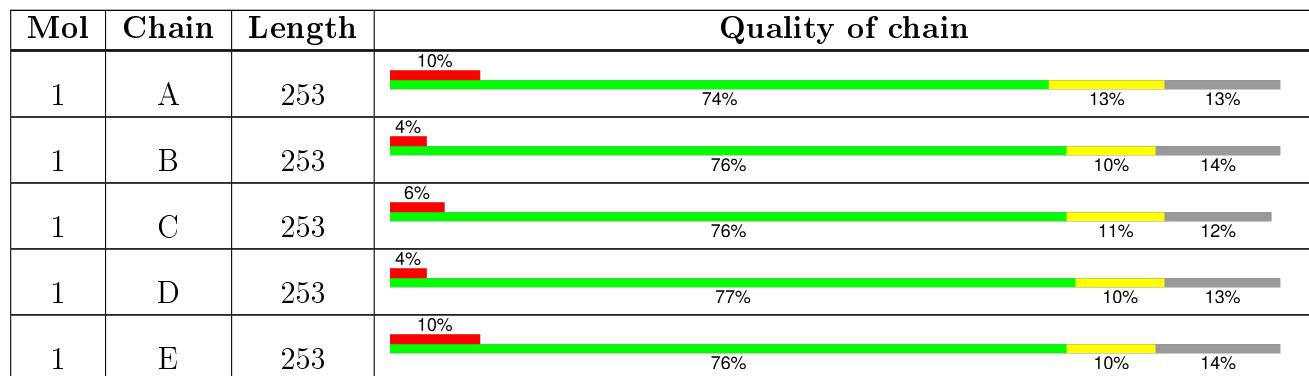
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Mol	Chain	Length	Quality of chain
1	F	253	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11933 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	220	Total 1815	C 1161	N 310	O 340	S 4	0	11	0
1	B	218	Total 1801	C 1149	N 314	O 333	S 5	0	11	0
1	C	222	Total 1826	C 1166	N 314	O 341	S 5	0	10	0
1	D	220	Total 1789	C 1140	N 308	O 336	S 5	0	8	0
1	E	218	Total 1785	C 1139	N 305	O 337	S 4	0	10	0
1	F	214	Total 1757	C 1123	N 303	O 327	S 4	0	9	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	THR	SER	engineered mutation	UNP Q79PF4
B	48	THR	SER	engineered mutation	UNP Q79PF4
C	48	THR	SER	engineered mutation	UNP Q79PF4
D	48	THR	SER	engineered mutation	UNP Q79PF4
E	48	THR	SER	engineered mutation	UNP Q79PF4
F	48	THR	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 1	Mg 1	0	0
2	E	1	Total 1	Mg 1	0	0
2	B	1	Total 1	Mg 1	0	0

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

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

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

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

AGS

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	146	Total 146	O 146	0	0
5	B	192	Total 192	O 192	0	0
5	C	175	Total 175	O 175	0	0
5	D	181	Total 181	O 181	0	0
5	E	138	Total 138	O 138	0	0
5	F	130	Total 130	O 130	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 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
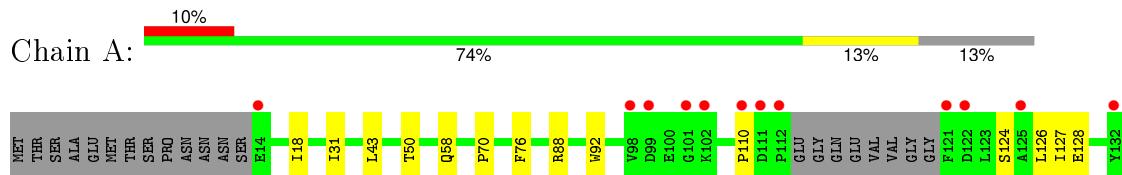
- Molecule 1: Circadian clock protein kinase KaiC
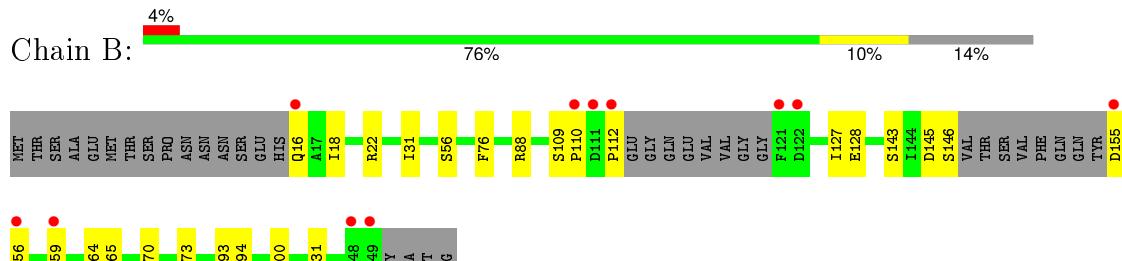
- Molecule 1: Circadian clock protein kinase KaiC
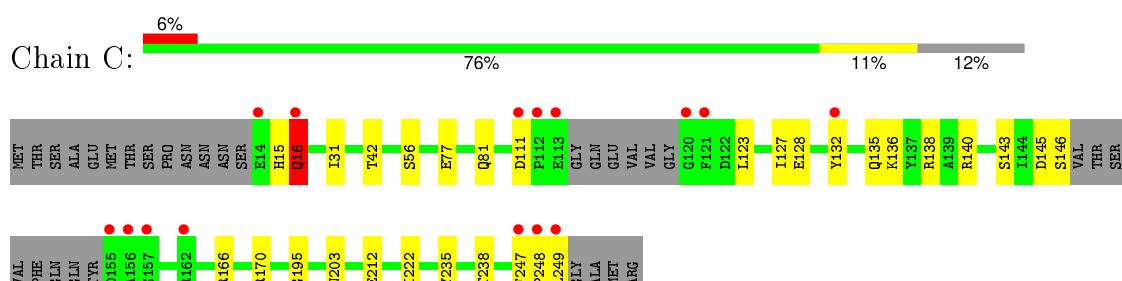
- Molecule 1: Circadian clock protein kinase KaiC
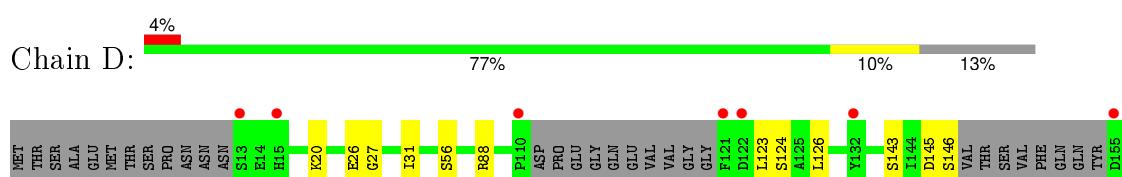
• Molecule 1: Circadian clock protein kinase KaiC
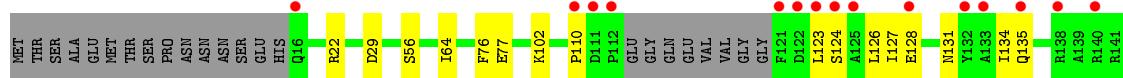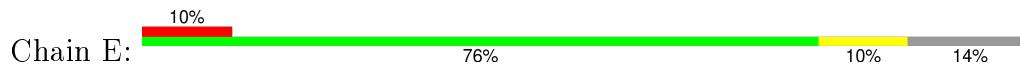
• Molecule 1: Circadian clock protein kinase KaiC

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.13Å 133.82Å 151.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.98 – 1.82 38.98 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.0 (38.98-1.82) 99.0 (38.98-1.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.07 (at 1.82Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.181 , 0.217 0.182 , 0.217	Depositor DCC
R_{free} test set	7219 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	21.8	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 57.5	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 143817 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11933	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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	0.40	0/1868	0.54	0/2518
1	B	0.45	0/1854	0.59	0/2495
1	C	0.46	0/1877	0.63	1/2528 (0.0%)
1	D	0.47	0/1835	0.61	0/2470
1	E	0.47	0/1837	0.60	0/2474
1	F	0.48	0/1802	0.63	1/2426 (0.0%)
All	All	0.46	0/11073	0.60	2/14911 (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	C	0	1

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	C	16	GLN	CA-CB-CG	-8.58	94.53	113.40
1	F	126	LEU	CB-CG-CD2	-5.14	102.26	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	16	GLN	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	1815	0	1849	23	0
1	B	1801	0	1844	22	0
1	C	1826	0	1854	28	0
1	D	1789	0	1816	19	0
1	E	1785	0	1819	20	1
1	F	1757	0	1796	25	1
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	0	0
4	E	31	0	12	0	0
4	F	31	0	12	0	0
5	A	146	0	0	1	0
5	B	192	0	0	4	0
5	C	175	0	0	5	0
5	D	181	0	0	3	0
5	E	138	0	0	0	1
5	F	130	0	0	0	1
All	All	11933	0	11050	123	2

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 (123) 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:D:164:LEU:HD11	1:D:180[B]:MET:HE1	1.53	0.89
1:B:193:ARG:NH1	1:C:195:GLY:O	2.14	0.80
1:A:173:GLN:NE2	5:A:507:HOH:O	2.01	0.79
1:A:124:SER:OG	1:A:166:ARG:NH1	2.14	0.79
1:A:195:GLY:O	1:F:193:ARG:NH2	2.20	0.75
1:E:131:ASN:OD1	1:E:135:GLN:NE2	2.19	0.75
1:A:31[B]:ILE:HD11	1:A:248:PRO:HG3	1.69	0.74
1:C:212:GLU:OE1	5:C:477:HOH:O	2.06	0.72
1:C:238:THR:HG23	1:C:247:PHE:HZ	1.53	0.72
1:F:183:GLU:OE2	1:F:193:ARG:NH1	2.24	0.70
1:B:112:PRO:O	1:C:166:ARG:NH1	2.25	0.69
1:E:110:PRO:HG3	1:F:162:ARG:HD3	1.76	0.68
1:C:238:THR:HG23	1:C:247:PHE:CZ	2.28	0.68
1:B:156:ALA:HB3	1:B:159:VAL:HG23	1.79	0.65
1:F:81:GLN:H	1:F:81:GLN:CD	2.00	0.65
1:A:247:PHE:O	1:A:249:LEU:HA	1.97	0.65
1:E:22:ARG:NH1	1:E:29:ASP:OD2	2.30	0.64
1:E:127:ILE:H	1:E:127:ILE:HD12	1.64	0.63
1:F:76:PHE:CE1	1:F:126:LEU:HD21	2.35	0.62
1:B:193:ARG:NH2	5:B:545:HOH:O	2.34	0.61
1:B:165:PHE:HB2	1:B:200:VAL:HG21	1.82	0.61
1:C:15:HIS:C	1:C:16:GLN:HG2	2.19	0.60
1:B:76:PHE:O	1:B:110:PRO:HD3	2.02	0.60
1:A:127:ILE:HD13	1:A:170:ARG:HG3	1.83	0.60
1:E:124:SER:HA	1:E:127:ILE:HD13	1.83	0.59
1:D:20:LYS:NZ	1:D:228:THR:HG21	2.18	0.59
1:A:58:GLN:HG2	1:A:92:TRP:CH2	2.39	0.58
1:E:110:PRO:HG2	1:F:165:PHE:CE2	2.39	0.58
1:B:22:ARG:NH1	5:B:578:HOH:O	2.37	0.58
1:D:56[A]:SER:HB2	1:D:143:SER:HB3	1.85	0.57
1:F:58:GLN:HG3	1:F:92:TRP:CH2	2.40	0.57
1:E:162:ARG:O	1:E:166:ARG:HG3	2.05	0.56
1:C:146[B]:SER:OG	5:C:543:HOH:O	2.17	0.56
1:D:124:SER:OG	1:D:166:ARG:NH2	2.38	0.56
1:D:156:ALA:HB3	1:D:159:VAL:HG23	1.88	0.56
1:B:155:ASP:OD1	1:B:194:TYR:HE1	1.88	0.56
1:C:77:GLU:OE1	1:D:162:ARG:NH1	2.38	0.56
1:E:124:SER:HA	1:E:127:ILE:CD1	2.35	0.55
1:B:76:PHE:O	1:B:109:SER:HA	2.07	0.55
1:C:248:PRO:O	1:C:249:LEU:HD12	2.08	0.54
1:D:228:THR:HG22	1:D:229:SER:N	2.23	0.54
1:C:128:GLU:OE2	1:C:170:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:ILE:HG23	1:E:102[B]:LYS:HD3	1.90	0.53
1:B:88:ARG:CZ	1:C:15:HIS:HB3	2.38	0.53
1:F:121:PHE:N	1:F:122:ASP:HA	2.23	0.53
1:C:135:GLN:HA	1:C:138:ARG:NH2	2.23	0.53
1:B:112:PRO:HB2	1:C:166:ARG:NH1	2.25	0.52
1:A:165:PHE:CE1	1:F:110:PRO:HG2	2.46	0.51
1:D:26:GLU:OE1	1:D:245:ASN:ND2	2.43	0.51
1:E:156:ALA:HB1	1:E:158:SER:OG	2.11	0.50
1:E:76:PHE:HZ	1:E:126:LEU:HD21	1.77	0.50
1:A:191[B]:ILE:HG23	1:A:206[B]:ILE:HD11	1.93	0.50
1:F:56[B]:SER:HB2	1:F:143:SER:HB3	1.95	0.49
1:E:156:ALA:HB3	1:E:159:VAL:HG22	1.95	0.49
1:D:123:LEU:HD12	1:D:126:LEU:HD23	1.95	0.49
1:D:56[B]:SER:HB3	1:D:143:SER:HB3	1.93	0.49
1:F:31[B]:ILE:HD13	1:F:231:MET:SD	2.53	0.48
1:A:18:ILE:HD13	1:F:85:LYS:HE3	1.96	0.48
1:E:123:LEU:O	1:E:127:ILE:HD12	2.13	0.48
1:A:248:PRO:HA	1:A:249:LEU:HB3	1.95	0.48
1:A:145[B]:ASP:HA	1:A:146[B]:SER:HA	1.61	0.47
1:F:191:ILE:HG23	1:F:206[B]:ILE:HD11	1.96	0.47
1:F:76:PHE:HE1	1:F:126:LEU:HD21	1.78	0.47
1:A:76:PHE:O	1:A:110:PRO:HD3	2.15	0.47
1:D:173:GLN:HG3	5:D:505:HOH:O	2.13	0.47
1:B:112:PRO:HB2	1:C:166:ARG:HH11	1.80	0.46
1:A:146[A]:SER:N	1:A:181:THR:OG1	2.45	0.46
1:A:88:ARG:HD2	1:B:16:GLN:OE1	2.15	0.46
1:B:145[A]:ASP:HA	1:B:146[A]:SER:HA	1.70	0.46
1:D:31[B]:ILE:HD13	1:D:231:MET:SD	2.56	0.46
1:E:124:SER:O	1:E:128:GLU:HG3	2.15	0.46
1:B:31:ILE:HG22	1:B:231[A]:MET:SD	2.55	0.46
1:F:31[A]:ILE:HG22	1:F:222:ILE:HD12	1.98	0.45
1:B:170[B]:ARG:NH1	1:B:173:GLN:OE1	2.47	0.45
1:D:88:ARG:NH1	5:D:579:HOH:O	2.48	0.45
1:C:56[A]:SER:HB2	1:C:143:SER:HB3	1.97	0.45
1:E:77[B]:GLU:HG2	1:F:165:PHE:HE1	1.81	0.45
1:A:31[B]:ILE:HD13	1:A:231:MET:SD	2.57	0.45
1:E:159:VAL:O	1:E:163:GLU:HG2	2.16	0.45
1:A:70:PRO:HB2	1:A:139:ALA:HA	1.98	0.45
1:C:127:ILE:HG21	1:C:170:ARG:HD3	2.00	0.44
1:F:122:ASP:HB2	1:F:125:ALA:H	1.82	0.44
1:D:20:LYS:HZ2	1:D:228:THR:HG21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:GLN:HA	1:C:138:ARG:HH22	1.81	0.44
1:B:127:ILE:HD13	1:B:170[A]:ARG:HG3	1.99	0.44
1:B:128:GLU:OE2	5:B:539:HOH:O	2.21	0.44
1:C:123:LEU:HD12	1:C:123:LEU:HA	1.86	0.44
1:C:145[A]:ASP:HA	1:C:146[A]:SER:HA	1.66	0.44
1:D:145[B]:ASP:HA	1:D:146[B]:SER:HA	1.68	0.44
1:A:110:PRO:HG2	1:B:165:PHE:CE2	2.53	0.43
1:B:173:GLN:HG3	5:B:494:HOH:O	2.18	0.43
1:B:56[B]:SER:HB2	1:B:143:SER:HB3	2.01	0.43
1:E:155:ASP:N	1:E:155:ASP:OD1	2.51	0.43
1:C:81:GLN:HG2	5:C:511:HOH:O	2.18	0.43
1:F:76:PHE:O	1:F:110:PRO:HD3	2.19	0.42
1:F:76:PHE:CZ	1:F:126:LEU:HD21	2.53	0.42
1:C:140:ARG:NE	5:C:536:HOH:O	2.52	0.42
1:C:56[B]:SER:HB3	1:C:143:SER:HB3	2.02	0.42
1:C:42:THR:HA	1:C:203:ASN:HB2	2.01	0.42
1:C:31:ILE:HG22	1:C:222:ILE:HD12	2.01	0.42
1:F:50:THR:HG22	1:F:209:ASN:HB2	2.02	0.42
1:C:140:ARG:HB3	1:C:140:ARG:HE	1.72	0.42
1:F:21:MET:HG3	1:F:141:ARG:NH2	2.35	0.42
1:E:134:ILE:HD11	1:E:142:VAL:HG21	2.02	0.42
1:F:222:ILE:HG21	1:F:225:LEU:HG	2.01	0.41
1:E:123:LEU:HD21	1:E:167:LEU:HB2	2.02	0.41
1:A:76:PHE:HZ	1:A:126:LEU:HD21	1.86	0.41
1:D:27:GLY:O	1:D:31[B]:ILE:HG12	2.21	0.41
1:F:27:GLY:O	1:F:31[B]:ILE:HG12	2.20	0.41
1:A:31[A]:ILE:HG22	1:A:222:ILE:HD12	2.02	0.41
1:C:235:TYR:CD1	1:C:249:LEU:HD22	2.56	0.41
1:A:191[B]:ILE:HG21	1:A:198:GLU:HB3	2.03	0.41
1:D:123:LEU:HD22	1:D:163:GLU:HB3	2.03	0.41
1:D:31[A]:ILE:HG22	1:D:222:ILE:HD12	2.03	0.41
1:C:123:LEU:HD23	5:C:487:HOH:O	2.21	0.41
1:F:145[A]:ASP:HA	1:F:146[A]:SER:HA	1.66	0.41
1:A:50:THR:HG22	1:A:209:ASN:HB2	2.02	0.40
1:F:170:ARG:O	1:F:174:ILE:HG13	2.22	0.40
1:B:164:LEU:HA	1:B:164:LEU:HD12	1.97	0.40
1:E:56[A]:SER:HB2	1:E:143:SER:HB3	2.02	0.40
1:D:170:ARG:HD3	5:D:497:HOH:O	2.21	0.40
1:C:132[B]:TYR:CE2	1:C:136:LYS:HD2	2.57	0.40
1:A:43:LEU:HD11	1:A:182:THR:CG2	2.52	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:404:HOH:O	5:F:401:HOH:O[4_455]	2.02	0.18
1:E:102[B]:LYS:NZ	1:F:212:GLU:OE1[4_455]	2.15	0.05

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	224/253 (88%)	218 (97%)	6 (3%)	0	100	100
1	B	222/253 (88%)	216 (97%)	6 (3%)	0	100	100
1	C	225/253 (89%)	221 (98%)	4 (2%)	0	100	100
1	D	221/253 (87%)	216 (98%)	5 (2%)	0	100	100
1	E	221/253 (87%)	212 (96%)	9 (4%)	0	100	100
1	F	216/253 (85%)	211 (98%)	5 (2%)	0	100	100
All	All	1329/1518 (88%)	1294 (97%)	35 (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	201/217 (93%)	198 (98%)	3 (2%)	72	62
1	B	199/217 (92%)	198 (100%)	1 (0%)	92	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	201/217 (93%)	200 (100%)	1 (0%)	92	90
1	D	197/217 (91%)	197 (100%)	0	100	100
1	E	198/217 (91%)	198 (100%)	0	100	100
1	F	194/217 (89%)	192 (99%)	2 (1%)	82	77
All	All	1190/1302 (91%)	1183 (99%)	7 (1%)	92	88

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128[A]	GLU
1	A	128[B]	GLU
1	A	162	ARG
1	B	18	ILE
1	C	111	ASP
1	F	155	ASP
1	F	170	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	0.79	1 (3%)	24,52,52	0.50	0
4	AGS	B	303	2	26,33,33	0.88	2 (7%)	24,52,52	0.59	0
4	AGS	C	303	2	26,33,33	1.00	1 (3%)	24,52,52	0.72	0
4	AGS	D	303	2	26,33,33	0.80	1 (3%)	24,52,52	0.72	0
4	AGS	E	303	2	26,33,33	0.77	0	24,52,52	0.74	1 (4%)
4	AGS	F	303	2	26,33,33	0.83	2 (7%)	24,52,52	0.75	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	303	2	-	0/17/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	303	AGS	PA-O2A	-2.17	1.45	1.55
4	F	303	AGS	PA-O2A	-2.16	1.45	1.55
4	F	303	AGS	PB-O2B	-2.10	1.46	1.55
4	B	303	AGS	PG-S1G	2.21	1.94	1.90
4	D	303	AGS	PG-S1G	2.33	1.94	1.90
4	A	303	AGS	PG-S1G	2.77	1.95	1.90
4	C	303	AGS	PG-S1G	4.06	1.97	1.90

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	303	AGS	O2A-PA-O3A	2.16	114.52	105.27

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(Å²)	Q<0.9
1	A	220/253 (86%)	0.53	25 (11%)	7	5	16, 31, 67, 105	0
1	B	218/253 (86%)	0.08	11 (5%)	32	27	14, 24, 54, 103	0
1	C	222/253 (87%)	0.10	15 (6%)	20	16	13, 24, 56, 99	1 (0%)
1	D	220/253 (86%)	0.06	10 (4%)	37	31	12, 23, 58, 92	0
1	E	218/253 (86%)	0.30	25 (11%)	6	5	12, 26, 69, 107	0
1	F	214/253 (84%)	0.20	16 (7%)	17	13	12, 26, 64, 108	0
All	All	1312/1518 (86%)	0.21	102 (7%)	16	12	12, 25, 63, 108	1 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	121	PHE	10.1
1	A	121	PHE	9.5
1	B	112	PRO	8.6
1	E	112	PRO	7.7
1	D	249	LEU	7.6
1	E	121	PHE	7.2
1	A	132	TYR	6.8
1	E	132	TYR	6.4
1	A	155	ASP	6.3
1	E	155	ASP	6.2
1	B	121	PHE	6.1
1	B	155	ASP	6.0
1	E	156	ALA	5.3
1	F	156	ALA	5.2
1	D	121	PHE	5.1
1	B	111	ASP	5.0
1	A	249	LEU	5.0
1	C	120	GLY	5.0
1	C	111	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	F	158	SER	4.8
1	C	249	LEU	4.7
1	C	155	ASP	4.6
1	E	124	SER	4.6
1	F	155	ASP	4.6
1	E	123	LEU	4.5
1	A	159	VAL	4.5
1	A	122	ASP	4.4
1	E	249	LEU	4.3
1	D	250	GLY	4.3
1	C	156	ALA	4.3
1	E	158	SER	4.1
1	F	111	ASP	4.1
1	C	247	PHE	4.0
1	B	122	ASP	3.9
1	E	248	PRO	3.8
1	A	156	ALA	3.8
1	E	111	ASP	3.7
1	B	156	ALA	3.7
1	C	121	PHE	3.6
1	E	247	PHE	3.6
1	E	159	VAL	3.5
1	A	158	SER	3.5
1	B	249	LEU	3.4
1	B	16	GLN	3.4
1	E	157	SER	3.4
1	F	110	PRO	3.4
1	E	16	GLN	3.3
1	A	14	GLU	3.3
1	B	248	PRO	3.2
1	D	132	TYR	3.2
1	F	157	SER	3.2
1	E	122	ASP	3.1
1	E	135	GLN	3.1
1	E	138	ARG	3.1
1	D	155	ASP	3.0
1	F	99	ASP	3.0
1	D	110	PRO	2.9
1	C	16	GLN	2.9
1	A	101	GLY	2.9
1	F	129	ARG	2.8
1	A	157	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	162	ARG	2.8
1	C	248	PRO	2.8
1	C	132[A]	TYR	2.8
1	C	113	GLU	2.8
1	A	248	PRO	2.7
1	A	99	ASP	2.7
1	E	110	PRO	2.7
1	D	122	ASP	2.7
1	C	157	SER	2.6
1	D	13	SER	2.6
1	F	162	ARG	2.6
1	F	122	ASP	2.6
1	E	133	ALA	2.5
1	E	140	ARG	2.5
1	F	247	PHE	2.5
1	C	112	PRO	2.4
1	F	124	SER	2.4
1	A	179	VAL	2.4
1	A	110	PRO	2.3
1	B	110	PRO	2.3
1	A	174	ILE	2.3
1	E	128	GLU	2.3
1	F	123	LEU	2.3
1	D	15	HIS	2.3
1	A	173	GLN	2.2
1	A	112	PRO	2.2
1	A	98	VAL	2.2
1	F	166	ARG	2.2
1	F	109	SER	2.2
1	A	162	ARG	2.2
1	D	156	ALA	2.2
1	A	135	GLN	2.2
1	A	125	ALA	2.1
1	A	102	LYS	2.1
1	B	159	VAL	2.1
1	C	162	ARG	2.1
1	A	111	ASP	2.1
1	E	194	TYR	2.1
1	A	138	ARG	2.1
1	C	14	GLU	2.0
1	E	125	ALA	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, 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	LLDF	B-factors(Å^2)	Q<0.9
4	AGS	B	303	31/31	0.98	0.09	-0.29	13,17,21,24	0
4	AGS	A	303	31/31	0.97	0.08	-0.73	18,22,27,28	0
4	AGS	E	303	31/31	0.97	0.08	-0.74	14,18,27,33	0
4	AGS	D	303	31/31	0.98	0.09	-0.88	12,16,22,25	0
4	AGS	C	303	31/31	0.98	0.07	-1.01	13,17,22,28	0
4	AGS	F	303	31/31	0.97	0.08	-1.25	14,18,28,35	0
2	MG	D	301	1/1	0.98	0.07	-2.78	17,17,17,17	0
2	MG	E	301	1/1	0.99	0.04	-2.89	20,20,20,20	0
2	MG	C	301	1/1	0.98	0.04	-2.93	19,19,19,19	0
2	MG	F	301	1/1	0.99	0.07	-3.93	22,22,22,22	0
2	MG	B	301	1/1	0.98	0.07	-4.02	19,19,19,19	0
2	MG	A	301	1/1	0.99	0.03	-6.95	22,22,22,22	0
3	CL	F	302	1/1	0.99	0.06	-	22,22,22,22	0
3	CL	C	302	1/1	1.00	0.06	-	21,21,21,21	0
3	CL	D	302	1/1	1.00	0.09	-	18,18,18,18	0
3	CL	E	302	1/1	0.98	0.04	-	22,22,22,22	0
3	CL	B	302	1/1	0.99	0.05	-	26,26,26,26	0
3	CL	A	302	1/1	0.99	0.05	-	25,25,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.