Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2020 – 09:06 AM GMT

PDB ID	:	6YS9
Title	:	T_926 truncate of ChlH from Thermosynechococcus elongatus at 1.64 A resolution
Authors	:	Bisson, C.; Hunter, C.N.
Deposited on	:	2020-04-21
Resolution	:	1.64 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 ⓘ symbol.

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

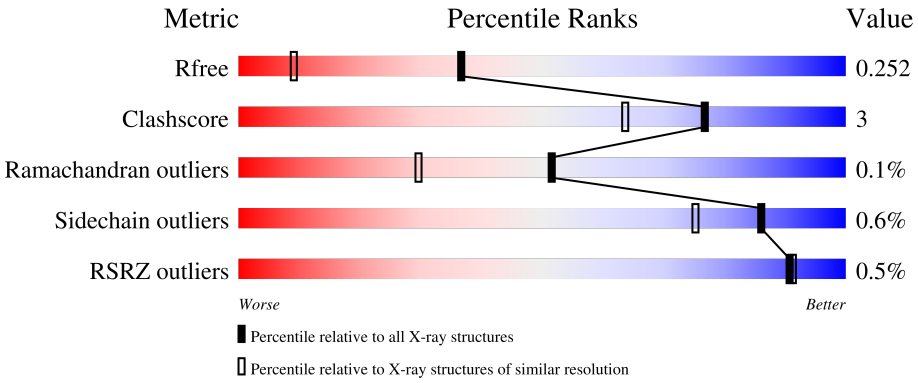
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 1.64 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}	130704	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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	410	85% 8% 7%
1	B	410	87% 6% 7%
1	C	410	. % 84% 8% 8%
1	D	410	85% 8% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12582 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 Magnesium-protoporphyrin methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	0
			3012	1891	525	586	10			
1	B	380	Total	C	N	O	S	0	0	0
			3005	1887	524	584	10			
1	C	378	Total	C	N	O	S	0	1	0
			2999	1884	522	583	10			
1	D	380	Total	C	N	O	S	0	1	0
			3008	1889	525	584	10			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8DM52
A	403	LEU	-	expression tag	UNP Q8DM52
A	404	GLU	-	expression tag	UNP Q8DM52
A	405	HIS	-	expression tag	UNP Q8DM52
A	406	HIS	-	expression tag	UNP Q8DM52
A	407	HIS	-	expression tag	UNP Q8DM52
A	408	HIS	-	expression tag	UNP Q8DM52
A	409	HIS	-	expression tag	UNP Q8DM52
A	410	HIS	-	expression tag	UNP Q8DM52
B	1	MET	-	initiating methionine	UNP Q8DM52
B	403	LEU	-	expression tag	UNP Q8DM52
B	404	GLU	-	expression tag	UNP Q8DM52
B	405	HIS	-	expression tag	UNP Q8DM52
B	406	HIS	-	expression tag	UNP Q8DM52
B	407	HIS	-	expression tag	UNP Q8DM52
B	408	HIS	-	expression tag	UNP Q8DM52
B	409	HIS	-	expression tag	UNP Q8DM52
B	410	HIS	-	expression tag	UNP Q8DM52
C	1	MET	-	initiating methionine	UNP Q8DM52
C	403	LEU	-	expression tag	UNP Q8DM52
C	404	GLU	-	expression tag	UNP Q8DM52

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Chain	Residue	Modelled	Actual	Comment	Reference
C	405	HIS	-	expression tag	UNP Q8DM52
C	406	HIS	-	expression tag	UNP Q8DM52
C	407	HIS	-	expression tag	UNP Q8DM52
C	408	HIS	-	expression tag	UNP Q8DM52
C	409	HIS	-	expression tag	UNP Q8DM52
C	410	HIS	-	expression tag	UNP Q8DM52
D	1	MET	-	initiating methionine	UNP Q8DM52
D	403	LEU	-	expression tag	UNP Q8DM52
D	404	GLU	-	expression tag	UNP Q8DM52
D	405	HIS	-	expression tag	UNP Q8DM52
D	406	HIS	-	expression tag	UNP Q8DM52
D	407	HIS	-	expression tag	UNP Q8DM52
D	408	HIS	-	expression tag	UNP Q8DM52
D	409	HIS	-	expression tag	UNP Q8DM52
D	410	HIS	-	expression tag	UNP Q8DM52

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total K 1 1	0	0
2	A	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0

- Molecule 3 is water.

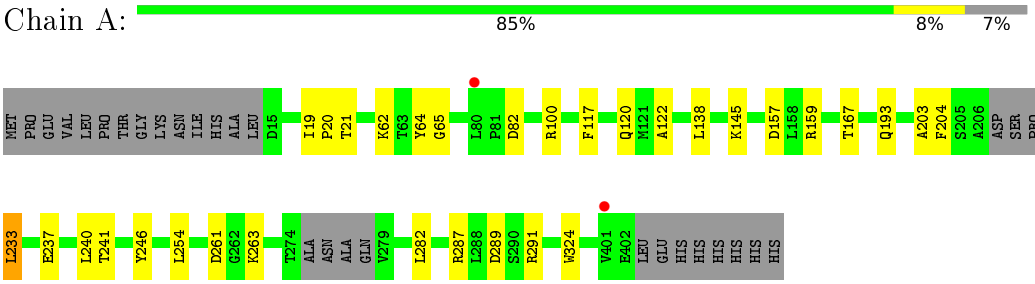
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	107	Total O 107 107	0	0
3	B	179	Total O 179 179	0	0
3	C	102	Total O 102 102	0	0
3	D	166	Total O 166 166	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

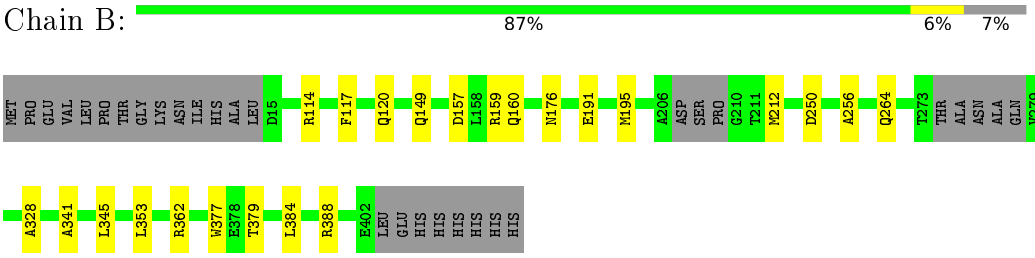
- Molecule 1: Magnesium-protoporphyrin methyltransferase

Chain A:



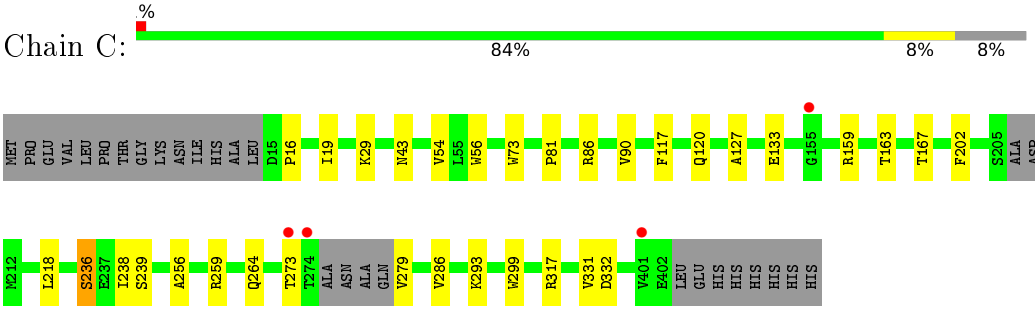
- Molecule 1: Magnesium-protoporphyrin methyltransferase

Chain B:



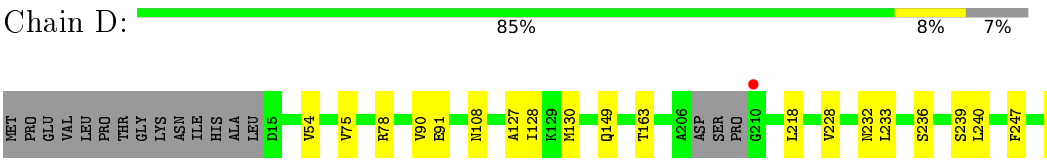
- Molecule 1: Magnesium-protoporphyrin methyltransferase

Chain C:



- Molecule 1: Magnesium-protoporphyrin methyltransferase

Chain D:




K266
T273
THR
ALA
ASN
ALA
Q278
V286
M303
G310
R317
T327
A328
R350
L390
V401
GLU
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.48Å 140.33Å 78.01Å 90.00° 108.66° 90.00°	Depositor
Resolution (Å)	64.38 – 1.64 64.38 – 1.64	Depositor EDS
% Data completeness (in resolution range)	86.2 (64.38-1.64) 90.9 (64.38-1.64)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 1.64Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.201 , 0.247 0.208 , 0.252	Depositor DCC
R_{free} test set	8572 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	18.8	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 20.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.050 for l,-k,h	Xtriage
Reported twinning fraction	0.893 for H, K, L 0.107 for -L, -K, -H	Depositor
Outliers	0 of 172694 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12582	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1657e-03.*

[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

5.1 Standard geometry

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

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	0.71	0/3064	0.82	2/4156 (0.0%)
1	B	0.75	0/3057	0.85	0/4146
1	C	0.73	0/3054	0.84	1/4142 (0.0%)
1	D	0.74	0/3063	0.84	0/4154
All	All	0.73	0/12238	0.84	3/16598 (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})
1	C	259	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	A	100	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	100	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3012	0	2970	22	0
1	B	3005	0	2963	16	0
1	C	2999	0	2960	15	0
1	D	3008	0	2970	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
3	A	107	0	0	2	0
3	B	179	0	0	4	0
3	C	102	0	0	1	0
3	D	166	0	0	4	0
All	All	12582	0	11863	72	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 (72) 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:149:GLN:OE1	3:D:601:HOH:O	1.87	0.93
1:A:291:ARG:NH2	3:A:601:HOH:O	2.33	0.61
1:A:19:ILE:HG23	1:A:65:GLY:HA3	1.85	0.58
1:C:279:VAL:N	3:C:603:HOH:O	2.35	0.58
1:B:362:ARG:NH1	3:B:602:HOH:O	2.37	0.55
1:D:130:MET:HE2	3:D:730:HOH:O	2.07	0.55
1:A:203:ALA:C	1:A:212:MET:HE3	2.28	0.54
1:C:256:ALA:HB2	1:C:264:GLN:HA	1.89	0.54
1:A:240:LEU:HG	1:A:324:TRP:CZ2	2.43	0.53
1:A:241:THR:OG1	1:A:289:ASP:OD2	2.25	0.53
1:C:29:LYS:HD2	1:C:73:TRP:CH2	2.44	0.52
1:A:122:ALA:HB2	1:A:204:PHE:CZ	2.44	0.52
1:C:163:THR:HB	1:C:218:LEU:HD21	1.92	0.52
1:D:130:MET:CE	3:D:730:HOH:O	2.59	0.50
1:D:232:ASN:C	1:D:233:LEU:HD12	2.31	0.50
1:D:254:LEU:C	1:D:254:LEU:HD23	2.33	0.49
1:D:149:GLN:NE2	3:D:607:HOH:O	2.45	0.49
1:A:203:ALA:O	1:A:212:MET:HE3	2.13	0.49
1:B:304:LEU:HD21	1:B:353:LEU:HD23	1.95	0.49
1:B:157:ASP:HB3	1:B:160:GLN:OE1	2.12	0.48
1:D:303:MET:O	1:D:310:GLY:HA3	2.12	0.48
1:D:350:ARG:HD2	1:D:390:LEU:CD1	2.43	0.48
1:A:117:PHE:HB3	1:A:120:GLN:HB2	1.95	0.48
1:A:62:LYS:NZ	1:A:237:GLU:OE1	2.46	0.48
1:C:236:SER:CB	1:C:273:THR:HG23	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ASP:OD1	1:A:159:ARG:N	2.42	0.48
1:D:163:THR:HB	1:D:218:LEU:HD21	1.96	0.47
1:C:43:ASN:ND2	1:C:43:ASN:O	2.47	0.47
1:D:350:ARG:HD2	1:D:390:LEU:HD11	1.96	0.47
1:B:117:PHE:HB3	1:B:120:GLN:HB2	1.97	0.47
1:B:149:GLN:NE2	3:B:601:HOH:O	2.34	0.47
1:B:191:GLU:O	1:B:195:MET:HG3	2.15	0.47
1:A:167:THR:HG22	1:A:212:MET:HE2	1.97	0.47
1:B:298:LYS:HD3	3:B:720:HOH:O	2.14	0.46
1:C:167:THR:O	1:C:202:PHE:HB2	2.16	0.46
1:C:16:PRO:O	1:C:19:ILE:HG12	2.16	0.46
1:D:78:ARG:HD2	1:D:91:GLU:OE2	2.15	0.45
1:B:250:ASP:OD2	1:B:328:ALA:HB2	2.16	0.45
1:D:75:VAL:HG11	1:D:128:ILE:HG12	1.97	0.45
1:A:233:LEU:HD12	1:A:246:TYR:CE2	2.52	0.44
1:B:256:ALA:HB2	1:B:264:GLN:HA	2.00	0.44
1:A:138:LEU:HD23	1:A:145:LYS:HA	1.98	0.44
1:B:176:ASN:O	1:B:195:MET:HE1	2.17	0.43
1:D:240:LEU:HD11	1:D:286:VAL:HG22	1.99	0.43
1:A:204:PHE:CD1	1:A:204:PHE:C	2.91	0.43
1:B:159:ARG:HG3	3:B:620:HOH:O	2.18	0.43
1:A:19:ILE:HA	1:A:20:PRO:HA	1.87	0.43
1:A:287:ARG:CZ	3:A:601:HOH:O	2.67	0.43
1:B:304:LEU:HD21	1:B:353:LEU:CD2	2.49	0.42
1:D:250:ASP:OD2	1:D:328:ALA:HB2	2.19	0.42
1:B:377:TRP:CH2	1:B:379:THR:HG21	2.54	0.42
1:B:114:ARG:CD	1:B:212:MET:HE1	2.49	0.42
1:C:133:GLU:OE2	1:C:159:ARG:HG3	2.19	0.42
1:C:286:VAL:HG11	1:C:331:VAL:HG22	2.01	0.42
1:C:293:LYS:HD3	1:C:299:TRP:CD1	2.55	0.42
1:C:117:PHE:HB3	1:C:120:GLN:HB2	2.01	0.41
1:D:54:VAL:HA	1:D:108:ASN:O	2.20	0.41
1:D:90:VAL:HG21	1:D:127:ALA:HB2	2.02	0.41
1:A:21:THR:HG23	1:A:64:TYR:HB3	2.01	0.41
1:D:247:PHE:O	1:D:327:THR:HG21	2.20	0.41
1:A:122:ALA:HA	1:A:204:PHE:CE1	2.55	0.41
1:B:341:ALA:HA	1:B:345:LEU:HD12	2.01	0.41
1:C:90:VAL:HG21	1:C:127:ALA:HB2	2.02	0.41
1:C:54:VAL:HG11	1:C:56:TRP:CE2	2.56	0.41
1:C:81:PRO:HA	1:C:86:ARG:O	2.21	0.41
1:D:228:VAL:HA	1:D:266:LYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LEU:HD21	1:A:282:LEU:HD11	2.02	0.41
1:A:193:GLN:HB3	1:A:254:LEU:HD13	2.03	0.41
1:A:261:ASP:CG	1:A:263:LYS:HG2	2.42	0.40
1:A:240:LEU:HG	1:A:324:TRP:CE2	2.57	0.40
1:B:384:LEU:O	1:B:388:ARG:HG3	2.21	0.40
1:D:236:SER:HB3	1:D:273:THR:HG23	2.04	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	375/410 (92%)	362 (96%)	12 (3%)	1 (0%)	41 21
1	B	374/410 (91%)	364 (97%)	10 (3%)	0	100 100
1	C	373/410 (91%)	359 (96%)	14 (4%)	0	100 100
1	D	375/410 (92%)	362 (96%)	13 (4%)	0	100 100
All	All	1497/1640 (91%)	1447 (97%)	49 (3%)	1 (0%)	51 29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ASP

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	324/349 (93%)	323 (100%)	1 (0%)	92 87
1	B	323/349 (93%)	323 (100%)	0	100 100
1	C	324/349 (93%)	319 (98%)	5 (2%)	65 42
1	D	324/349 (93%)	322 (99%)	2 (1%)	86 75
All	All	1295/1396 (93%)	1287 (99%)	8 (1%)	86 75

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	LEU
1	C	236	SER
1	C	238	ILE
1	C	239	SER
1	C	317	ARG
1	C	332	ASP
1	D	239	SER
1	D	317	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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

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^{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	381/410 (92%)	-0.17	2 (0%) 91 91	11, 25, 60, 104	0
1	B	380/410 (92%)	-0.39	0 100 100	8, 19, 45, 76	0
1	C	378/410 (92%)	-0.17	4 (1%) 80 81	12, 24, 60, 85	0
1	D	380/410 (92%)	-0.38	2 (0%) 91 91	9, 20, 47, 80	0
All	All	1519/1640 (92%)	-0.28	8 (0%) 91 91	8, 22, 55, 104	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	210	GLY	6.6
1	A	401	VAL	3.1
1	C	273	THR	2.8
1	A	80	LEU	2.7
1	D	401	VAL	2.7
1	C	274	THR	2.4
1	C	401	VAL	2.4
1	C	155	GLY	2.3

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 monosaccharides 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, 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	B-factors(Å^2)	Q<0.9
2	K	A	501	1/1	0.96	0.06	35,35,35,35	0
2	K	D	501	1/1	0.99	0.03	23,23,23,23	0
2	K	C	501	1/1	0.99	0.04	27,27,27,27	0
2	K	B	501	1/1	0.99	0.03	25,25,25,25	0

6.5 Other polymers

There are no such residues in this entry.