Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:16 am BST

PDB ID	:	4O9A
Title	:	Crystal structure of Beta-ketothiolase (PhaA) from Ralstonia eutropha H16
Authors	:	Kim, E.J.; Kim, J.; Kim, S.; Kim, K.J.
Deposited on	:	2014-01-02
Resolution	:	1.52 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:

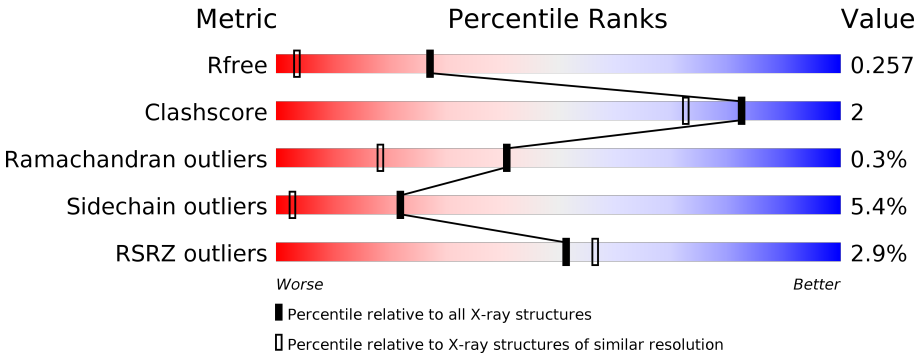
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.52 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	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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	398	2% 89% 9%
1	B	398	3% 90% 7%
1	C	398	3% 87% 10%
1	D	398	4% 89% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11616 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 Acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			2827	1769	501	538	19			
1	B	392	Total	C	N	O	S	0	0	0
			2827	1769	501	538	19			
1	C	392	Total	C	N	O	S	0	0	0
			2827	1769	501	538	19			
1	D	392	Total	C	N	O	S	0	0	0
			2827	1769	501	538	19			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	EXPRESSION TAG	UNP P14611
A	-3	HIS	-	EXPRESSION TAG	UNP P14611
A	-2	HIS	-	EXPRESSION TAG	UNP P14611
A	-1	HIS	-	EXPRESSION TAG	UNP P14611
A	0	HIS	-	EXPRESSION TAG	UNP P14611
A	1	HIS	-	EXPRESSION TAG	UNP P14611
A	88	SER	CYS	ENGINEERED MUTATION	UNP P14611
B	-4	HIS	-	EXPRESSION TAG	UNP P14611
B	-3	HIS	-	EXPRESSION TAG	UNP P14611
B	-2	HIS	-	EXPRESSION TAG	UNP P14611
B	-1	HIS	-	EXPRESSION TAG	UNP P14611
B	0	HIS	-	EXPRESSION TAG	UNP P14611
B	1	HIS	-	EXPRESSION TAG	UNP P14611
B	88	SER	CYS	ENGINEERED MUTATION	UNP P14611
C	-4	HIS	-	EXPRESSION TAG	UNP P14611
C	-3	HIS	-	EXPRESSION TAG	UNP P14611
C	-2	HIS	-	EXPRESSION TAG	UNP P14611
C	-1	HIS	-	EXPRESSION TAG	UNP P14611
C	0	HIS	-	EXPRESSION TAG	UNP P14611
C	1	HIS	-	EXPRESSION TAG	UNP P14611
C	88	SER	CYS	ENGINEERED MUTATION	UNP P14611

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	HIS	-	EXPRESSION TAG	UNP P14611
D	-3	HIS	-	EXPRESSION TAG	UNP P14611
D	-2	HIS	-	EXPRESSION TAG	UNP P14611
D	-1	HIS	-	EXPRESSION TAG	UNP P14611
D	0	HIS	-	EXPRESSION TAG	UNP P14611
D	1	HIS	-	EXPRESSION TAG	UNP P14611
D	88	SER	CYS	ENGINEERED MUTATION	UNP P14611

- Molecule 2 is water.

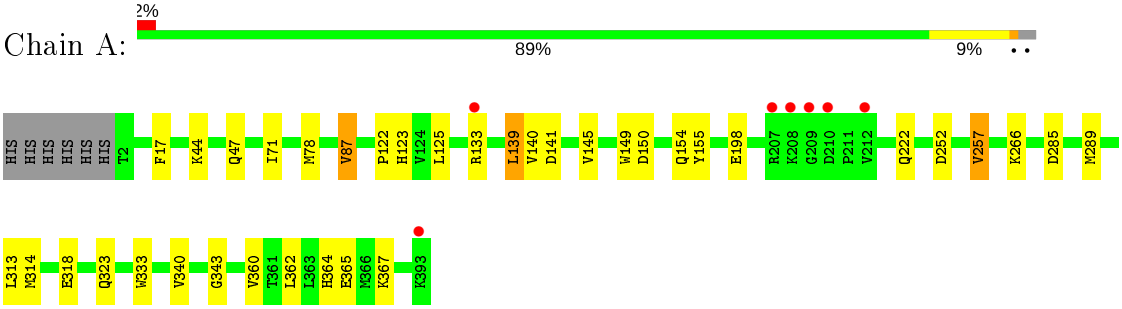
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	79	Total O 79 79	0	0
2	B	102	Total O 102 102	0	0
2	C	62	Total O 62 62	0	0
2	D	65	Total O 65 65	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

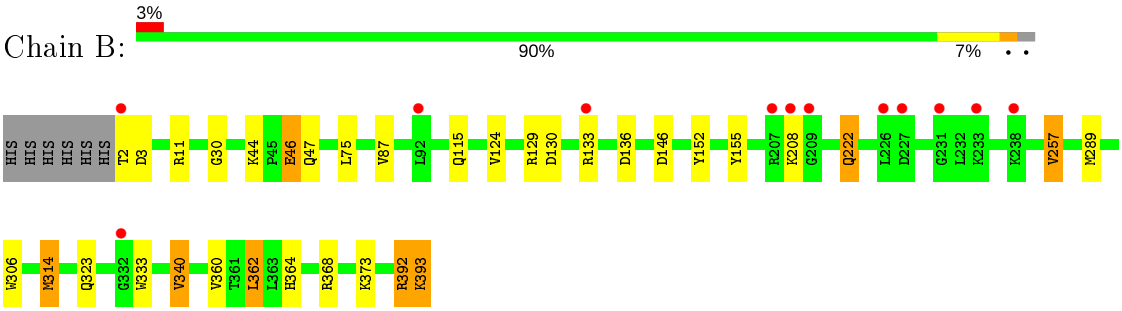
- Molecule 1: Acetyl-CoA acetyltransferase

Chain A:



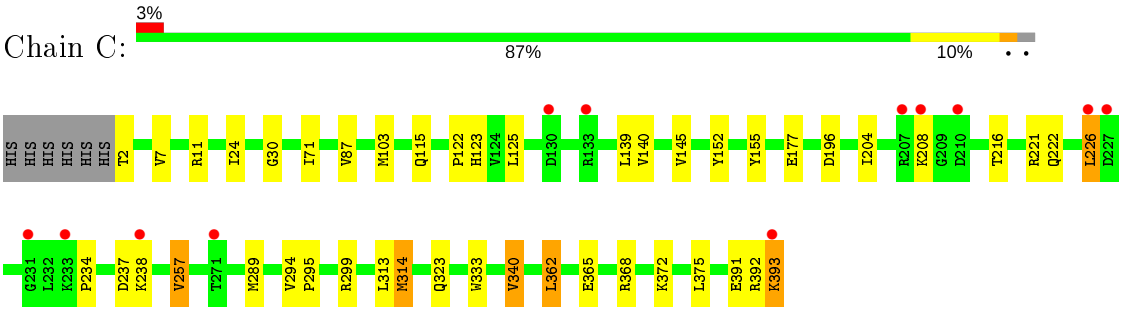
- Molecule 1: Acetyl-CoA acetyltransferase

Chain B:



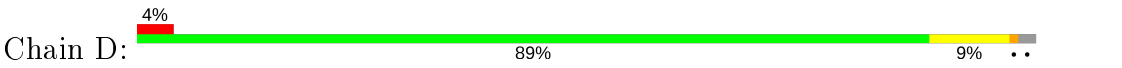
- Molecule 1: Acetyl-CoA acetyltransferase

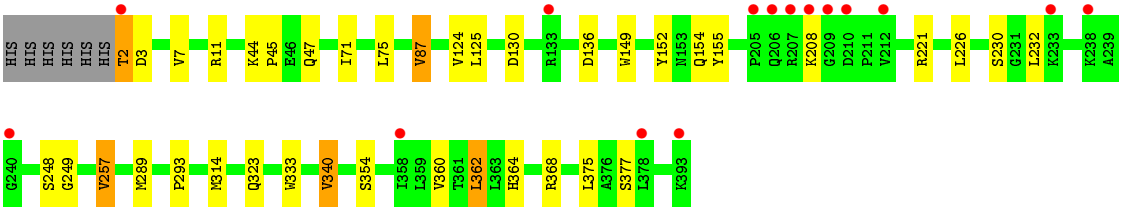
Chain C:



- Molecule 1: Acetyl-CoA acetyltransferase

Chain D:




HIS
HIS
HIS
HIS
HIS
T2
D3
V7
R11
K44
P45
E46
Q47
I71
L75
V87
V124
L125
D130
R133
D136
W149
Y152
N153
Q154
Y155
P205
Q206
R207
K208
G209
D210
P211
V212
R221
L226
S230
G231
L232
K233
K238
A239
G240
S248
G249
V257
M289
P293
M314
Q323
W333
V340
S354
I358
L359
V360
T361
L362
L363
H364
R368
L375
A376
S377
L378
R393

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.27Å 104.70Å 106.91Å 90.00° 106.12° 90.00°	Depositor
Resolution (Å)	27.86 – 1.52 27.86 – 1.52	Depositor EDS
% Data completeness (in resolution range)	91.2 (27.86-1.52) 91.2 (27.86-1.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 1.52Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.218 , 0.254 0.222 , 0.257	Depositor DCC
R_{free} test set	10085 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	13.0	Xtriage
Anisotropy	1.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 36.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11616	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.95	0/2867	1.05	6/3876 (0.2%)
1	B	0.95	1/2867 (0.0%)	1.03	12/3876 (0.3%)
1	C	0.92	0/2867	1.03	13/3876 (0.3%)
1	D	0.89	0/2867	1.01	16/3876 (0.4%)
All	All	0.93	1/11468 (0.0%)	1.03	47/15504 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	146	ASP	CB-CG	5.42	1.63	1.51

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	368	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	C	340	VAL	CG1-CB-CG2	8.99	125.29	110.90
1	A	257	VAL	CG1-CB-CG2	8.82	125.02	110.90
1	B	257	VAL	CG1-CB-CG2	8.56	124.59	110.90
1	D	221	ARG	NE-CZ-NH1	8.55	124.57	120.30
1	B	368	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	D	3	ASP	N-CA-CB	-8.06	96.10	110.60
1	D	368	ARG	NE-CZ-NH2	7.88	124.24	120.30
1	B	368	ARG	NE-CZ-NH2	-7.71	116.45	120.30
1	D	11	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	D	257	VAL	CG1-CB-CG2	7.33	122.64	110.90
1	D	340	VAL	CG1-CB-CG2	7.25	122.50	110.90
1	C	257	VAL	CG1-CB-CG2	7.22	122.46	110.90
1	B	340	VAL	CG1-CB-CG2	7.18	122.38	110.90
1	C	362	LEU	CB-CG-CD2	7.05	122.98	111.00
1	B	3	ASP	N-CA-CB	-6.95	98.09	110.60
1	D	221	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	B	340	VAL	CA-CB-CG2	6.59	120.79	110.90
1	B	392	ARG	NE-CZ-NH1	6.53	123.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	375	LEU	CA-CB-CG	6.27	129.73	115.30
1	D	362	LEU	CB-CG-CD2	6.24	121.61	111.00
1	C	299	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	150	ASP	CB-CG-OD2	6.07	123.77	118.30
1	B	136	ASP	CB-CG-OD1	5.87	123.58	118.30
1	D	375	LEU	CA-CB-CG	5.84	128.74	115.30
1	C	11	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	C	11	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	257	VAL	CA-CB-CG1	5.65	119.37	110.90
1	B	362	LEU	CA-CB-CG	5.63	128.25	115.30
1	D	257	VAL	N-CA-CB	-5.49	99.42	111.50
1	D	230	SER	CB-CA-C	-5.47	99.71	110.10
1	C	299	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	D	368	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	141	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	11	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	252	ASP	CB-CG-OD2	5.33	123.10	118.30
1	D	3	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	C	221	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	C	196	ASP	CB-CG-OD1	5.25	123.03	118.30
1	C	257	VAL	CA-CB-CG1	5.23	118.75	110.90
1	D	257	VAL	CA-CB-CG1	5.22	118.73	110.90
1	A	198	GLU	OE1-CD-OE2	5.18	129.52	123.30
1	C	340	VAL	N-CA-CB	-5.17	100.13	111.50
1	B	257	VAL	N-CA-CB	-5.16	100.15	111.50
1	A	285	ASP	CB-CG-OD1	5.08	122.87	118.30
1	D	136	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	D	226	LEU	CB-CG-CD2	-5.01	102.48	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2827	0	2895	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2827	0	2895	17	0
1	C	2827	0	2895	19	0
1	D	2827	0	2895	14	0
2	A	79	0	0	0	0
2	B	102	0	0	2	0
2	C	62	0	0	0	0
2	D	65	0	0	3	0
All	All	11616	0	11580	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 2.

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:D:44:LYS:H	1:D:47:GLN:HE21	1.35	0.72
1:D:364:HIS:HE1	2:D:445:HOH:O	1.75	0.69
1:B:364:HIS:HE1	2:B:453:HOH:O	1.79	0.65
1:B:222:GLN:HE21	1:B:222:GLN:H	1.47	0.61
1:B:392:ARG:O	1:B:393:LYS:CD	2.48	0.60
1:A:140:VAL:CG1	1:A:145:VAL:HG21	2.31	0.60
1:A:313:LEU:HD21	1:A:365:GLU:HG3	1.85	0.58
1:C:313:LEU:HD21	1:C:365:GLU:HG3	1.86	0.57
1:A:44:LYS:H	1:A:47:GLN:NE2	2.03	0.57
1:C:392:ARG:O	1:C:393:LYS:HD3	2.06	0.56
1:B:392:ARG:O	1:B:393:LYS:HD2	2.07	0.55
1:C:140:VAL:CG1	1:C:145:VAL:HG21	2.37	0.54
1:D:2:THR:N	2:D:441:HOH:O	2.42	0.53
1:A:149:TRP:HE1	1:A:154:GLN:NE2	2.06	0.53
1:C:392:ARG:O	1:C:393:LYS:CD	2.57	0.53
1:A:123:HIS:HB3	1:A:139:LEU:HD23	1.92	0.52
1:D:45:PRO:HB3	1:D:75:LEU:HD23	1.92	0.51
1:D:44:LYS:H	1:D:47:GLN:NE2	2.07	0.51
1:C:7:VAL:HG12	1:C:7:VAL:O	2.11	0.50
1:C:140:VAL:HG11	1:C:145:VAL:HG21	1.93	0.50
1:C:24:ILE:HD11	1:C:204:ILE:HD12	1.94	0.49
1:C:24:ILE:HD11	1:C:204:ILE:CD1	2.42	0.49
1:B:392:ARG:O	1:B:393:LYS:HD3	2.13	0.48
1:D:293:PRO:HB3	1:D:377:SER:OG	2.13	0.48
1:D:7:VAL:O	1:D:7:VAL:HG12	2.14	0.48
1:D:360:VAL:O	1:D:364:HIS:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:HIS:CE1	2:B:453:HOH:O	2.62	0.46
1:C:123:HIS:HB3	1:C:139:LEU:HD22	1.98	0.46
1:B:46:GLU:HG3	1:B:46:GLU:H	1.27	0.45
1:B:306:TRP:CE2	1:B:373:LYS:HD3	2.51	0.45
1:D:364:HIS:CE1	2:D:445:HOH:O	2.60	0.45
1:C:152:TYR:CZ	1:D:71:ILE:HD12	2.52	0.45
1:C:30:GLY:HA3	1:C:115:GLN:NE2	2.32	0.44
1:A:140:VAL:HG13	1:A:145:VAL:HG21	2.00	0.44
1:C:177:GLU:HG2	1:C:226:LEU:HD11	1.99	0.44
1:B:44:LYS:HB2	1:B:47:GLN:HG2	2.00	0.43
1:D:248:SER:OG	1:D:249:GLY:N	2.49	0.43
1:D:149:TRP:HE1	1:D:154:GLN:NE2	2.16	0.43
1:B:30:GLY:HA3	1:B:115:GLN:NE2	2.34	0.43
1:A:122:PRO:CG	1:B:124:VAL:HG21	2.49	0.42
1:C:2:THR:CG2	1:C:103:MET:HA	2.49	0.42
1:A:17:PHE:CZ	1:B:129:ARG:HD3	2.54	0.42
1:C:234:PRO:HB2	1:C:237:ASP:O	2.20	0.42
1:A:44:LYS:H	1:A:47:GLN:HE21	1.67	0.42
1:A:140:VAL:HG11	1:A:145:VAL:HG21	2.01	0.41
1:C:314:MET:SD	1:C:314:MET:N	2.93	0.41
1:B:75:LEU:HD12	1:B:75:LEU:N	2.34	0.41
1:C:372:LYS:O	1:C:391:GLU:HA	2.20	0.41
1:B:222:GLN:HE21	1:B:222:GLN:N	2.17	0.41
1:C:294:VAL:HB	1:C:295:PRO:CD	2.51	0.41
1:C:122:PRO:HB2	1:D:124:VAL:HG22	2.03	0.41
1:A:318:GLU:CD	1:A:343:GLY:HA3	2.42	0.40
1:C:71:ILE:HD12	1:D:152:TYR:CZ	2.56	0.40
1:A:71:ILE:HD12	1:B:152:TYR:CZ	2.56	0.40
1:A:360:VAL:O	1:A:364:HIS:HD2	2.04	0.40
1:B:314:MET:SD	1:B:314:MET:N	2.95	0.40
1:B:360:VAL:O	1:B:364:HIS:HD2	2.05	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	390/398 (98%)	379 (97%)	10 (3%)	1 (0%)	41	18
1	B	390/398 (98%)	380 (97%)	9 (2%)	1 (0%)	41	18
1	C	390/398 (98%)	379 (97%)	10 (3%)	1 (0%)	41	18
1	D	390/398 (98%)	375 (96%)	14 (4%)	1 (0%)	41	18
All	All	1560/1592 (98%)	1513 (97%)	43 (3%)	4 (0%)	41	18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	VAL
1	B	87	VAL
1	C	87	VAL
1	D	87	VAL

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	284/290 (98%)	268 (94%)	16 (6%)	21	2
1	B	284/290 (98%)	269 (95%)	15 (5%)	22	3
1	C	284/290 (98%)	269 (95%)	15 (5%)	22	3
1	D	284/290 (98%)	269 (95%)	15 (5%)	22	3
All	All	1136/1160 (98%)	1075 (95%)	61 (5%)	22	3

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	MET
1	A	87	VAL
1	A	125	LEU
1	A	133	ARG

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Mol	Chain	Res	Type
1	A	139	LEU
1	A	155	TYR
1	A	222	GLN
1	A	257	VAL
1	A	266	LYS
1	A	289	MET
1	A	314	MET
1	A	323	GLN
1	A	333	TRP
1	A	340	VAL
1	A	362	LEU
1	A	367	LYS
1	B	2	THR
1	B	46	GLU
1	B	130	ASP
1	B	133	ARG
1	B	155	TYR
1	B	208	LYS
1	B	222	GLN
1	B	257	VAL
1	B	289	MET
1	B	314	MET
1	B	323	GLN
1	B	333	TRP
1	B	340	VAL
1	B	362	LEU
1	B	393	LYS
1	C	125	LEU
1	C	155	TYR
1	C	208	LYS
1	C	216	THR
1	C	222	GLN
1	C	226	LEU
1	C	238	LYS
1	C	257	VAL
1	C	289	MET
1	C	314	MET
1	C	323	GLN
1	C	333	TRP
1	C	340	VAL
1	C	362	LEU
1	C	393	LYS

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Mol	Chain	Res	Type
1	D	2	THR
1	D	87	VAL
1	D	125	LEU
1	D	130	ASP
1	D	155	TYR
1	D	208	LYS
1	D	232	LEU
1	D	257	VAL
1	D	289	MET
1	D	314	MET
1	D	323	GLN
1	D	333	TRP
1	D	340	VAL
1	D	354	SER
1	D	362	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	115	GLN
1	A	154	GLN
1	A	184	ASN
1	A	329	GLN
1	A	330	GLN
1	A	364	HIS
1	B	115	GLN
1	B	154	GLN
1	B	184	ASN
1	B	222	GLN
1	B	364	HIS
1	C	115	GLN
1	C	154	GLN
1	C	364	HIS
1	D	47	GLN
1	D	115	GLN
1	D	154	GLN
1	D	184	ASN
1	D	222	GLN
1	D	364	HIS

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

There are no ligands in this entry.

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	392/398 (98%)	0.01	7 (1%) 68 73	10, 16, 30, 59	0
1	B	392/398 (98%)	0.02	12 (3%) 49 54	9, 17, 32, 55	0
1	C	392/398 (98%)	0.13	12 (3%) 49 54	10, 18, 34, 58	0
1	D	392/398 (98%)	0.11	15 (3%) 40 45	11, 19, 33, 66	0
All	All	1568/1592 (98%)	0.07	46 (2%) 51 56	9, 17, 33, 66	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	207	ARG	6.2
1	B	207	ARG	5.2
1	C	207	ARG	4.2
1	D	209	GLY	4.0
1	A	208	LYS	4.0
1	B	208	LYS	3.9
1	A	207	ARG	3.9
1	C	208	LYS	3.7
1	D	238	LYS	3.5
1	D	393	LYS	3.5
1	B	209	GLY	3.5
1	D	2	THR	3.4
1	A	133	ARG	3.3
1	B	226	LEU	3.2
1	B	227	ASP	3.1
1	C	133	ARG	2.9
1	D	208	LYS	2.8
1	D	233	LYS	2.8
1	A	209	GLY	2.8
1	A	212	VAL	2.7
1	C	210	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	358	ILE	2.7
1	C	226	LEU	2.7
1	C	231	GLY	2.7
1	A	393	LYS	2.6
1	D	210	ASP	2.6
1	D	240	GLY	2.6
1	D	133	ARG	2.6
1	C	130	ASP	2.6
1	B	238	LYS	2.6
1	D	212	VAL	2.5
1	B	231	GLY	2.4
1	C	238	LYS	2.4
1	B	133	ARG	2.4
1	C	393	LYS	2.4
1	D	205	PRO	2.3
1	B	92	LEU	2.3
1	C	227	ASP	2.3
1	A	210	ASP	2.3
1	D	206	GLN	2.2
1	B	332	GLY	2.1
1	C	271	THR	2.1
1	B	233	LYS	2.1
1	B	2	THR	2.0
1	D	378	LEU	2.0
1	C	233	LYS	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.