Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:56 PM GMT

PDB ID	:	4QFW
Title	:	Crystal structure of acyl-CoA thioesterase tesB from Yersinia pestis
Authors	:	Swarbrick, C.M.D.; Forwood, J.K.
Deposited on	:	2014-05-21
Resolution	:	2.00 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:

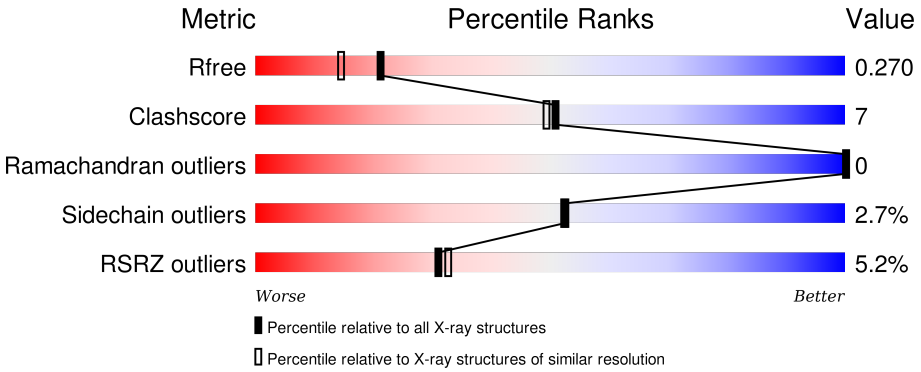
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	288	3%, 83%, 7%, 9%
1	B	288	2%, 77%, 15%, 8%
1	C	288	3%, 81%, 11%, 7%
1	D	288	10%, 74%, 17%, 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8667 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 Acyl-CoA thioesterase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2097	1334	367	389	7			
1	B	265	Total	C	N	O	S	0	0	0
			2114	1346	369	392	7			
1	C	269	Total	C	N	O	S	0	0	0
			2152	1373	376	396	7			
1	D	263	Total	C	N	O	S	0	0	0
			2097	1334	367	389	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	287	SER	-	EXPRESSION TAG	UNP Q0WCE2
A	288	ASN	-	EXPRESSION TAG	UNP Q0WCE2
B	287	SER	-	EXPRESSION TAG	UNP Q0WCE2
B	288	ASN	-	EXPRESSION TAG	UNP Q0WCE2
C	287	SER	-	EXPRESSION TAG	UNP Q0WCE2
C	288	ASN	-	EXPRESSION TAG	UNP Q0WCE2
D	287	SER	-	EXPRESSION TAG	UNP Q0WCE2
D	288	ASN	-	EXPRESSION TAG	UNP Q0WCE2

- Molecule 2 is water.

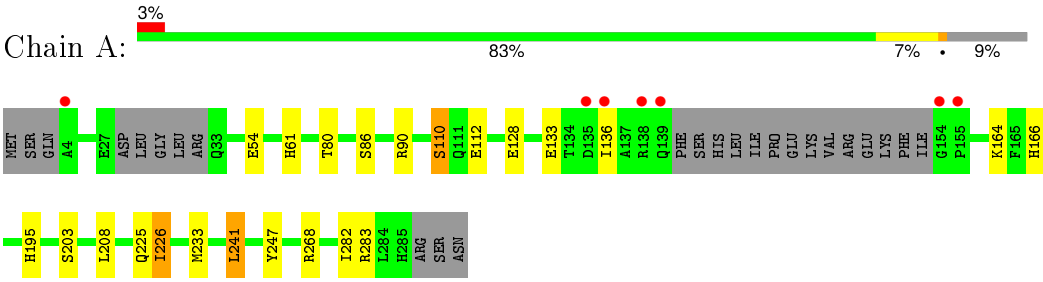
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	79	Total	O	0	0
			79	79		
2	B	42	Total	O	0	0
			42	42		
2	C	62	Total	O	0	0
			62	62		
2	D	24	Total	O	0	0
			24	24		

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.

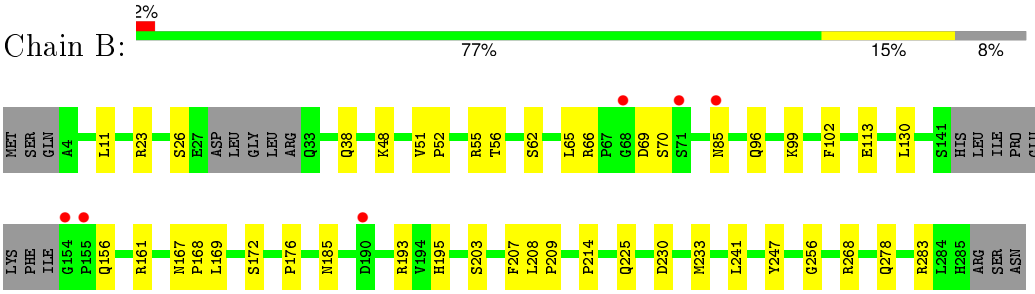
- Molecule 1: Acyl-CoA thioesterase II

Chain A:



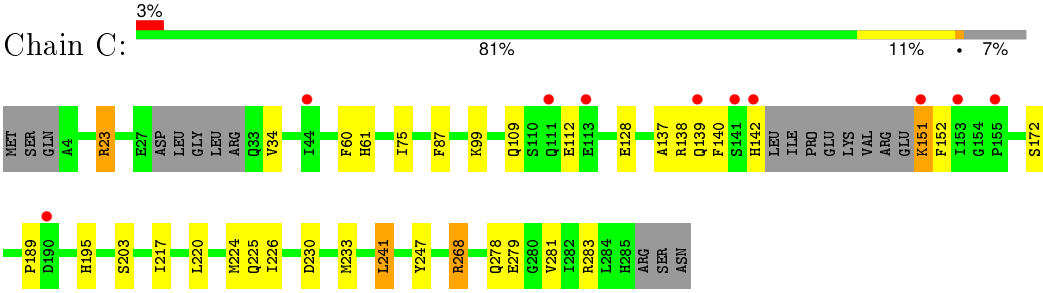
- Molecule 1: Acyl-CoA thioesterase II

Chain B:



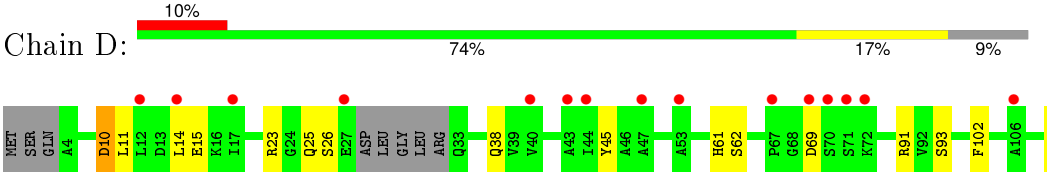
- Molecule 1: Acyl-CoA thioesterase II

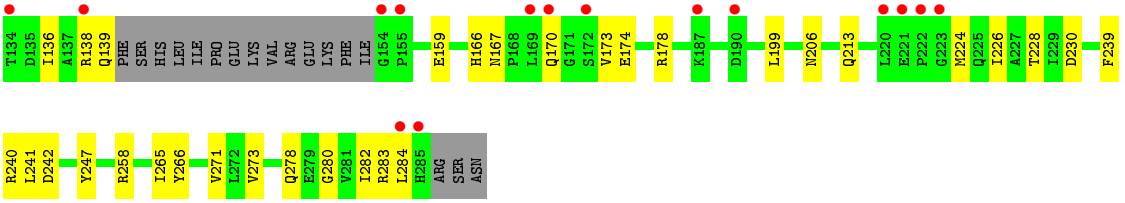
Chain C:



- Molecule 1: Acyl-CoA thioesterase II

Chain D:




T134
D135
I136
A137
R138
Q139
PHE
SER
HIS
LEU
ILE
PRO
GLU
LYS
VAL
ARG
GLU
LYS
PHE
ILE
G154
P155
E159
H166
N167
P168
L169
Q170
G171
S172
V173
E174
R178
K187
D190
L199
N206
Q213
L220
E221
P222
G223
M224
Q225
I226
A227
T228
I229
D230
F239

R240
L241
D242
Y247
R258
I265
Y266
V271
L272
V273
Q278
E279
G280
V281
I282
R283
L284
H285
ARG
SER
ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.23Å 171.62Å 73.70Å 90.00° 109.62° 90.00°	Depositor
Resolution (Å)	24.29 – 2.00 24.29 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.7 (24.29-2.00) 93.7 (24.29-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.36 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.221 , 0.268 0.227 , 0.270	Depositor DCC
R_{free} test set	3827 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	22.9	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 49.5	EDS
Estimated twinning fraction	0.032 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 75499 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8667	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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

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	0.87	0/2152	0.85	0/2915
1	B	0.84	0/2170	0.86	3/2939 (0.1%)
1	C	0.91	0/2210	0.91	2/2992 (0.1%)
1	D	0.84	0/2152	0.87	1/2915 (0.0%)
All	All	0.87	0/8684	0.88	6/11761 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	23	ARG	NE-CZ-NH2	6.02	123.31	120.30
1	B	55	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	C	268	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	B	23	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	D	91	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	65	LEU	CB-CG-CD1	-5.29	102.01	111.00

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	2097	0	2024	21	0
1	B	2114	0	2038	37	0
1	C	2152	0	2078	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2097	0	2024	34	0
2	A	79	0	0	0	0
2	B	42	0	0	0	0
2	C	62	0	0	1	0
2	D	24	0	0	0	0
All	All	8667	0	8164	114	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 7.

All (114) 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:C:138:ARG:O	1:C:139:GLN:HB2	1.68	0.90
1:B:26:SER:HA	1:B:38:GLN:HE22	1.35	0.89
1:B:69:ASP:H	1:B:96:GLN:HE22	1.21	0.85
1:B:26:SER:HA	1:B:38:GLN:NE2	1.96	0.81
1:A:195:HIS:HD2	1:A:241:LEU:H	1.29	0.81
1:D:284:LEU:O	1:D:284:LEU:HD12	1.81	0.80
1:C:195:HIS:HD2	1:C:241:LEU:H	1.31	0.77
1:A:54:GLU:OE1	1:A:110:SER:HB3	1.86	0.76
1:C:99:LYS:HE2	2:C:320:HOH:O	1.85	0.75
1:C:112:GLU:OE1	1:D:283:ARG:NH1	2.22	0.73
1:B:11:LEU:HD21	1:B:38:GLN:NE2	2.03	0.72
1:A:195:HIS:CD2	1:A:241:LEU:H	2.08	0.72
1:A:203:SER:OG	1:A:233:MET:HE1	1.89	0.72
1:D:136:ILE:O	1:D:139:GLN:HB3	1.92	0.69
1:A:203:SER:OG	1:A:233:MET:CE	2.41	0.68
1:D:10:ASP:OD1	1:D:11:LEU:N	2.26	0.68
1:D:166:HIS:ND1	1:D:174:GLU:OE2	2.29	0.64
1:C:195:HIS:CD2	1:C:241:LEU:H	2.15	0.64
1:D:15:GLU:OE1	1:D:23:ARG:NH2	2.31	0.63
1:D:178:ARG:HH11	1:D:206:ASN:HD22	1.46	0.63
1:C:151:LYS:HG3	1:C:220:LEU:HD11	1.80	0.62
1:A:112:GLU:OE1	1:B:283:ARG:NH2	2.32	0.62
1:B:203:SER:CB	1:B:233:MET:HE2	2.29	0.62
1:A:128:GLU:OE2	1:A:268:ARG:NH2	2.33	0.62
1:C:225:GLN:NE2	1:C:283:ARG:HH21	1.97	0.61
1:C:217:ILE:HG21	1:C:224:MET:HE3	1.83	0.61
1:C:138:ARG:O	1:C:139:GLN:CB	2.42	0.60
1:C:128:GLU:OE2	1:C:268:ARG:NH2	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:HIS:CD2	1:B:241:LEU:H	2.21	0.58
1:B:195:HIS:HD2	1:B:241:LEU:H	1.52	0.58
1:B:203:SER:OG	1:B:233:MET:HE1	2.04	0.57
1:D:166:HIS:CE1	1:D:174:GLU:OE2	2.57	0.57
1:B:268:ARG:HH11	1:B:268:ARG:HG2	1.70	0.57
1:D:226:ILE:HG22	1:D:282:ILE:HG22	1.86	0.57
1:C:203:SER:OG	1:C:233:MET:HE1	2.07	0.55
1:B:26:SER:CA	1:B:38:GLN:HE22	2.12	0.55
1:C:151:LYS:O	1:C:151:LYS:HD3	2.06	0.55
1:C:87:PHE:CE1	1:C:109:GLN:HG3	2.42	0.54
1:C:225:GLN:NE2	1:C:283:ARG:NH2	2.56	0.54
1:C:172:SER:O	1:C:174:GLU:HG2	2.08	0.54
1:C:61:HIS:HE1	1:D:230:ASP:HB2	1.72	0.54
1:B:203:SER:OG	1:B:233:MET:CE	2.56	0.53
1:A:226:ILE:HD12	1:A:282:ILE:HG22	1.90	0.53
1:D:11:LEU:HD11	1:D:25:GLN:O	2.09	0.52
1:B:130:LEU:O	1:B:161:ARG:HD3	2.09	0.52
1:D:167:ASN:ND2	1:D:170:GLN:OE1	2.43	0.52
1:B:167:ASN:ND2	1:B:169:LEU:H	2.08	0.51
1:A:133:GLU:HA	1:A:136:ILE:HG22	1.93	0.51
1:C:203:SER:OG	1:C:233:MET:CE	2.59	0.50
1:C:60:PHE:CZ	1:C:233:MET:HE3	2.46	0.50
1:B:156:GLN:O	1:B:185:ASN:ND2	2.43	0.50
1:D:14:LEU:HB2	1:D:45:TYR:CE2	2.48	0.49
1:D:199:LEU:HD22	1:D:239:PHE:CZ	2.48	0.49
1:C:137:ALA:HA	1:C:140:PHE:CE1	2.47	0.49
1:D:265:ILE:O	1:D:273:VAL:HG22	2.13	0.48
1:D:15:GLU:CD	1:D:23:ARG:HH21	2.17	0.48
1:D:15:GLU:OE1	1:D:23:ARG:NE	2.46	0.48
1:C:225:GLN:HE22	1:C:283:ARG:NH2	2.12	0.48
1:D:167:ASN:HB3	1:D:170:GLN:HB3	1.96	0.48
1:A:164:LYS:HD2	1:A:166:HIS:CE1	2.49	0.47
1:A:203:SER:CB	1:A:233:MET:HE2	2.45	0.47
1:B:85:ASN:O	1:B:85:ASN:OD1	2.33	0.46
1:C:225:GLN:HE21	1:C:283:ARG:HD2	1.81	0.46
1:D:228:THR:HG23	1:D:278:GLN:CD	2.36	0.46
1:D:26:SER:HA	1:D:38:GLN:NE2	2.30	0.45
1:D:226:ILE:HG13	1:D:226:ILE:O	2.16	0.45
1:D:224:MET:HE2	1:D:284:LEU:HA	1.98	0.45
1:B:66:ARG:HE	1:B:99:LYS:NZ	2.13	0.45
1:B:11:LEU:HD21	1:B:38:GLN:HE21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:ARG:CZ	1:D:138:ARG:HB2	2.47	0.45
1:B:69:ASP:N	1:B:96:GLN:HE22	2.02	0.45
1:D:174:GLU:HG3	1:D:213:GLN:HB3	1.99	0.45
1:B:66:ARG:CZ	1:B:99:LYS:HE2	2.47	0.45
1:B:48:LYS:HE3	1:B:193:ARG:HD2	1.98	0.45
1:D:132:SER:OG	1:D:159:GLU:OE2	2.36	0.44
1:A:112:GLU:OE2	1:B:283:ARG:NH2	2.48	0.44
1:C:283:ARG:NE	1:D:112:GLU:OE2	2.50	0.44
1:D:62:SER:HB2	1:D:102:PHE:CE1	2.53	0.44
1:C:142:HIS:H	1:C:142:HIS:CD2	2.36	0.44
1:A:208:LEU:HG	1:A:226:ILE:HD11	1.99	0.44
1:D:258:ARG:HA	1:D:280:GLY:O	2.18	0.44
1:C:226:ILE:HA	1:C:281:VAL:O	2.18	0.44
1:A:225:GLN:OE1	1:A:283:ARG:NH2	2.42	0.44
1:B:167:ASN:HD22	1:B:169:LEU:H	1.66	0.44
1:A:112:GLU:O	1:B:256:GLY:HA2	2.18	0.44
1:C:230:ASP:HB2	1:D:61:HIS:HE1	1.83	0.44
1:B:203:SER:HB3	1:B:233:MET:HE2	1.99	0.43
1:C:189:PRO:O	1:C:195:HIS:HE1	2.01	0.43
1:D:14:LEU:HB2	1:D:45:TYR:CD2	2.54	0.43
1:C:230:ASP:OD1	1:C:279:GLU:HB3	2.18	0.43
1:A:80:THR:HA	1:A:90:ARG:HD3	2.00	0.43
1:A:203:SER:OG	1:A:233:MET:HE2	2.15	0.43
1:C:230:ASP:O	1:C:278:GLN:HG3	2.19	0.43
1:B:203:SER:CB	1:B:233:MET:CE	2.95	0.43
1:C:230:ASP:HB2	1:D:61:HIS:CE1	2.53	0.43
1:A:128:GLU:CD	1:A:268:ARG:HH22	2.21	0.43
1:A:112:GLU:CD	1:B:283:ARG:NH2	2.72	0.42
1:B:167:ASN:HA	1:B:168:PRO:HD3	1.85	0.42
1:A:61:HIS:HE1	1:B:230:ASP:HB2	1.84	0.42
1:B:230:ASP:O	1:B:278:GLN:HG3	2.19	0.42
1:D:266:TYR:HA	1:D:271:VAL:O	2.19	0.42
1:B:62:SER:HB2	1:B:102:PHE:CE1	2.54	0.42
1:B:176:PRO:HB3	1:B:214:PRO:HG3	2.01	0.42
1:B:51:VAL:HG13	1:B:52:PRO:HD2	2.02	0.42
1:A:203:SER:CB	1:A:233:MET:CE	2.98	0.42
1:D:62:SER:HB2	1:D:102:PHE:CZ	2.55	0.42
1:B:233:MET:HB2	1:B:233:MET:HE3	1.72	0.42
1:C:225:GLN:HE22	1:C:283:ARG:HH21	1.63	0.41
1:B:208:LEU:N	1:B:209:PRO:CD	2.83	0.41
1:C:23:ARG:HB2	1:C:75:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:PHE:CE1	1:B:278:GLN:HB3	2.55	0.41
1:C:151:LYS:CG	1:C:220:LEU:HD11	2.49	0.41
1:B:268:ARG:HH11	1:B:268:ARG:CG	2.32	0.41
1:D:240:ARG:HB3	1:D:242:ASP:OD1	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	257/288 (89%)	253 (98%)	4 (2%)	0	100	100
1	B	259/288 (90%)	254 (98%)	5 (2%)	0	100	100
1	C	263/288 (91%)	259 (98%)	4 (2%)	0	100	100
1	D	257/288 (89%)	250 (97%)	7 (3%)	0	100	100
All	All	1036/1152 (90%)	1016 (98%)	20 (2%)	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	224/248 (90%)	218 (97%)	6 (3%)	52	52
1	B	226/248 (91%)	220 (97%)	6 (3%)	52	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	230/248 (93%)	224 (97%)	6 (3%)	54 54
1	D	224/248 (90%)	218 (97%)	6 (3%)	52 52
All	All	904/992 (91%)	880 (97%)	24 (3%)	52 52

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	SER
1	A	110	SER
1	A	190	ASP
1	A	226	ILE
1	A	241	LEU
1	A	247	TYR
1	B	56	THR
1	B	70	SER
1	B	113	GLU
1	B	172	SER
1	B	225	GLN
1	B	247	TYR
1	C	34	VAL
1	C	151	LYS
1	C	152	PHE
1	C	180	VAL
1	C	241	LEU
1	C	247	TYR
1	D	10	ASP
1	D	69	ASP
1	D	93	SER
1	D	173	VAL
1	D	241	LEU
1	D	247	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	A	195	HIS
1	A	215	HIS
1	B	38	GLN
1	B	96	GLN

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Mol	Chain	Res	Type
1	B	167	ASN
1	B	195	HIS
1	B	215	HIS
1	C	139	GLN
1	C	142	HIS
1	C	195	HIS
1	C	215	HIS
1	C	225	GLN
1	C	285	HIS
1	D	38	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

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	263/288 (91%)	-0.05	9 (3%) 49 50	11, 24, 48, 97	0
1	B	265/288 (92%)	0.10	6 (2%) 64 64	14, 30, 49, 67	0
1	C	269/288 (93%)	-0.05	10 (3%) 45 47	11, 22, 44, 65	0
1	D	263/288 (91%)	0.63	30 (11%) 7 7	19, 34, 60, 86	0
All	All	1060/1152 (92%)	0.15	55 (5%) 31 33	11, 28, 53, 97	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	155	PRO	7.5
1	B	154	GLY	6.8
1	D	284	LEU	6.3
1	A	154	GLY	5.9
1	A	139	GLN	5.9
1	C	153	ILE	5.8
1	B	155	PRO	5.4
1	D	154	GLY	5.1
1	D	169	LEU	4.8
1	A	135	ASP	4.7
1	D	223	GLY	4.3
1	D	170	GLN	4.3
1	D	285	HIS	4.1
1	A	136	ILE	3.8
1	A	138	ARG	3.8
1	C	141	SER	3.7
1	D	44	ILE	3.7
1	B	190	ASP	3.4
1	D	190	ASP	3.3
1	D	12	LEU	3.2
1	A	155	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	221	GLU	3.1
1	B	68	GLY	3.0
1	D	220	LEU	2.9
1	D	71	SER	2.8
1	D	69	ASP	2.8
1	C	190	ASP	2.8
1	D	14	LEU	2.7
1	D	222	PRO	2.7
1	C	139	GLN	2.7
1	D	17	ILE	2.7
1	D	134	THR	2.6
1	D	172	SER	2.6
1	D	187	LYS	2.5
1	C	142	HIS	2.5
1	D	43	ALA	2.5
1	D	70	SER	2.5
1	A	187	LYS	2.5
1	C	113	GLU	2.4
1	B	85	ASN	2.4
1	D	47	ALA	2.3
1	D	67	PRO	2.3
1	C	151	LYS	2.2
1	D	27	GLU	2.2
1	C	44	ILE	2.2
1	C	155	PRO	2.2
1	A	4	ALA	2.2
1	D	72	LYS	2.2
1	D	40	VAL	2.1
1	B	71	SER	2.1
1	D	106	ALA	2.1
1	D	138	ARG	2.1
1	C	111	GLN	2.1
1	D	53	ALA	2.1
1	A	190	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.