Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2021 – 05:20 PM EST

PDB ID	:	3I4F
Title	:	Structure of putative 3-oxoacyl-reductase from bacillus thuringiensis
Authors	:	Ramagopal, U.A.; Kim, J.; Toro, R.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2009-07-01
Resolution	:	2.39 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:

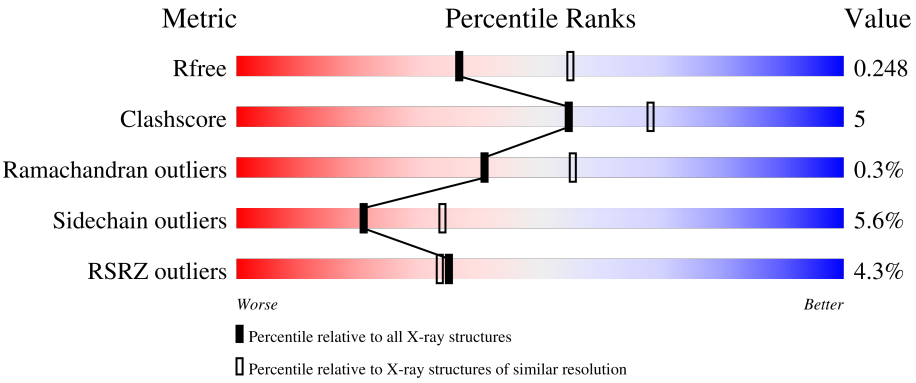
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 of 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	264	4% 76% 14% • 8%
1	B	264	4% 75% 16% • 8%
1	C	264	5% 77% 13% • 9%
1	D	264	3% 78% 13% • 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7541 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 3-oxoacyl-[acyl-carrier protein] reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	1	0
			1865	1186	314	355	10			
1	B	242	Total	C	N	O	S	0	1	0
			1875	1192	314	359	10			
1	C	240	Total	C	N	O	S	0	0	0
			1862	1182	312	358	10			
1	D	242	Total	C	N	O	S	0	0	0
			1879	1192	315	362	10			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	MET	-	expression tag	UNP C3ERL8
A	33	SER	-	expression tag	UNP C3ERL8
A	34	LEU	-	expression tag	UNP C3ERL8
A	35	GLY	-	expression tag	UNP C3ERL8
A	36	ARG	-	expression tag	UNP C3ERL8
A	288	GLU	-	expression tag	UNP C3ERL8
A	289	GLY	-	expression tag	UNP C3ERL8
A	290	HIS	-	expression tag	UNP C3ERL8
A	291	HIS	-	expression tag	UNP C3ERL8
A	292	HIS	-	expression tag	UNP C3ERL8
A	293	HIS	-	expression tag	UNP C3ERL8
A	294	HIS	-	expression tag	UNP C3ERL8
A	295	HIS	-	expression tag	UNP C3ERL8
B	32	MET	-	expression tag	UNP C3ERL8
B	33	SER	-	expression tag	UNP C3ERL8
B	34	LEU	-	expression tag	UNP C3ERL8
B	35	GLY	-	expression tag	UNP C3ERL8
B	36	ARG	-	expression tag	UNP C3ERL8
B	288	GLU	-	expression tag	UNP C3ERL8
B	289	GLY	-	expression tag	UNP C3ERL8
B	290	HIS	-	expression tag	UNP C3ERL8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	291	HIS	-	expression tag	UNP C3ERL8
B	292	HIS	-	expression tag	UNP C3ERL8
B	293	HIS	-	expression tag	UNP C3ERL8
B	294	HIS	-	expression tag	UNP C3ERL8
B	295	HIS	-	expression tag	UNP C3ERL8
C	32	MET	-	expression tag	UNP C3ERL8
C	33	SER	-	expression tag	UNP C3ERL8
C	34	LEU	-	expression tag	UNP C3ERL8
C	35	GLY	-	expression tag	UNP C3ERL8
C	36	ARG	-	expression tag	UNP C3ERL8
C	288	GLU	-	expression tag	UNP C3ERL8
C	289	GLY	-	expression tag	UNP C3ERL8
C	290	HIS	-	expression tag	UNP C3ERL8
C	291	HIS	-	expression tag	UNP C3ERL8
C	292	HIS	-	expression tag	UNP C3ERL8
C	293	HIS	-	expression tag	UNP C3ERL8
C	294	HIS	-	expression tag	UNP C3ERL8
C	295	HIS	-	expression tag	UNP C3ERL8
D	32	MET	-	expression tag	UNP C3ERL8
D	33	SER	-	expression tag	UNP C3ERL8
D	34	LEU	-	expression tag	UNP C3ERL8
D	35	GLY	-	expression tag	UNP C3ERL8
D	36	ARG	-	expression tag	UNP C3ERL8
D	288	GLU	-	expression tag	UNP C3ERL8
D	289	GLY	-	expression tag	UNP C3ERL8
D	290	HIS	-	expression tag	UNP C3ERL8
D	291	HIS	-	expression tag	UNP C3ERL8
D	292	HIS	-	expression tag	UNP C3ERL8
D	293	HIS	-	expression tag	UNP C3ERL8
D	294	HIS	-	expression tag	UNP C3ERL8
D	295	HIS	-	expression tag	UNP C3ERL8

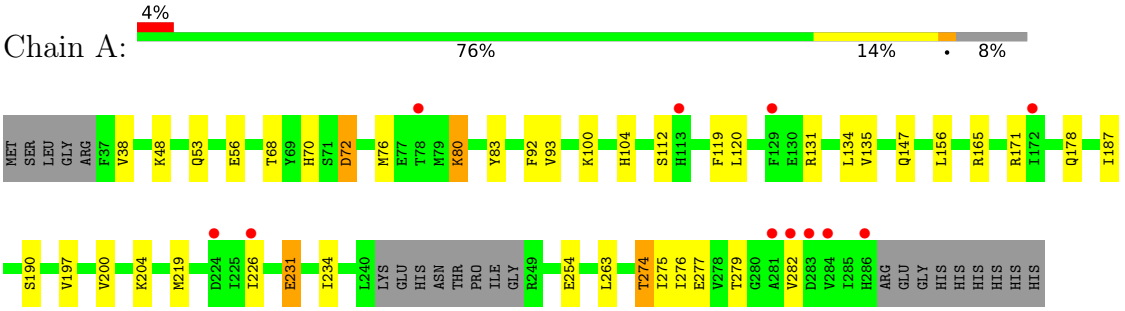
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	18	Total O 18 18	0	0
2	B	19	Total O 19 19	0	0
2	C	10	Total O 10 10	0	0
2	D	13	Total O 13 13	0	0

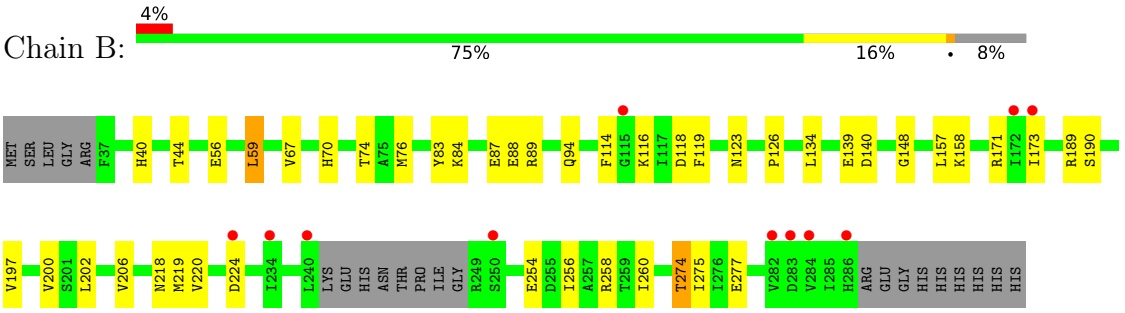
3 Residue-property plots (i)

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.

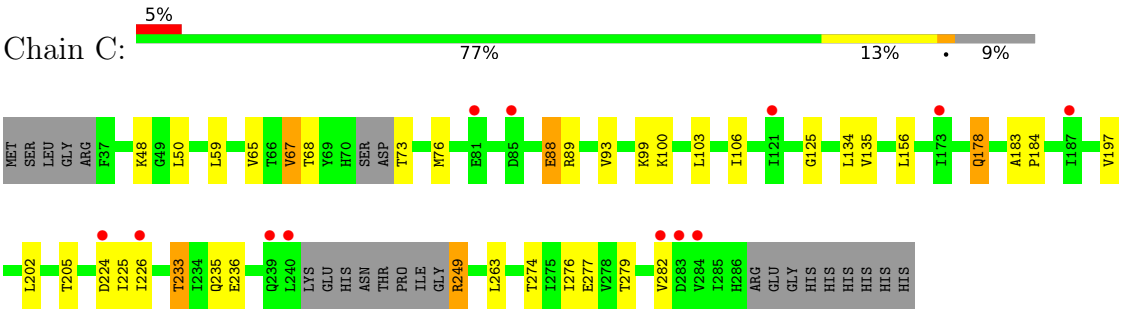
• Molecule 1: 3-oxoacyl-[acyl-carrier protein] reductase



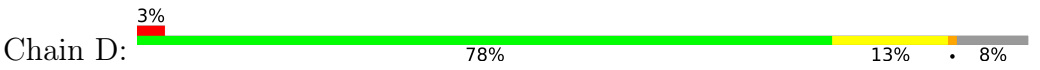
• Molecule 1: 3-oxoacyl-[acyl-carrier protein] reductase

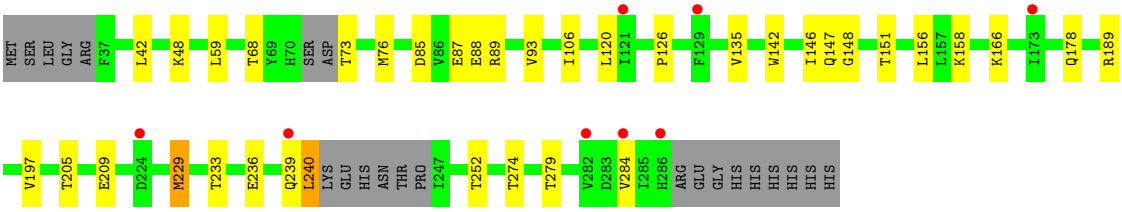


• Molecule 1: 3-oxoacyl-[acyl-carrier protein] reductase



• Molecule 1: 3-oxoacyl-[acyl-carrier protein] reductase




MET SER LEU GLY ARG F37 L42 K48 L59 T68 Y69 H70 SER ASP T73 M76 D85 V86 E87 E88 R89 V93 I106 L120 I121 P126 F129 V135 W142 I146 Q147 G148 T151 L156 L157 K158 K166 I173 Q178 R189
V197 T205 E209 D224 M229 T233 E236 Q239 L240 LYS GLU HIS ASN THR PRO I247 T252 T274 T279 V282 D283 V284 I285 H286 ARG GLU GLY 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	69.42Å 86.59Å 78.41Å 90.00° 97.05° 90.00°	Depositor
Resolution (Å)	27.60 – 2.39 27.06 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.3 (27.60-2.39) 99.3 (27.06-2.39)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.05 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.248 0.193 , 0.248	Depositor DCC
R_{free} test set	1841 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	44.5	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 40.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7541	wwPDB-VP
Average B, all atoms (Å^2)	38.0	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 36.12 % 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 5.2492e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.49	0/1899	0.59	0/2567
1	B	0.50	0/1909	0.57	0/2579
1	C	0.49	0/1891	0.58	0/2553
1	D	0.52	0/1908	0.60	0/2574
All	All	0.50	0/7607	0.58	0/10273

There are no bond length outliers.

There are no bond angle outliers.

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	1865	0	1844	27	0
1	B	1875	0	1856	25	0
1	C	1862	0	1847	25	0
1	D	1879	0	1867	19	0
2	A	18	0	0	0	0
2	B	19	0	0	0	0
2	C	10	0	0	0	0
2	D	13	0	0	0	0
All	All	7541	0	7414	78	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 5.

All (78) 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:B:190:SER:HB3	1:C:205:THR:HG21	1.65	0.78
1:D:239:GLN:O	1:D:240:LEU:HB2	1.84	0.78
1:C:249:ARG:HH21	1:C:249:ARG:HG3	1.48	0.78
1:A:178:GLN:HG3	1:A:279:THR:HG21	1.75	0.69
1:B:134:LEU:CD1	1:C:202:LEU:HD11	2.26	0.65
1:A:56:GLU:HG2	1:A:83:TYR:OH	1.97	0.65
1:A:204:LYS:HE3	1:A:275:ILE:HD11	1.80	0.64
1:A:48:LYS:HE2	1:A:72:ASP:OD2	1.98	0.63
1:B:134:LEU:HD13	1:C:202:LEU:HD11	1.82	0.61
1:B:126:PRO:HG2	1:B:148:GLY:HA3	1.83	0.59
1:A:120:LEU:HD11	1:A:156:LEU:HD13	1.85	0.58
1:B:190:SER:CB	1:C:205:THR:HG21	2.34	0.56
1:B:44:THR:O	1:B:123:ASN:HB3	2.06	0.56
1:B:202:LEU:HD11	1:C:134:LEU:HD22	1.86	0.56
1:B:56:GLU:HG2	1:B:83:TYR:OH	2.05	0.55
1:C:263:LEU:HD11	1:C:276:ILE:HD12	1.89	0.55
1:A:135:VAL:O	1:D:158:LYS:HE3	2.08	0.54
1:A:282:VAL:HG13	1:A:282:VAL:O	2.07	0.53
1:A:190:SER:HB3	1:D:205:THR:HG21	1.90	0.53
1:C:106:ILE:HD11	1:C:156:LEU:HD21	1.91	0.52
1:A:165:ARG:NH2	1:D:135:VAL:HG11	2.23	0.52
1:B:157:LEU:HD13	1:B:206:VAL:HG21	1.91	0.52
1:D:233:THR:HG23	1:D:236:GLU:H	1.76	0.51
1:C:233:THR:CG2	1:C:236:GLU:H	2.24	0.50
1:A:197:VAL:HG12	1:D:197:VAL:HG12	1.93	0.50
1:C:59:LEU:O	1:C:89:ARG:NH2	2.45	0.50
1:D:178:GLN:HB2	1:D:279:THR:HG21	1.93	0.50
1:A:80:LYS:HE3	1:A:92:PHE:CE2	2.47	0.50
1:B:277:GLU:O	1:D:274:THR:HG21	2.11	0.50
1:D:229:MET:HG3	1:D:252:THR:HG22	1.94	0.50
1:B:254:GLU:O	1:B:258:ARG:HG2	2.13	0.49
1:D:120:LEU:HD11	1:D:156:LEU:HD13	1.94	0.49
1:D:42:LEU:HD11	1:D:106:ILE:HD12	1.94	0.48
1:A:274:THR:HG21	1:C:277:GLU:O	2.13	0.48
1:B:116:LYS:HD3	1:B:118:ASP:OD2	2.12	0.48
1:B:197:VAL:HG12	1:C:197:VAL:HG12	1.96	0.48
1:A:277:GLU:HB2	1:C:274:THR:HG22	1.96	0.47
1:B:220:VAL:HG11	1:B:256:ILE:HG23	1.97	0.47
1:A:187:ILE:HG13	1:D:209:GLU:HG2	1.96	0.47
1:C:279:THR:O	1:C:282:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:ARG:NH2	1:C:249:ARG:HG3	2.22	0.46
1:C:103:LEU:O	1:C:106:ILE:HG12	2.16	0.46
1:C:68:THR:HA	1:C:93:VAL:O	2.16	0.45
1:D:233:THR:CG2	1:D:236:GLU:H	2.29	0.45
1:A:80:LYS:HE3	1:A:92:PHE:HE2	1.82	0.45
1:B:173:ILE:HG21	1:B:260:ILE:HG12	1.99	0.45
1:B:40:HIS:CE1	1:B:114:PHE:CD2	3.05	0.45
1:C:183:ALA:N	1:C:184:PRO:HD3	2.32	0.45
1:D:126:PRO:HG2	1:D:148:GLY:HA3	1.99	0.45
1:B:59:LEU:O	1:B:89:ARG:NH2	2.50	0.45
1:B:84:LYS:O	1:B:87:GLU:HG3	2.17	0.45
1:A:100:LYS:HE2	1:A:104[B]:HIS:HE1	1.82	0.44
1:C:178:GLN:HB2	1:C:178:GLN:HE21	1.67	0.44
1:C:65:VAL:HG12	1:C:67:VAL:HG12	1.99	0.44
1:D:59:LEU:O	1:D:89:ARG:NH2	2.50	0.44
1:B:218:ASN:OD1	1:B:274:THR:HG23	2.18	0.44
1:A:204:LYS:HE3	1:A:275:ILE:CD1	2.46	0.44
1:A:274:THR:HG22	1:C:277:GLU:HB2	1.99	0.43
1:D:68:THR:HA	1:D:93:VAL:O	2.18	0.43
1:C:88:GLU:HG2	1:C:89:ARG:N	2.33	0.43
1:A:68:THR:HA	1:A:93:VAL:O	2.19	0.43
1:A:200:VAL:HG22	1:A:219:MET:SD	2.58	0.43
1:B:202:LEU:HD11	1:C:134:LEU:CD2	2.48	0.42
1:A:263:LEU:HD11	1:A:276:ILE:HD12	2.01	0.42
1:A:119:PHE:HD1	1:A:171:ARG:HB2	1.85	0.41
1:B:200:VAL:HG22	1:B:219:MET:SD	2.61	0.41
1:D:142:TRP:O	1:D:146:ILE:HG12	2.20	0.41
1:B:119:PHE:HD1	1:B:171:ARG:HB2	1.85	0.41
1:D:178:GLN:NE2	1:D:284:VAL:H	2.19	0.41
1:B:70:HIS:O	1:B:94:GLN:NE2	2.40	0.41
1:D:147:GLN:HA	1:D:151:THR:HB	2.02	0.41
1:A:134:LEU:HD23	1:A:134:LEU:C	2.41	0.41
1:A:234:ILE:HG13	1:A:254:GLU:HB3	2.01	0.41
1:A:156:LEU:HA	1:A:156:LEU:HD23	1.84	0.41
1:A:277:GLU:O	1:C:274:THR:HG21	2.21	0.40
1:A:53:GLN:NE2	1:A:231:GLU:O	2.55	0.40
1:B:219:MET:HB3	1:B:275:ILE:HG13	2.03	0.40
1:B:158:LYS:HA	1:C:135:VAL: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	239/264 (90%)	229 (96%)	8 (3%)	2 (1%)	19 29
1	B	239/264 (90%)	231 (97%)	8 (3%)	0	100 100
1	C	234/264 (89%)	231 (99%)	2 (1%)	1 (0%)	34 48
1	D	236/264 (89%)	231 (98%)	5 (2%)	0	100 100
All	All	948/1056 (90%)	922 (97%)	23 (2%)	3 (0%)	41 55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	72	ASP
1	C	125	GLY

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	194/221 (88%)	185 (95%)	9 (5%)	27 43
1	B	196/221 (89%)	186 (95%)	10 (5%)	24 39
1	C	196/221 (89%)	181 (92%)	15 (8%)	13 20
1	D	198/221 (90%)	188 (95%)	10 (5%)	24 39
All	All	784/884 (89%)	740 (94%)	44 (6%)	21 34

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	76	MET
1	A	80	LYS
1	A	112	SER
1	A	131	ARG
1	A	147	GLN
1	A	226	ILE
1	A	231	GLU
1	A	274	THR
1	B	59	LEU
1	B	67	VAL
1	B	74	THR
1	B	76	MET
1	B	88	GLU
1	B	139	GLU
1	B	140	ASP
1	B	189	ARG
1	B	224	ASP
1	B	274	THR
1	C	48	LYS
1	C	50	LEU
1	C	67	VAL
1	C	73	THR
1	C	76	MET
1	C	88	GLU
1	C	99	LYS
1	C	100	LYS
1	C	178	GLN
1	C	224	ASP
1	C	225	ILE
1	C	226	ILE
1	C	233	THR
1	C	235	GLN
1	C	249	ARG
1	D	48	LYS
1	D	73	THR
1	D	76	MET
1	D	85	ASP
1	D	87	GLU
1	D	88	GLU
1	D	166	LYS
1	D	189	ARG
1	D	229	MET

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Mol	Chain	Res	Type
1	D	240	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	147	GLN
1	A	286	HIS
1	B	113	HIS
1	B	123	ASN
1	B	147	GLN
1	C	123	ASN
1	C	178	GLN
1	D	70	HIS
1	D	123	ASN
1	D	178	GLN

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)

There are no ligands in this entry.

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	242/264 (91%)	0.31	11 (4%)	33	31	28, 36, 50, 62	0
1	B	242/264 (91%)	0.32	11 (4%)	33	31	29, 38, 53, 70	0
1	C	240/264 (90%)	0.33	12 (5%)	28	27	27, 37, 50, 52	0
1	D	242/264 (91%)	0.27	8 (3%)	46	45	26, 37, 47, 56	0
All	All	966/1056 (91%)	0.31	42 (4%)	35	33	26, 37, 50, 70	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	284	VAL	4.8
1	B	250	SER	4.7
1	B	284	VAL	4.6
1	B	286	HIS	4.2
1	D	282	VAL	4.1
1	C	284	VAL	4.0
1	B	283	ASP	4.0
1	C	226	ILE	3.9
1	D	286	HIS	3.9
1	A	286	HIS	3.7
1	B	224	ASP	3.5
1	A	282	VAL	3.4
1	A	284	VAL	3.3
1	C	85	ASP	3.3
1	D	224	ASP	3.3
1	D	129	PHE	3.3
1	C	240	LEU	3.0
1	C	224	ASP	3.0
1	A	113	HIS	3.0
1	C	283	ASP	2.9
1	D	173	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	239	GLN	2.8
1	A	283	ASP	2.7
1	B	282	VAL	2.6
1	C	187	ILE	2.6
1	A	224	ASP	2.5
1	C	173	ILE	2.5
1	B	240	LEU	2.4
1	C	282	VAL	2.4
1	A	78	THR	2.3
1	A	226	ILE	2.3
1	A	129	PHE	2.3
1	A	172	ILE	2.3
1	B	172	ILE	2.3
1	A	281	ALA	2.3
1	C	239	GLN	2.3
1	D	121	ILE	2.2
1	B	234	ILE	2.2
1	B	115	GLY	2.2
1	C	81	GLU	2.2
1	C	121	ILE	2.2
1	B	173	ILE	2.1

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 monosaccharides 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.