



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:44 PM GMT

PDB ID : 3FTP
Title : Crystal structure of 3-Ketoacyl-(acyl-carrier-protein)reductase from
Burkholderia pseudomallei at 2.05 Å resolution
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2009-01-13
Resolution : 2.05 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

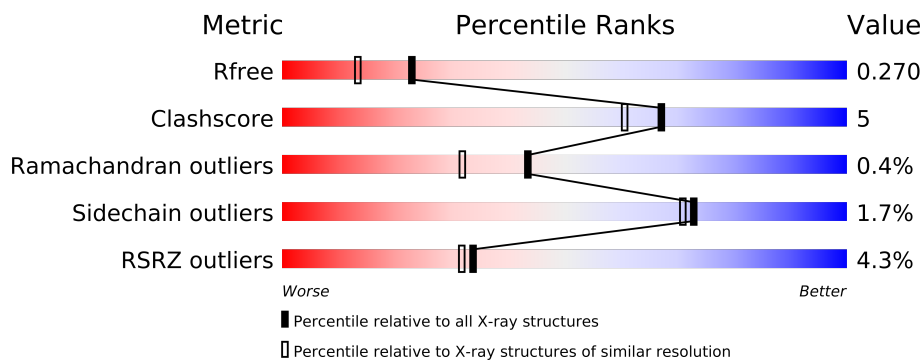
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.05 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}	66092	1380 (2.06-2.02)
Clashscore	79885	1577 (2.06-2.02)
Ramachandran outliers	78287	1565 (2.06-2.02)
Sidechain outliers	78261	1565 (2.06-2.02)
RSRZ outliers	66119	1381 (2.06-2.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	270	
1	B	270	
1	C	270	
1	D	270	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7369 atoms, of which 0 are hydrogen and 0 are deuterium.

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-carrierprotein] reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1735	1077	316	333	9			
1	B	248	Total	C	N	O	S	0	0	0
			1748	1084	319	337	8			
1	C	244	Total	C	N	O	S	0	0	0
			1704	1057	312	327	8			
1	D	241	Total	C	N	O	S	0	0	0
			1702	1057	310	327	8			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP Q63S85
A	-19	ALA	-	EXPRESSION TAG	UNP Q63S85
A	-18	HIS	-	EXPRESSION TAG	UNP Q63S85
A	-17	HIS	-	EXPRESSION TAG	UNP Q63S85
A	-16	HIS	-	EXPRESSION TAG	UNP Q63S85
A	-15	HIS	-	EXPRESSION TAG	UNP Q63S85
A	-14	HIS	-	EXPRESSION TAG	UNP Q63S85
A	-13	HIS	-	EXPRESSION TAG	UNP Q63S85
A	-12	MET	-	EXPRESSION TAG	UNP Q63S85
A	-11	GLY	-	EXPRESSION TAG	UNP Q63S85
A	-10	THR	-	EXPRESSION TAG	UNP Q63S85
A	-9	LEU	-	EXPRESSION TAG	UNP Q63S85
A	-8	GLU	-	EXPRESSION TAG	UNP Q63S85
A	-7	ALA	-	EXPRESSION TAG	UNP Q63S85
A	-6	GLN	-	EXPRESSION TAG	UNP Q63S85
A	-5	THR	-	EXPRESSION TAG	UNP Q63S85
A	-4	GLN	-	EXPRESSION TAG	UNP Q63S85
A	-3	GLY	-	EXPRESSION TAG	UNP Q63S85
A	-2	PRO	-	EXPRESSION TAG	UNP Q63S85
A	-1	GLY	-	EXPRESSION TAG	UNP Q63S85
A	0	SER	-	EXPRESSION TAG	UNP Q63S85

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	EXPRESSION TAG	UNP Q63S85
B	-19	ALA	-	EXPRESSION TAG	UNP Q63S85
B	-18	HIS	-	EXPRESSION TAG	UNP Q63S85
B	-17	HIS	-	EXPRESSION TAG	UNP Q63S85
B	-16	HIS	-	EXPRESSION TAG	UNP Q63S85
B	-15	HIS	-	EXPRESSION TAG	UNP Q63S85
B	-14	HIS	-	EXPRESSION TAG	UNP Q63S85
B	-13	HIS	-	EXPRESSION TAG	UNP Q63S85
B	-12	MET	-	EXPRESSION TAG	UNP Q63S85
B	-11	GLY	-	EXPRESSION TAG	UNP Q63S85
B	-10	THR	-	EXPRESSION TAG	UNP Q63S85
B	-9	LEU	-	EXPRESSION TAG	UNP Q63S85
B	-8	GLU	-	EXPRESSION TAG	UNP Q63S85
B	-7	ALA	-	EXPRESSION TAG	UNP Q63S85
B	-6	GLN	-	EXPRESSION TAG	UNP Q63S85
B	-5	THR	-	EXPRESSION TAG	UNP Q63S85
B	-4	GLN	-	EXPRESSION TAG	UNP Q63S85
B	-3	GLY	-	EXPRESSION TAG	UNP Q63S85
B	-2	PRO	-	EXPRESSION TAG	UNP Q63S85
B	-1	GLY	-	EXPRESSION TAG	UNP Q63S85
B	0	SER	-	EXPRESSION TAG	UNP Q63S85
C	-20	MET	-	EXPRESSION TAG	UNP Q63S85
C	-19	ALA	-	EXPRESSION TAG	UNP Q63S85
C	-18	HIS	-	EXPRESSION TAG	UNP Q63S85
C	-17	HIS	-	EXPRESSION TAG	UNP Q63S85
C	-16	HIS	-	EXPRESSION TAG	UNP Q63S85
C	-15	HIS	-	EXPRESSION TAG	UNP Q63S85
C	-14	HIS	-	EXPRESSION TAG	UNP Q63S85
C	-13	HIS	-	EXPRESSION TAG	UNP Q63S85
C	-12	MET	-	EXPRESSION TAG	UNP Q63S85
C	-11	GLY	-	EXPRESSION TAG	UNP Q63S85
C	-10	THR	-	EXPRESSION TAG	UNP Q63S85
C	-9	LEU	-	EXPRESSION TAG	UNP Q63S85
C	-8	GLU	-	EXPRESSION TAG	UNP Q63S85
C	-7	ALA	-	EXPRESSION TAG	UNP Q63S85
C	-6	GLN	-	EXPRESSION TAG	UNP Q63S85
C	-5	THR	-	EXPRESSION TAG	UNP Q63S85
C	-4	GLN	-	EXPRESSION TAG	UNP Q63S85
C	-3	GLY	-	EXPRESSION TAG	UNP Q63S85
C	-2	PRO	-	EXPRESSION TAG	UNP Q63S85
C	-1	GLY	-	EXPRESSION TAG	UNP Q63S85
C	0	SER	-	EXPRESSION TAG	UNP Q63S85

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	EXPRESSION TAG	UNP Q63S85
D	-19	ALA	-	EXPRESSION TAG	UNP Q63S85
D	-18	HIS	-	EXPRESSION TAG	UNP Q63S85
D	-17	HIS	-	EXPRESSION TAG	UNP Q63S85
D	-16	HIS	-	EXPRESSION TAG	UNP Q63S85
D	-15	HIS	-	EXPRESSION TAG	UNP Q63S85
D	-14	HIS	-	EXPRESSION TAG	UNP Q63S85
D	-13	HIS	-	EXPRESSION TAG	UNP Q63S85
D	-12	MET	-	EXPRESSION TAG	UNP Q63S85
D	-11	GLY	-	EXPRESSION TAG	UNP Q63S85
D	-10	THR	-	EXPRESSION TAG	UNP Q63S85
D	-9	LEU	-	EXPRESSION TAG	UNP Q63S85
D	-8	GLU	-	EXPRESSION TAG	UNP Q63S85
D	-7	ALA	-	EXPRESSION TAG	UNP Q63S85
D	-6	GLN	-	EXPRESSION TAG	UNP Q63S85
D	-5	THR	-	EXPRESSION TAG	UNP Q63S85
D	-4	GLN	-	EXPRESSION TAG	UNP Q63S85
D	-3	GLY	-	EXPRESSION TAG	UNP Q63S85
D	-2	PRO	-	EXPRESSION TAG	UNP Q63S85
D	-1	GLY	-	EXPRESSION TAG	UNP Q63S85
D	0	SER	-	EXPRESSION TAG	UNP Q63S85

- Molecule 2 is water.

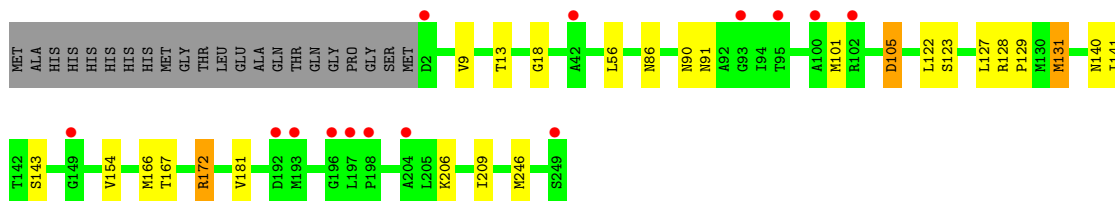
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	111	Total 111	O 111	0	0
2	B	140	Total 140	O 140	0	0
2	C	108	Total 108	O 108	0	0
2	D	121	Total 121	O 121	0	0

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.

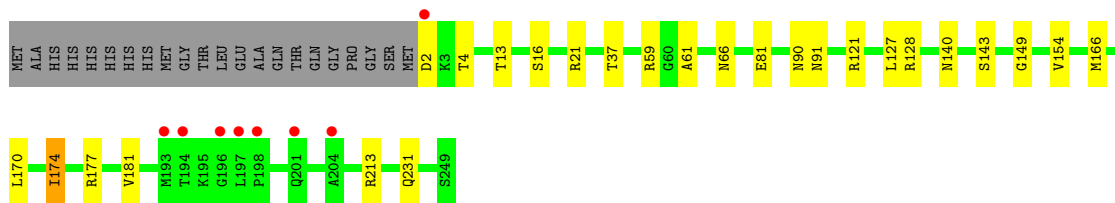
- Molecule 1: 3-oxoacyl-[acyl-carrierprotein] reductase

Chain A: 



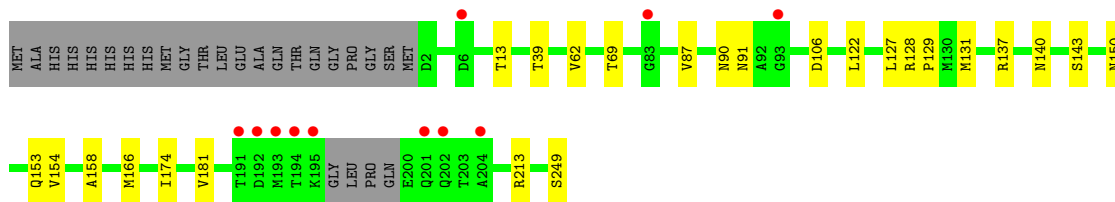
- Molecule 1: 3-oxoacyl-[acyl-carrierprotein] reductase

Chain B: 



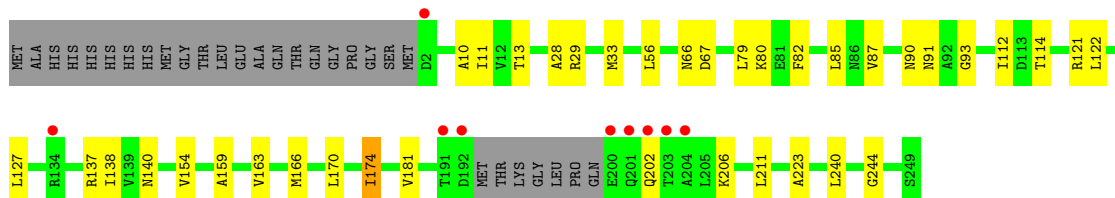
- Molecule 1: 3-oxoacyl-[acyl-carrierprotein] reductase

Chain C: 



- Molecule 1: 3-oxoacyl-[acyl-carrierprotein] reductase

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.62Å 89.90Å 120.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.68 – 2.05 19.68 – 2.05	Depositor EDS
% Data completeness (in resolution range)	88.9 (19.68-2.05) 88.9 (19.68-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.67 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.208 , 0.268 0.211 , 0.270	Depositor DCC
R_{free} test set	2690 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.8	EDS
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 52958 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7369	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

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	0.70	0/1753	0.75	2/2380 (0.1%)
1	B	0.74	0/1766	0.79	0/2396
1	C	0.73	0/1720	0.74	0/2333
1	D	0.72	0/1718	0.76	1/2328 (0.0%)
All	All	0.72	0/6957	0.76	3/9437 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	29	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	172	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	172	ARG	NE-CZ-NH1	5.13	122.87	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1735	0	1729	16	0
1	B	1748	0	1749	20	0
1	C	1704	0	1688	16	0
1	D	1702	0	1711	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	111	0	0	1	0
2	B	140	0	0	6	0
2	C	108	0	0	4	0
2	D	121	0	0	2	0
All	All	7369	0	6877	69	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (69) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:128:ARG:NH2	2:C:460:HOH:O	2.13	0.80
1:A:9:VAL:H	1:A:86:ASN:HD22	1.30	0.76
1:D:93:GLY:HA2	1:D:114:THR:HG22	1.75	0.68
1:D:28:ALA:HB3	1:D:56:LEU:HD13	1.75	0.68
1:C:150:ASN:HD22	1:C:153:GLN:HE21	1.43	0.66
1:B:16:SER:O	1:B:21:ARG:NH2	2.29	0.66
1:C:213:ARG:NH1	2:C:471:HOH:O	2.20	0.62
1:D:11:ILE:HD12	1:D:85:LEU:HD11	1.81	0.61
1:C:39:THR:O	1:C:62:VAL:HG13	2.02	0.59
1:A:167:THR:HG23	1:A:181:VAL:HG12	1.83	0.59
1:A:127:LEU:O	1:A:131:MET:HB2	2.04	0.57
1:D:87:VAL:HG22	1:D:137:ARG:HB2	1.86	0.57
1:C:13:THR:O	1:C:91:ASN:HB3	2.05	0.57
1:B:213:ARG:NH1	2:B:280:HOH:O	2.27	0.57
1:D:174:ILE:HD11	1:D:181:VAL:CG2	2.35	0.56
1:C:90:ASN:HB2	1:C:140:ASN:HD22	1.71	0.56
1:B:174:ILE:HD11	1:B:181:VAL:HG23	1.88	0.55
1:A:123:SER:O	1:A:127:LEU:HG	2.06	0.55
1:A:166:MET:HG3	1:B:154:VAL:HG13	1.88	0.55
1:A:166:MET:HG3	1:B:154:VAL:CG1	2.37	0.53
1:B:21:ARG:NH1	2:B:274:HOH:O	2.40	0.53
1:B:4:THR:CG2	1:B:231:GLN:HE22	2.20	0.53
1:D:127:LEU:HD11	1:D:170:LEU:HD11	1.90	0.53
1:C:106:ASP:HB3	2:C:295:HOH:O	2.08	0.52
1:B:90:ASN:HB2	1:B:140:ASN:HD22	1.74	0.52
1:C:166:MET:HG3	1:D:154:VAL:HG13	1.91	0.52
1:A:90:ASN:HB2	1:A:140:ASN:HD22	1.75	0.52
1:B:231:GLN:NE2	2:B:322:HOH:O	2.41	0.52
1:B:4:THR:HG22	1:B:231:GLN:HE22	1.76	0.51
1:A:206:LYS:HA	1:A:209:ILE:HD12	1.93	0.51
1:D:66:ASN:O	1:D:121:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:154:VAL:HG13	1:D:166:MET:HG3	1.93	0.51
1:A:101:MET:HE1	1:B:128:ARG:HA	1.95	0.47
1:B:59:ARG:NH1	1:B:81:GLU:OE2	2.35	0.47
1:C:174:ILE:HD11	1:C:181:VAL:CG2	2.44	0.47
1:D:211:LEU:HD12	1:D:244:GLY:HA2	1.97	0.47
1:B:127:LEU:HD11	1:B:170:LEU:HD23	1.96	0.46
1:C:127:LEU:O	1:C:131:MET:HE2	2.15	0.46
1:D:79:LEU:O	1:D:80:LYS:C	2.51	0.46
1:D:170:LEU:HG	1:D:174:ILE:HD13	1.97	0.46
1:D:138:ILE:HB	1:D:181:VAL:HG13	1.98	0.46
1:A:105:ASP:OD2	1:B:121:ARG:NH2	2.49	0.45
1:D:13:THR:O	1:D:91:ASN:HB3	2.16	0.45
1:A:91:ASN:HD22	1:A:141:ILE:HB	1.82	0.45
1:D:10:ALA:HA	1:D:87:VAL:O	2.17	0.44
1:A:13:THR:O	1:A:91:ASN:HB3	2.16	0.44
1:C:87:VAL:HG22	1:C:137:ARG:HB2	1.98	0.44
1:A:128:ARG:HB2	1:A:129:PRO:CD	2.48	0.44
1:D:90:ASN:HB2	1:D:140:ASN:HD22	1.83	0.43
1:D:67:ASP:OD1	1:D:67:ASP:C	2.57	0.43
1:C:150:ASN:HD22	1:C:153:GLN:NE2	2.14	0.43
1:C:128:ARG:HB2	1:C:129:PRO:CD	2.49	0.43
1:B:166:MET:HG3	1:B:170:LEU:CD1	2.49	0.43
1:B:13:THR:O	1:B:91:ASN:HB3	2.19	0.43
1:D:66:ASN:ND2	2:D:314:HOH:O	2.41	0.42
1:D:33:MET:HG2	1:D:82:PHE:CE1	2.54	0.42
1:B:37:THR:HA	1:B:61:ALA:O	2.19	0.42
1:B:2:ASP:N	2:B:503:HOH:O	2.52	0.42
1:D:223:ALA:HB1	1:D:240:LEU:HD23	2.01	0.42
1:B:66:ASN:ND2	2:B:343:HOH:O	2.28	0.42
1:D:159:ALA:O	1:D:163:VAL:HG23	2.19	0.42
1:C:158:ALA:HB2	1:D:166:MET:HB2	2.01	0.42
1:A:56:LEU:O	2:A:400:HOH:O	2.22	0.41
1:D:28:ALA:CB	1:D:56:LEU:HD13	2.48	0.41
1:A:154:VAL:HG23	2:B:409:HOH:O	2.21	0.40
1:D:202:GLN:O	1:D:206:LYS:HG3	2.21	0.40
1:A:172:ARG:NH1	1:B:149:GLY:O	2.54	0.40
1:D:121:ARG:HD2	2:D:267:HOH:O	2.21	0.40
1:C:249:SER:HA	2:C:317:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	246/270 (91%)	231 (94%)	13 (5%)	2 (1%)	27	14
1	B	246/270 (91%)	233 (95%)	12 (5%)	1 (0%)	43	32
1	C	240/270 (89%)	231 (96%)	8 (3%)	1 (0%)	43	32
1	D	237/270 (88%)	224 (94%)	13 (6%)	0	100	100
All	All	969/1080 (90%)	919 (95%)	46 (5%)	4 (0%)	43	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	GLY
1	B	143	SER
1	A	143	SER
1	C	143	SER

5.3.2 Protein sidechains ⓘ

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	165/197 (84%)	161 (98%)	4 (2%)	61	57
1	B	168/197 (85%)	166 (99%)	2 (1%)	82	81
1	C	160/197 (81%)	158 (99%)	2 (1%)	80	79
1	D	164/197 (83%)	161 (98%)	3 (2%)	71	68
All	All	657/788 (83%)	646 (98%)	11 (2%)	73	71

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ASP
1	A	122	LEU
1	A	131	MET
1	A	246	MET
1	B	174	ILE
1	B	177	ARG
1	C	69	THR
1	C	122	LEU
1	D	112	ILE
1	D	122	LEU
1	D	174	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	86	ASN
1	A	90	ASN
1	A	91	ASN
1	A	140	ASN
1	B	8	GLN
1	B	53	GLN
1	B	90	ASN
1	B	91	ASN
1	B	140	ASN
1	B	202	GLN
1	C	66	ASN
1	C	90	ASN
1	C	140	ASN
1	C	153	GLN
1	D	66	ASN
1	D	90	ASN
1	D	140	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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, 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(Å ²)	Q<0.9
1	A	248/270 (91%)	0.35	14 (5%) 24 22	18, 33, 52, 64	0
1	B	248/270 (91%)	0.16	8 (3%) 45 45	17, 27, 46, 62	0
1	C	244/270 (90%)	0.19	11 (4%) 32 30	17, 31, 47, 65	0
1	D	241/270 (89%)	0.28	9 (3%) 39 39	18, 31, 46, 63	0
All	All	981/1080 (90%)	0.25	42 (4%) 34 32	17, 30, 50, 65	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	196	GLY	5.5
1	C	193	MET	4.9
1	D	192	ASP	4.9
1	A	102	ARG	4.8
1	B	193	MET	4.8
1	D	200	GLU	4.6
1	C	201	GLN	4.1
1	D	201	GLN	4.1
1	B	194	THR	4.0
1	C	192	ASP	3.6
1	A	197	LEU	3.4
1	A	196	GLY	3.4
1	D	2	ASP	3.4
1	A	149	GLY	3.1
1	D	191	THR	3.1
1	B	198	PRO	3.0
1	C	204	ALA	2.9
1	D	203	THR	2.9
1	C	195	LYS	2.8
1	C	194	THR	2.8
1	A	95	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	192	ASP	2.6
1	B	2	ASP	2.6
1	D	204	ALA	2.6
1	B	204	ALA	2.6
1	A	204	ALA	2.6
1	A	100	ALA	2.5
1	A	249	SER	2.5
1	A	198	PRO	2.5
1	B	197	LEU	2.4
1	C	191	THR	2.4
1	C	83	GLY	2.2
1	B	201	GLN	2.2
1	A	193	MET	2.2
1	C	202	GLN	2.2
1	D	202	GLN	2.2
1	C	93	GLY	2.1
1	A	42	ALA	2.1
1	C	6	ASP	2.1
1	D	134	ARG	2.1
1	A	93	GLY	2.0
1	A	2	ASP	2.0

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 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.