Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:51 PM GMT

PDB ID	:	3V8B
Title	:	Crystal Structure of a 3-ketoacyl-ACP reductase from Sinorhizobium meliloti 1021
Authors	:	Kumaran, D.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; Lafleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on	:	2011-12-22
Resolution	:	2.70 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:

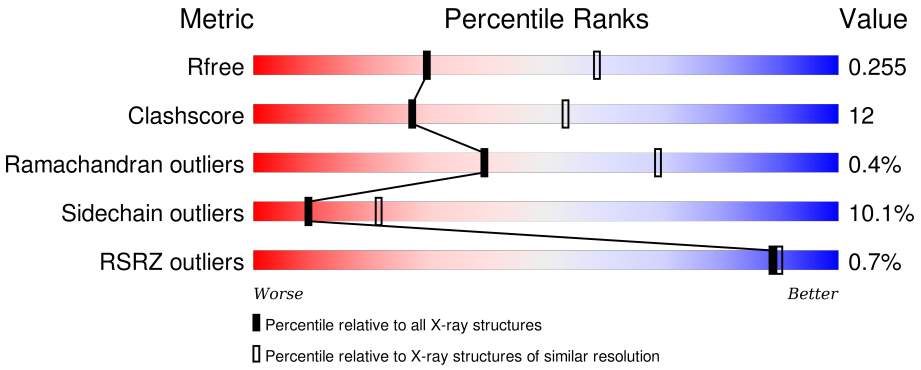
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	283	65% 23% • 9%
1	B	283	68% 18% 5% 9%
1	C	283	67% 19% • 10%
1	D	283	2% 62% 24% • 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7663 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 Putative dehydrogenase, possibly 3-oxoacyl-[acyl-carrier protein] reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	Se	0	0	0
			1908	1198	342	366	1	1			
1	B	257	Total	C	N	O	S	Se	0	0	0
			1908	1198	342	366	1	1			
1	C	255	Total	C	N	O	S	Se	0	0	0
			1895	1190	340	363	1	1			
1	D	256	Total	C	N	O	S	Se	0	0	0
			1901	1193	341	365	1	1			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MSE	-	EXPRESSION TAG	UNP Q92U42
A	-21	HIS	-	EXPRESSION TAG	UNP Q92U42
A	-20	HIS	-	EXPRESSION TAG	UNP Q92U42
A	-19	HIS	-	EXPRESSION TAG	UNP Q92U42
A	-18	HIS	-	EXPRESSION TAG	UNP Q92U42
A	-17	HIS	-	EXPRESSION TAG	UNP Q92U42
A	-16	HIS	-	EXPRESSION TAG	UNP Q92U42
A	-15	SER	-	EXPRESSION TAG	UNP Q92U42
A	-14	SER	-	EXPRESSION TAG	UNP Q92U42
A	-13	GLY	-	EXPRESSION TAG	UNP Q92U42
A	-12	VAL	-	EXPRESSION TAG	UNP Q92U42
A	-11	ASP	-	EXPRESSION TAG	UNP Q92U42
A	-10	LEU	-	EXPRESSION TAG	UNP Q92U42
A	-9	GLY	-	EXPRESSION TAG	UNP Q92U42
A	-8	THR	-	EXPRESSION TAG	UNP Q92U42
A	-7	GLU	-	EXPRESSION TAG	UNP Q92U42
A	-6	ASN	-	EXPRESSION TAG	UNP Q92U42
A	-5	LEU	-	EXPRESSION TAG	UNP Q92U42
A	-4	TYR	-	EXPRESSION TAG	UNP Q92U42
A	-3	PHE	-	EXPRESSION TAG	UNP Q92U42

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLN	-	EXPRESSION TAG	UNP Q92U42
A	-1	SER	-	EXPRESSION TAG	UNP Q92U42
A	0	MSE	-	EXPRESSION TAG	UNP Q92U42
B	-22	MSE	-	EXPRESSION TAG	UNP Q92U42
B	-21	HIS	-	EXPRESSION TAG	UNP Q92U42
B	-20	HIS	-	EXPRESSION TAG	UNP Q92U42
B	-19	HIS	-	EXPRESSION TAG	UNP Q92U42
B	-18	HIS	-	EXPRESSION TAG	UNP Q92U42
B	-17	HIS	-	EXPRESSION TAG	UNP Q92U42
B	-16	HIS	-	EXPRESSION TAG	UNP Q92U42
B	-15	SER	-	EXPRESSION TAG	UNP Q92U42
B	-14	SER	-	EXPRESSION TAG	UNP Q92U42
B	-13	GLY	-	EXPRESSION TAG	UNP Q92U42
B	-12	VAL	-	EXPRESSION TAG	UNP Q92U42
B	-11	ASP	-	EXPRESSION TAG	UNP Q92U42
B	-10	LEU	-	EXPRESSION TAG	UNP Q92U42
B	-9	GLY	-	EXPRESSION TAG	UNP Q92U42
B	-8	THR	-	EXPRESSION TAG	UNP Q92U42
B	-7	GLU	-	EXPRESSION TAG	UNP Q92U42
B	-6	ASN	-	EXPRESSION TAG	UNP Q92U42
B	-5	LEU	-	EXPRESSION TAG	UNP Q92U42
B	-4	TYR	-	EXPRESSION TAG	UNP Q92U42
B	-3	PHE	-	EXPRESSION TAG	UNP Q92U42
B	-2	GLN	-	EXPRESSION TAG	UNP Q92U42
B	-1	SER	-	EXPRESSION TAG	UNP Q92U42
B	0	MSE	-	EXPRESSION TAG	UNP Q92U42
C	-22	MSE	-	EXPRESSION TAG	UNP Q92U42
C	-21	HIS	-	EXPRESSION TAG	UNP Q92U42
C	-20	HIS	-	EXPRESSION TAG	UNP Q92U42
C	-19	HIS	-	EXPRESSION TAG	UNP Q92U42
C	-18	HIS	-	EXPRESSION TAG	UNP Q92U42
C	-17	HIS	-	EXPRESSION TAG	UNP Q92U42
C	-16	HIS	-	EXPRESSION TAG	UNP Q92U42
C	-15	SER	-	EXPRESSION TAG	UNP Q92U42
C	-14	SER	-	EXPRESSION TAG	UNP Q92U42
C	-13	GLY	-	EXPRESSION TAG	UNP Q92U42
C	-12	VAL	-	EXPRESSION TAG	UNP Q92U42
C	-11	ASP	-	EXPRESSION TAG	UNP Q92U42
C	-10	LEU	-	EXPRESSION TAG	UNP Q92U42
C	-9	GLY	-	EXPRESSION TAG	UNP Q92U42
C	-8	THR	-	EXPRESSION TAG	UNP Q92U42
C	-7	GLU	-	EXPRESSION TAG	UNP Q92U42

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	ASN	-	EXPRESSION TAG	UNP Q92U42
C	-5	LEU	-	EXPRESSION TAG	UNP Q92U42
C	-4	TYR	-	EXPRESSION TAG	UNP Q92U42
C	-3	PHE	-	EXPRESSION TAG	UNP Q92U42
C	-2	GLN	-	EXPRESSION TAG	UNP Q92U42
C	-1	SER	-	EXPRESSION TAG	UNP Q92U42
C	0	MSE	-	EXPRESSION TAG	UNP Q92U42
D	-22	MSE	-	EXPRESSION TAG	UNP Q92U42
D	-21	HIS	-	EXPRESSION TAG	UNP Q92U42
D	-20	HIS	-	EXPRESSION TAG	UNP Q92U42
D	-19	HIS	-	EXPRESSION TAG	UNP Q92U42
D	-18	HIS	-	EXPRESSION TAG	UNP Q92U42
D	-17	HIS	-	EXPRESSION TAG	UNP Q92U42
D	-16	HIS	-	EXPRESSION TAG	UNP Q92U42
D	-15	SER	-	EXPRESSION TAG	UNP Q92U42
D	-14	SER	-	EXPRESSION TAG	UNP Q92U42
D	-13	GLY	-	EXPRESSION TAG	UNP Q92U42
D	-12	VAL	-	EXPRESSION TAG	UNP Q92U42
D	-11	ASP	-	EXPRESSION TAG	UNP Q92U42
D	-10	LEU	-	EXPRESSION TAG	UNP Q92U42
D	-9	GLY	-	EXPRESSION TAG	UNP Q92U42
D	-8	THR	-	EXPRESSION TAG	UNP Q92U42
D	-7	GLU	-	EXPRESSION TAG	UNP Q92U42
D	-6	ASN	-	EXPRESSION TAG	UNP Q92U42
D	-5	LEU	-	EXPRESSION TAG	UNP Q92U42
D	-4	TYR	-	EXPRESSION TAG	UNP Q92U42
D	-3	PHE	-	EXPRESSION TAG	UNP Q92U42
D	-2	GLN	-	EXPRESSION TAG	UNP Q92U42
D	-1	SER	-	EXPRESSION TAG	UNP Q92U42
D	0	MSE	-	EXPRESSION TAG	UNP Q92U42

- Molecule 2 is water.

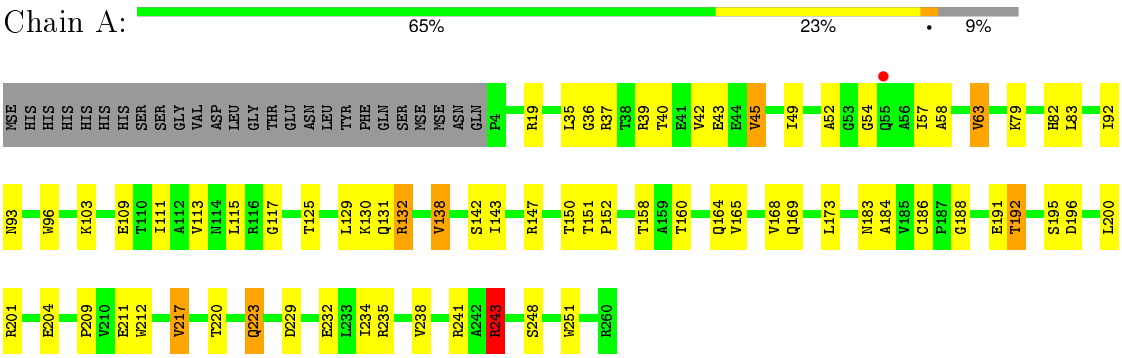
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	11	Total O 11 11	0	0
2	B	16	Total O 16 16	0	0
2	C	9	Total O 9 9	0	0
2	D	15	Total O 15 15	0	0

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.

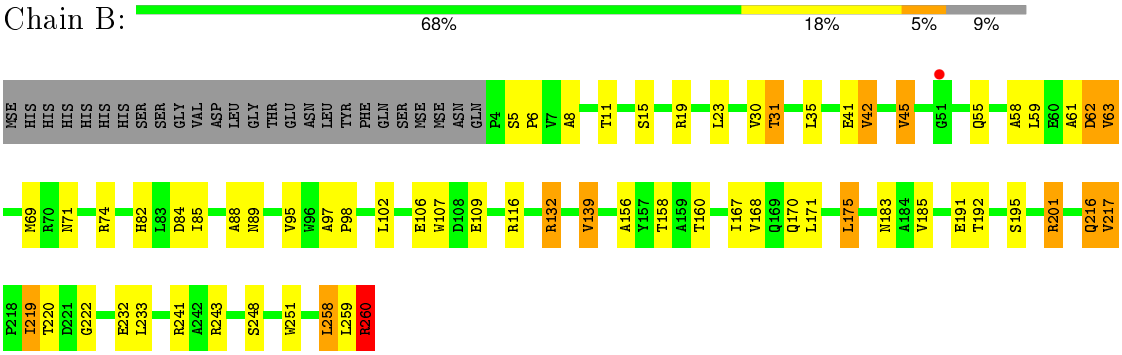
- Molecule 1: Putative dehydrogenase, possibly 3-oxoacyl-[acyl-carrier protein] reductase

Chain A:



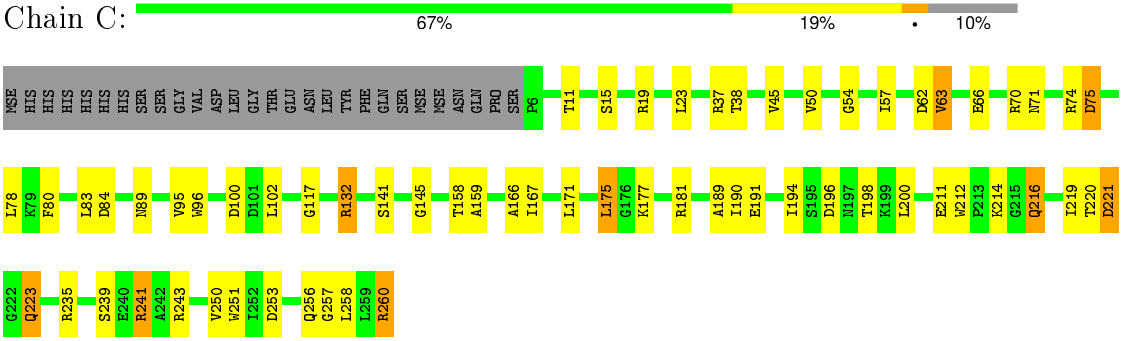
- Molecule 1: Putative dehydrogenase, possibly 3-oxoacyl-[acyl-carrier protein] reductase

Chain B:



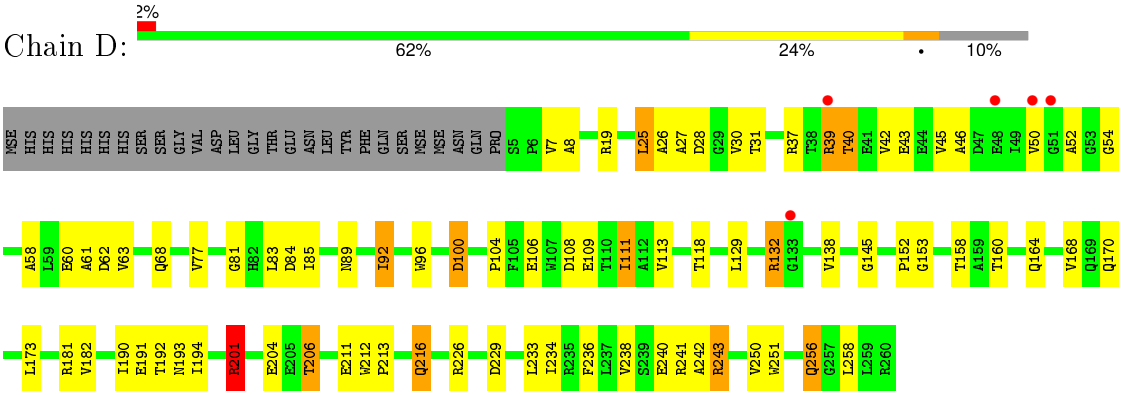
- Molecule 1: Putative dehydrogenase, possibly 3-oxoacyl-[acyl-carrier protein] reductase

Chain C:



• Molecule 1: Putative dehydrogenase, possibly 3-oxoacyl-[acyl-carrier protein] reductase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	114.79Å 143.92Å 66.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.92 – 2.70 48.92 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.92-2.70) 99.8 (48.92-2.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.59 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.187 , 0.255 0.188 , 0.255	Depositor DCC
R_{free} test set	1570 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	36.3	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 33.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 31060 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7663	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% 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	0.69	1/1939 (0.1%)	0.82	3/2643 (0.1%)
1	B	0.72	2/1939 (0.1%)	0.87	3/2643 (0.1%)
1	C	0.69	1/1925 (0.1%)	0.83	1/2623 (0.0%)
1	D	0.69	3/1931 (0.2%)	0.84	3/2632 (0.1%)
All	All	0.70	7/7734 (0.1%)	0.84	10/10541 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	251	TRP	CD2-CE2	6.40	1.49	1.41
1	B	251	TRP	CD2-CE2	5.62	1.48	1.41
1	D	212	TRP	CD2-CE2	5.56	1.48	1.41
1	C	251	TRP	CD2-CE2	5.55	1.48	1.41
1	D	96	TRP	CD2-CE2	5.32	1.47	1.41
1	B	107	TRP	CD2-CE2	5.31	1.47	1.41
1	A	212	TRP	CD2-CE2	5.09	1.47	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	243	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	B	260	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	D	201	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	D	108	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	116	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	A	52	ALA	N-CA-C	-5.22	96.91	111.00
1	D	256	GLN	C-N-CA	-5.20	111.38	122.30
1	C	62	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	A	147	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	B	201	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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	1908	0	1928	45	0
1	B	1908	0	1928	52	0
1	C	1895	0	1916	37	0
1	D	1901	0	1920	64	0
2	A	11	0	0	0	0
2	B	16	0	0	0	0
2	C	9	0	0	0	0
2	D	15	0	0	0	0
All	All	7663	0	7692	183	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 12.

All (183) 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:260:ARG:HG2	1:C:260:ARG:HH11	1.23	0.98
1:D:118:THR:HG21	1:D:164:GLN:HE21	1.26	0.97
1:B:31:THR:HB	1:B:55:GLN:HB2	1.42	0.97
1:B:260:ARG:HH11	1:B:260:ARG:HG2	1.29	0.96
1:B:35:LEU:HD21	1:B:69:MSE:HE1	1.46	0.94
1:A:158:THR:HG21	1:D:170:GLN:HG3	1.50	0.93
1:C:84:ASP:OD1	1:C:132:ARG:HD3	1.77	0.84
1:A:200:LEU:HD12	1:A:201:ARG:H	1.45	0.82
1:A:57:ILE:HG21	1:A:79:LYS:HD3	1.62	0.82
1:D:25:LEU:O	1:D:30:VAL:HB	1.80	0.80
1:D:118:THR:HG21	1:D:164:GLN:NE2	1.96	0.80
1:B:61:ALA:CB	1:B:69:MSE:HE2	2.16	0.76
1:B:61:ALA:HB1	1:B:69:MSE:HE2	1.68	0.75
1:A:243:ARG:HG2	1:A:243:ARG:HH11	1.54	0.73
1:D:26:ALA:O	1:D:28:ASP:N	2.20	0.73
1:D:233:LEU:HD21	1:D:250:VAL:HG13	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LEU:HD11	1:B:258:LEU:HB3	1.71	0.72
1:D:92:ILE:HD11	1:D:113:VAL:HG21	1.73	0.70
1:D:152:PRO:CB	1:D:206:THR:HG22	2.22	0.69
1:C:260:ARG:HG2	1:C:260:ARG:NH1	1.99	0.69
1:B:132:ARG:O	1:B:132:ARG:HG3	1.94	0.67
1:C:260:ARG:CG	1:C:260:ARG:HH11	2.03	0.67
1:D:42:VAL:HG23	1:D:58:ALA:HB1	1.78	0.66
1:B:167:ILE:HD11	1:C:159:ALA:HB2	1.77	0.66
1:D:26:ALA:C	1:D:28:ASP:H	1.99	0.65
1:D:152:PRO:HB2	1:D:206:THR:HG22	1.79	0.65
1:A:183:ASN:HD22	1:A:248:SER:H	1.44	0.64
1:B:260:ARG:NH1	1:B:260:ARG:HG2	2.08	0.64
1:B:71:ASN:ND2	1:B:74:ARG:NH2	2.46	0.64
1:B:88:ALA:HB3	1:B:139:VAL:HB	1.80	0.62
1:C:66:GLU:O	1:C:70:ARG:HG3	1.99	0.62
1:B:216:GLN:OE1	1:B:260:ARG:HD2	2.00	0.62
1:B:71:ASN:HD22	1:B:74:ARG:NH2	1.98	0.61
1:B:156:ALA:O	1:B:160:THR:HG23	2.00	0.61
1:C:19:ARG:HG3	1:C:45:VAL:HG21	1.83	0.60
1:A:130:LYS:HE3	1:D:100:ASP:OD2	2.01	0.60
1:D:84:ASP:OD1	1:D:132:ARG:HD2	2.01	0.60
1:B:42:VAL:HG13	1:B:58:ALA:HB1	1.84	0.60
1:A:42:VAL:HG23	1:A:58:ALA:HB1	1.84	0.60
1:D:62:ASP:H	1:D:68:GLN:NE2	2.01	0.59
1:B:35:LEU:HA	1:B:59:LEU:O	2.03	0.58
1:B:42:VAL:CG1	1:B:58:ALA:HB1	2.34	0.58
1:A:217:VAL:O	1:A:217:VAL:HG22	2.03	0.58
1:A:109:GLU:O	1:A:113:VAL:HG23	2.03	0.58
1:A:200:LEU:HD12	1:A:201:ARG:N	2.17	0.58
1:B:63:VAL:HA	1:B:69:MSE:HE3	1.85	0.58
1:B:260:ARG:CG	1:B:260:ARG:HH11	2.08	0.58
1:D:43:GLU:HA	1:D:58:ALA:HB2	1.86	0.57
1:C:71:ASN:OD1	1:C:74:ARG:NH2	2.37	0.57
1:B:183:ASN:ND2	1:B:248:SER:H	2.03	0.56
1:B:185:VAL:CG2	1:B:233:LEU:HD23	2.34	0.56
1:A:19:ARG:HG3	1:A:45:VAL:HG11	1.87	0.56
1:A:158:THR:HG21	1:D:170:GLN:CG	2.28	0.56
1:B:71:ASN:ND2	1:B:74:ARG:HH21	2.03	0.56
1:B:217:VAL:HG22	1:B:220:THR:OG1	2.06	0.56
1:D:216:GLN:O	1:D:256:GLN:HB2	2.05	0.56
1:D:39:ARG:HD2	1:D:40:THR:N	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:VAL:HG23	1:B:233:LEU:HD23	1.88	0.55
1:D:233:LEU:HD11	1:D:250:VAL:HG11	1.88	0.55
1:C:63:VAL:HG13	1:C:117:GLY:HA3	1.89	0.55
1:A:209:PRO:HG2	1:C:214:LYS:HG2	1.89	0.55
1:A:130:LYS:CE	1:D:100:ASP:OD2	2.55	0.54
1:C:57:ILE:HG22	1:C:80:PHE:HE2	1.72	0.54
1:A:235:ARG:HH21	1:A:241:ARG:HH22	1.56	0.54
1:B:106:GLU:CD	1:B:201:ARG:HH22	2.10	0.54
1:A:192:THR:HG22	1:A:196:ASP:OD2	2.08	0.54
1:B:35:LEU:CD2	1:B:69:MSE:HE1	2.31	0.54
1:D:226:ARG:O	1:D:229:ASP:HB2	2.07	0.54
1:B:8:ALA:HA	1:B:85:ILE:O	2.08	0.53
1:D:61:ALA:HA	1:D:68:GLN:HE21	1.73	0.53
1:D:50:VAL:C	1:D:52:ALA:H	2.11	0.53
1:A:19:ARG:HG3	1:A:45:VAL:CG1	2.38	0.53
1:D:92:ILE:HD11	1:D:113:VAL:CG2	2.38	0.53
1:C:11:THR:O	1:C:89:ASN:HB3	2.09	0.53
1:D:233:LEU:HD21	1:D:250:VAL:CG1	2.37	0.53
1:D:61:ALA:HA	1:D:68:GLN:NE2	2.23	0.52
1:A:183:ASN:ND2	1:A:248:SER:H	2.08	0.52
1:A:83:LEU:HD22	1:A:129:LEU:CD1	2.40	0.52
1:D:19:ARG:NH1	1:D:45:VAL:HG12	2.25	0.51
1:C:96:TRP:HB2	1:C:200:LEU:HD13	1.91	0.51
1:C:220:THR:O	1:C:221:ASP:C	2.48	0.51
1:B:6:PRO:HB2	1:B:30:VAL:HG22	1.93	0.50
1:B:61:ALA:HB3	1:B:69:MSE:HE2	1.90	0.50
1:A:229:ASP:OD1	1:B:243:ARG:NH1	2.44	0.50
1:D:168:VAL:HG13	1:D:182:VAL:HG12	1.94	0.50
1:D:111:ILE:HD12	1:D:160:THR:HG22	1.94	0.49
1:A:83:LEU:HD22	1:A:129:LEU:HD11	1.94	0.49
1:C:181:ARG:HD3	1:C:243:ARG:O	2.12	0.49
1:D:152:PRO:CB	1:D:206:THR:CG2	2.89	0.49
1:A:35:LEU:HD23	1:A:35:LEU:C	2.33	0.49
1:B:158:THR:HG22	1:C:166:ALA:HB1	1.95	0.49
1:D:50:VAL:HA	1:D:54:GLY:O	2.12	0.48
1:A:49:ILE:HG22	1:A:54:GLY:HA3	1.94	0.48
1:A:165:VAL:O	1:A:169:GLN:HG3	2.13	0.48
1:A:143:ILE:HG12	1:A:188:GLY:HA2	1.96	0.48
1:D:77:VAL:O	1:D:81:GLY:N	2.36	0.48
1:B:15:SER:HA	1:B:19:ARG:HB2	1.96	0.48
1:C:171:LEU:O	1:C:175:LEU:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:GLU:OE1	1:D:201:ARG:NH2	2.46	0.48
1:B:216:GLN:OE1	1:B:260:ARG:CD	2.61	0.47
1:C:74:ARG:NH1	1:C:75:ASP:OD1	2.47	0.47
1:A:160:THR:O	1:A:164:GLN:HG3	2.14	0.47
1:D:89:ASN:CG	1:D:89:ASN:O	2.52	0.47
1:A:232:GLU:OE2	1:B:241:ARG:NH1	2.47	0.47
1:C:258:LEU:HB2	1:D:173:LEU:HD21	1.96	0.47
1:A:138:VAL:HA	1:A:183:ASN:O	2.14	0.47
1:A:243:ARG:NH1	1:A:243:ARG:HG2	2.25	0.47
1:A:92:ILE:HG13	1:A:92:ILE:O	2.13	0.47
1:B:139:VAL:HG13	1:B:168:VAL:CG2	2.44	0.47
1:D:26:ALA:C	1:D:28:ASP:N	2.67	0.47
1:C:223:GLN:HE21	1:C:223:GLN:H	1.63	0.47
1:D:152:PRO:CA	1:D:206:THR:CG2	2.93	0.47
1:B:61:ALA:HB3	1:B:69:MSE:CE	2.45	0.47
1:C:145:GLY:HA2	1:C:158:THR:HG23	1.98	0.46
1:D:46:ALA:O	1:D:50:VAL:HG23	2.16	0.46
1:D:106:GLU:CD	1:D:201:ARG:HH22	2.19	0.46
1:B:41:GLU:O	1:B:45:VAL:HG12	2.15	0.46
1:B:217:VAL:HG13	1:B:222:GLY:C	2.36	0.46
1:C:219:ILE:HA	1:C:219:ILE:HD12	1.82	0.46
1:C:189:ALA:O	1:C:190:ILE:HD13	2.15	0.46
1:A:234:ILE:O	1:A:238:VAL:HG22	2.16	0.46
1:D:7:VAL:HG22	1:D:31:THR:HB	1.98	0.46
1:D:152:PRO:HB2	1:D:206:THR:CG2	2.44	0.46
1:B:11:THR:O	1:B:89:ASN:HB3	2.16	0.46
1:C:253:ASP:OD2	1:C:257:GLY:HA3	2.16	0.46
1:D:211:GLU:O	1:D:213:PRO:HD3	2.17	0.45
1:D:106:GLU:OE2	1:D:201:ARG:NH2	2.46	0.45
1:C:50:VAL:HA	1:C:54:GLY:O	2.15	0.45
1:A:93:ASN:ND2	1:A:96:TRP:HZ2	2.14	0.45
1:B:185:VAL:HG23	1:B:233:LEU:CD2	2.46	0.45
1:C:212:TRP:CD1	1:C:216:GLN:HG2	2.52	0.45
1:D:190:ILE:C	1:D:192:THR:H	2.20	0.45
1:B:82:HIS:HD2	1:B:84:ASP:OD2	2.01	0.44
1:C:239:SER:OG	1:C:241:ARG:HB2	2.16	0.44
1:D:83:LEU:HA	1:D:83:LEU:HD12	1.73	0.44
1:A:151:THR:HA	1:A:152:PRO:HD3	1.75	0.44
1:A:168:VAL:HG21	1:A:184:ALA:HB2	1.98	0.44
1:D:39:ARG:HA	1:D:42:VAL:HG22	2.00	0.44
1:D:60:GLU:O	1:D:61:ALA:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:ILE:HG13	1:D:113:VAL:HG11	2.00	0.44
1:A:35:LEU:HD23	1:A:36:GLY:N	2.33	0.44
1:C:250:VAL:HG22	1:D:250:VAL:HG23	1.99	0.44
1:D:8:ALA:HB2	1:D:85:ILE:HB	2.00	0.44
1:D:8:ALA:HA	1:D:85:ILE:O	2.18	0.44
1:B:171:LEU:HB3	1:B:175:LEU:HD22	2.00	0.44
1:D:181:ARG:HD3	1:D:243:ARG:O	2.17	0.44
1:A:186:CYS:HB2	1:A:251:TRP:CD1	2.53	0.43
1:B:219:ILE:HD12	1:B:219:ILE:HA	1.81	0.43
1:B:170:GLN:HG3	1:C:158:THR:HG21	2.01	0.43
1:C:19:ARG:HG3	1:C:45:VAL:CG2	2.48	0.43
1:B:216:GLN:HE21	1:B:216:GLN:H	1.65	0.43
1:A:63:VAL:HG13	1:A:117:GLY:HA3	2.00	0.43
1:D:190:ILE:O	1:D:192:THR:N	2.47	0.43
1:D:191:GLU:OE1	1:D:191:GLU:HA	2.19	0.43
1:D:39:ARG:HD2	1:D:40:THR:H	1.82	0.43
1:B:62:ASP:C	1:B:62:ASP:OD2	2.57	0.43
1:C:74:ARG:O	1:C:78:LEU:HG	2.19	0.42
1:B:5:SER:HA	1:B:6:PRO:HD3	1.79	0.42
1:C:216:GLN:OE1	1:C:260:ARG:NE	2.53	0.42
1:D:240:GLU:O	1:D:243:ARG:NH1	2.47	0.42
1:D:153:GLY:N	1:D:206:THR:HG21	2.34	0.42
1:C:171:LEU:HD23	1:C:171:LEU:HA	1.85	0.42
1:A:150:THR:HG22	1:D:173:LEU:HD13	2.00	0.42
1:D:152:PRO:C	1:D:206:THR:HG21	2.40	0.42
1:B:95:VAL:HG11	1:B:201:ARG:NH2	2.35	0.42
1:B:97:ALA:HB1	1:B:98:PRO:HD2	2.02	0.42
1:A:115:LEU:HA	1:A:115:LEU:HD12	1.70	0.42
1:D:83:LEU:HB3	1:D:129:LEU:HD12	2.03	0.41
1:A:40:THR:HA	1:A:43:GLU:HG3	2.01	0.41
1:C:216:GLN:HE22	1:C:256:GLN:HE21	1.67	0.41
1:B:82:HIS:CD2	1:B:132:ARG:NH1	2.88	0.41
1:A:82:HIS:HB2	1:A:132:ARG:HG3	2.01	0.41
1:C:15:SER:CA	1:C:19:ARG:HB2	2.51	0.41
1:D:145:GLY:HA2	1:D:158:THR:HG23	2.02	0.41
1:A:39:ARG:O	1:A:43:GLU:HG3	2.21	0.41
1:D:234:ILE:O	1:D:238:VAL:HG13	2.21	0.41
1:A:130:LYS:NZ	1:D:100:ASP:OD2	2.54	0.40
1:A:220:THR:OG1	1:A:223:GLN:O	2.34	0.40
1:D:236:PHE:CE2	1:D:242:ALA:HB2	2.56	0.40
1:C:194:ILE:HG21	1:C:260:ARG:HE	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:SER:CA	1:B:19:ARG:HB2	2.52	0.40
1:B:183:ASN:HD22	1:B:248:SER:H	1.68	0.40
1:C:100:ASP:N	1:C:100:ASP:OD1	2.54	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	255/283 (90%)	245 (96%)	10 (4%)	0	100	100
1	B	255/283 (90%)	240 (94%)	15 (6%)	0	100	100
1	C	253/283 (89%)	237 (94%)	13 (5%)	3 (1%)	16	39
1	D	254/283 (90%)	233 (92%)	20 (8%)	1 (0%)	39	69
All	All	1017/1132 (90%)	955 (94%)	58 (6%)	4 (0%)	39	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	221	ASP
1	D	27	ALA
1	C	191	GLU
1	C	198	THR

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	198/218 (91%)	180 (91%)	18 (9%)	12 26
1	B	198/218 (91%)	177 (89%)	21 (11%)	8 19
1	C	196/218 (90%)	176 (90%)	20 (10%)	9 21
1	D	197/218 (90%)	176 (89%)	21 (11%)	8 19
All	All	789/872 (90%)	709 (90%)	80 (10%)	9 21

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	45	VAL
1	A	63	VAL
1	A	103	LYS
1	A	111	ILE
1	A	125	THR
1	A	131	GLN
1	A	132	ARG
1	A	138	VAL
1	A	142	SER
1	A	191	GLU
1	A	192	THR
1	A	195	SER
1	A	204	GLU
1	A	211	GLU
1	A	217	VAL
1	A	223	GLN
1	A	243	ARG
1	B	23	LEU
1	B	31	THR
1	B	42	VAL
1	B	45	VAL
1	B	62	ASP
1	B	63	VAL
1	B	102	LEU
1	B	109	GLU
1	B	132	ARG
1	B	139	VAL
1	B	175	LEU
1	B	191	GLU
1	B	192	THR

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Mol	Chain	Res	Type
1	B	195	SER
1	B	216	GLN
1	B	217	VAL
1	B	219	ILE
1	B	232	GLU
1	B	258	LEU
1	B	259	LEU
1	B	260	ARG
1	C	23	LEU
1	C	37	ARG
1	C	38	THR
1	C	63	VAL
1	C	75	ASP
1	C	83	LEU
1	C	95	VAL
1	C	102	LEU
1	C	132	ARG
1	C	141	SER
1	C	167	ILE
1	C	175	LEU
1	C	177	LYS
1	C	196	ASP
1	C	211	GLU
1	C	216	GLN
1	C	223	GLN
1	C	235	ARG
1	C	241	ARG
1	C	260	ARG
1	D	25	LEU
1	D	37	ARG
1	D	39	ARG
1	D	40	THR
1	D	63	VAL
1	D	92	ILE
1	D	100	ASP
1	D	104	PRO
1	D	109	GLU
1	D	111	ILE
1	D	132	ARG
1	D	138	VAL
1	D	193	ASN
1	D	194	ILE

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Mol	Chain	Res	Type
1	D	201	ARG
1	D	204	GLU
1	D	206	THR
1	D	216	GLN
1	D	241	ARG
1	D	243	ARG
1	D	258	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	68	GLN
1	A	93	ASN
1	A	131	GLN
1	A	183	ASN
1	A	223	GLN
1	B	71	ASN
1	B	169	GLN
1	B	183	ASN
1	C	216	GLN
1	C	223	GLN
1	D	68	GLN
1	D	183	ASN
1	D	193	ASN

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	256/283 (90%)	-0.20	1 (0%) 93 94	16, 27, 49, 78	0
1	B	256/283 (90%)	-0.28	1 (0%) 93 94	15, 26, 50, 66	0
1	C	254/283 (89%)	-0.38	0 100 100	17, 29, 53, 63	0
1	D	255/283 (90%)	-0.06	5 (1%) 68 69	17, 32, 58, 74	0
All	All	1021/1132 (90%)	-0.23	7 (0%) 89 90	15, 29, 54, 78	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	51	GLY	4.2
1	A	55	GLN	2.7
1	D	133	GLY	2.5
1	D	39	ARG	2.2
1	D	48	GLU	2.2
1	D	50	VAL	2.1
1	B	51	GLY	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 (i)

There are no such residues in this entry.