Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:26 AM GMT

PDB ID	:	3EMK
Title	:	2.5A crystal structure of glucose/ribitol dehydrogenase from brucella melitensis
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2008-09-24
Resolution	:	2.50 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:

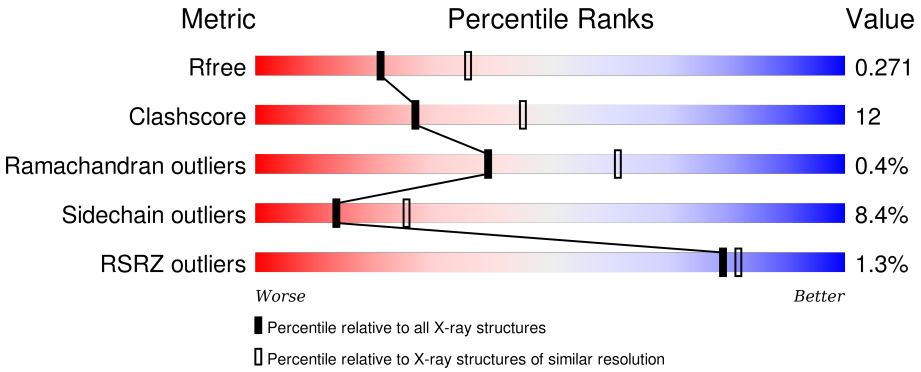
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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	246	2% 76% 19%
1	B	246	2% 67% 26% 6%
1	C	246	% 71% 22%
1	D	246	% 73% 20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7138 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 GLUCOSE/RIBITOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1784	1110	321	340	13			
1	B	232	Total	C	N	O	S	0	0	0
			1711	1067	309	323	12			
1	C	236	Total	C	N	O	S	0	0	0
			1748	1088	316	332	12			
1	D	238	Total	C	N	O	S	0	0	0
			1765	1099	318	336	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q8YFP3
B	0	SER	-	expression tag	UNP Q8YFP3
C	0	SER	-	expression tag	UNP Q8YFP3
D	0	SER	-	expression tag	UNP Q8YFP3

- Molecule 2 is water.

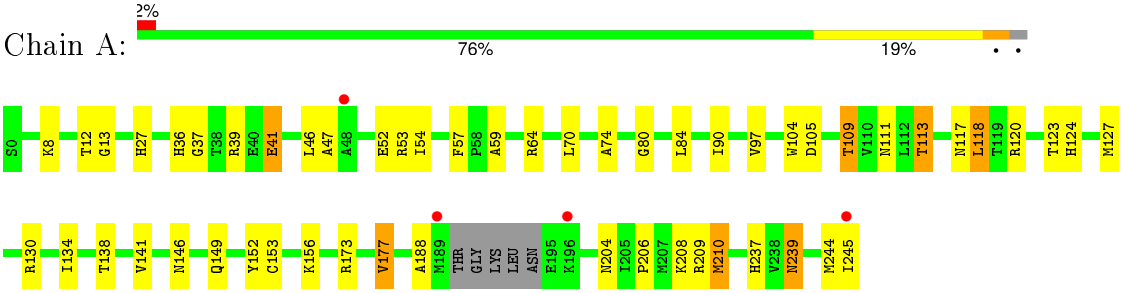
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	37	Total	O	0	0
			37	37		
2	B	28	Total	O	0	0
			28	28		
2	C	29	Total	O	0	0
			29	29		
2	D	36	Total	O	0	0
			36	36		

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.

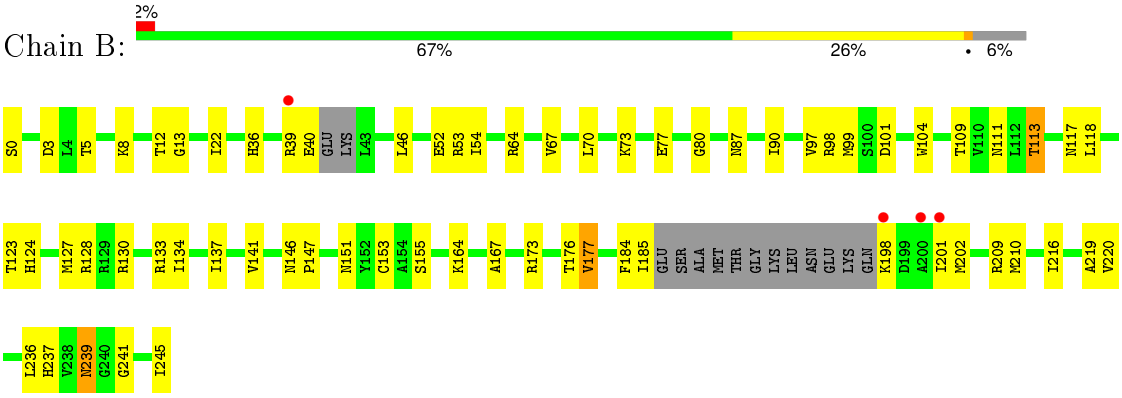
- Molecule 1: GLUCOSE/RIBITOL DEHYDROGENASE

Chain A:



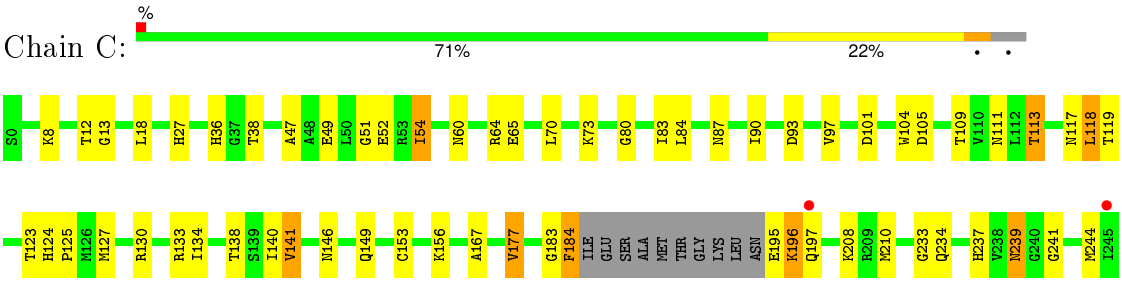
- Molecule 1: GLUCOSE/RIBITOL DEHYDROGENASE

Chain B:



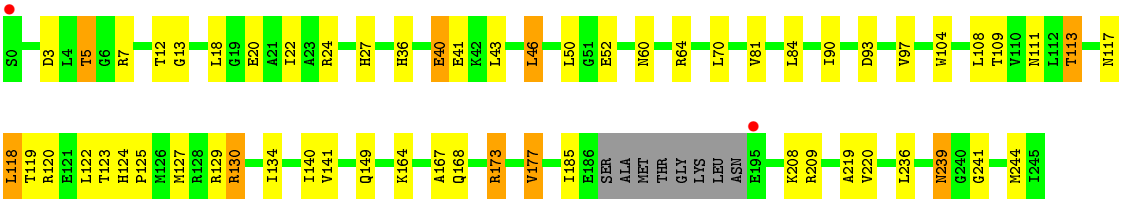
- Molecule 1: GLUCOSE/RIBITOL DEHYDROGENASE

Chain C:



- Molecule 1: GLUCOSE/RIBITOL DEHYDROGENASE

Chain D:


S0
D3
L4
T5
G6
R7
T12
G13
L18
G19
E20
A21
I22
A23
R24
H27
H36
E40
E41
K42
L43
L46
L50
G51
E52
N60
R64
L70
V81
L84
I90
D93
V97
W104
L108
T109
V110
N111
L112
T113
N117
L118
T119
R120
E121
L122
T123
H124
P125
M126
M127
R128
R129
R130
I134
I140
V141
Q149
K164
A167
Q168
R173
V177
I185
E186
SER
ALA
MET
THR
GLY
LYS
LEU
ASN
E195
K208
R209
A219
V220
L236
M239
G240
G241
M244
I245

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	99.49Å 147.94Å 63.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 44.18 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.7 (50.00-2.50) 94.7 (44.18-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.268 0.203 , 0.271	Depositor DCC
R_{free} test set	1598 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	30.8	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 34.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 31701 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7138	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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	0.60	0/1803	0.70	0/2429
1	B	0.58	0/1729	0.73	0/2331
1	C	0.58	0/1767	0.69	1/2381 (0.0%)
1	D	0.56	0/1784	0.69	0/2404
All	All	0.58	0/7083	0.70	1/9545 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	18	LEU	CA-CB-CG	5.59	128.16	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	184	PHE	Peptide

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	1784	0	1814	44	0
1	B	1711	0	1742	50	0
1	C	1748	0	1778	54	0
1	D	1765	0	1795	40	0
2	A	37	0	0	1	0
2	B	28	0	0	2	0
2	C	29	0	0	4	0
2	D	36	0	0	0	0
All	All	7138	0	7129	170	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 (170) 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:99:MET:HE1	1:B:151:ASN:HB3	1.40	1.04
1:C:105:ASP:O	1:C:109:THR:HG23	1.64	0.98
1:D:90:ILE:H	1:D:111:ASN:HD21	1.17	0.89
1:A:109:THR:HA	1:A:113:THR:HG23	1.51	0.89
1:A:104:TRP:HE1	1:C:113:THR:HB	1.39	0.87
1:B:13:GLY:H	1:B:36:HIS:HD2	1.20	0.86
1:B:99:MET:CE	1:B:151:ASN:HB3	2.07	0.84
1:C:119:THR:O	1:C:123:THR:HG23	1.76	0.84
1:A:124:HIS:HA	1:A:127:MET:HE3	1.64	0.79
1:B:90:ILE:H	1:B:111:ASN:HD21	1.28	0.79
1:A:123:THR:HG22	1:A:134:ILE:HD11	1.65	0.79
1:C:64:ARG:HH11	1:C:117:ASN:HD21	1.33	0.75
1:B:3:ASP:OD1	1:B:5:THR:HG23	1.86	0.75
1:A:104:TRP:NE1	1:C:113:THR:HB	2.01	0.75
1:C:195:GLU:O	1:C:197:GLN:N	2.20	0.75
1:C:183:GLY:O	1:C:184:PHE:HB3	1.85	0.74
1:B:209:ARG:HG3	1:B:210:MET:O	1.86	0.74
1:A:141:VAL:HG22	1:A:146:ASN:HB2	1.70	0.73
1:C:141:VAL:HG22	1:C:146:ASN:HB2	1.70	0.73
1:C:64:ARG:NH1	1:C:117:ASN:HD21	1.86	0.73
1:C:141:VAL:HG13	1:C:153:CYS:SG	2.29	0.72
1:B:141:VAL:HG22	1:B:146:ASN:HB2	1.70	0.72
1:A:141:VAL:HG13	1:A:153:CYS:SG	2.30	0.71
1:A:90:ILE:H	1:A:111:ASN:HD21	1.36	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:ILE:H	1:C:111:ASN:HD21	1.37	0.70
1:B:141:VAL:HG13	1:B:153:CYS:SG	2.33	0.68
1:D:13:GLY:H	1:D:36:HIS:HD2	1.41	0.68
1:A:97:VAL:HG11	1:C:124:HIS:HB2	1.75	0.67
1:B:239:ASN:HD22	1:B:241:GLY:H	1.43	0.67
1:B:64:ARG:HE	1:B:117:ASN:HD21	1.43	0.66
1:C:8:LYS:HE2	1:C:80:GLY:O	1.95	0.66
1:A:124:HIS:CD2	1:C:97:VAL:HG21	2.30	0.66
1:B:239:ASN:ND2	1:B:241:GLY:H	1.93	0.66
1:B:239:ASN:HD22	1:B:239:ASN:C	2.00	0.65
1:B:99:MET:CE	1:B:104:TRP:HE3	2.10	0.65
1:C:64:ARG:HH11	1:C:117:ASN:ND2	1.94	0.64
1:B:104:TRP:NE1	1:D:113:THR:HB	2.13	0.64
1:D:239:ASN:HD22	1:D:241:GLY:H	1.45	0.64
1:B:198:LYS:HA	1:B:201:ILE:HD12	1.79	0.64
1:B:73:LYS:HE2	1:B:77:GLU:OE2	1.98	0.63
1:A:13:GLY:H	1:A:36:HIS:HD2	1.45	0.63
1:D:109:THR:HA	1:D:113:THR:HG23	1.79	0.63
1:A:97:VAL:CG1	1:C:124:HIS:HB2	2.28	0.62
1:A:105:ASP:O	1:A:109:THR:HG23	1.99	0.62
1:D:119:THR:O	1:D:123:THR:HG23	1.99	0.61
1:A:237:HIS:HD2	2:A:273:HOH:O	1.84	0.60
1:D:134:ILE:HB	1:D:177:VAL:HB	1.84	0.60
1:A:84:LEU:HD11	1:A:118:LEU:HD13	1.85	0.59
1:D:27:HIS:HE1	1:D:52:GLU:O	1.86	0.59
1:B:109:THR:HA	1:B:113:THR:HG23	1.84	0.59
1:D:40:GLU:HA	1:D:43:LEU:HD12	1.85	0.58
1:D:64:ARG:HE	1:D:117:ASN:HD21	1.50	0.58
1:C:239:ASN:C	1:C:239:ASN:HD22	2.05	0.58
1:D:18:LEU:HD21	1:D:185:ILE:HG21	1.86	0.58
1:C:239:ASN:HD22	1:C:241:GLY:H	1.52	0.58
1:D:239:ASN:C	1:D:239:ASN:HD22	2.06	0.57
1:B:12:THR:HA	1:B:36:HIS:HB3	1.85	0.57
1:A:27:HIS:HE1	1:A:52:GLU:O	1.87	0.57
1:C:109:THR:HA	1:C:113:THR:HG23	1.88	0.56
1:B:99:MET:HE1	1:B:104:TRP:HE3	1.71	0.56
1:D:239:ASN:ND2	1:D:241:GLY:H	2.03	0.56
1:C:47:ALA:HB1	1:C:54:ILE:HG21	1.90	0.54
1:B:111:ASN:HB2	1:B:155:SER:HB2	1.89	0.54
1:C:52:GLU:HA	1:C:52:GLU:OE2	2.06	0.54
1:D:12:THR:HA	1:D:36:HIS:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ARG:HE	1:A:117:ASN:HD21	1.56	0.54
1:B:237:HIS:CE1	1:B:245:ILE:HD13	2.42	0.54
1:A:113:THR:HB	1:C:104:TRP:HE1	1.73	0.53
1:D:41:GLU:H	1:D:41:GLU:CD	2.12	0.53
1:B:104:TRP:HE1	1:D:113:THR:HB	1.72	0.52
1:C:123:THR:HG22	1:C:134:ILE:HD11	1.92	0.52
1:D:123:THR:HG22	1:D:134:ILE:HD11	1.90	0.52
1:C:93:ASP:OD1	1:C:149:GLN:HG2	2.08	0.52
1:D:46:LEU:HD22	1:D:50:LEU:CD1	2.39	0.52
1:A:39:ARG:HD3	1:A:41:GLU:OE1	2.10	0.52
1:C:124:HIS:HA	1:C:127:MET:CE	2.39	0.52
1:D:46:LEU:HD22	1:D:50:LEU:HD11	1.90	0.52
1:C:134:ILE:HB	1:C:177:VAL:HB	1.90	0.52
1:B:167:ALA:HA	1:B:177:VAL:HG13	1.92	0.52
1:B:239:ASN:ND2	2:B:269:HOH:O	2.42	0.52
1:A:123:THR:HG22	1:A:134:ILE:CD1	2.36	0.51
1:B:124:HIS:CD2	1:B:128:ARG:HD3	2.45	0.51
1:A:138:THR:HA	1:A:156:LYS:HD2	1.93	0.51
1:D:3:ASP:OD1	1:D:5:THR:HG22	2.11	0.51
1:A:57:PHE:CZ	1:A:74:ALA:HA	2.46	0.51
1:A:36:HIS:HE1	1:A:59:ALA:O	1.94	0.51
1:C:239:ASN:ND2	1:C:241:GLY:H	2.09	0.50
1:A:13:GLY:H	1:A:36:HIS:CD2	2.27	0.50
1:A:90:ILE:N	1:A:111:ASN:HD21	2.07	0.50
1:A:149:GLN:HB3	1:A:152:TYR:HB3	1.94	0.50
1:C:124:HIS:HB3	1:C:125:PRO:HD3	1.93	0.49
1:D:130:ARG:HH22	1:D:173:ARG:HH11	1.59	0.49
1:B:22:ILE:HG12	1:B:220:VAL:HG21	1.94	0.49
1:A:209:ARG:HG3	1:A:210:MET:O	2.13	0.49
1:A:244:MET:HB3	1:B:164:LYS:HG2	1.94	0.49
1:B:99:MET:HE2	1:B:104:TRP:HE3	1.76	0.49
1:B:13:GLY:H	1:B:36:HIS:CD2	2.12	0.49
1:B:134:ILE:HB	1:B:177:VAL:HB	1.94	0.49
1:D:93:ASP:OD1	1:D:149:GLN:HG2	2.13	0.49
1:B:111:ASN:N	1:B:111:ASN:HD22	2.09	0.48
1:A:124:HIS:HD2	1:C:97:VAL:HG21	1.73	0.48
1:B:123:THR:O	1:B:127:MET:HG3	2.13	0.48
1:A:113:THR:HB	1:C:104:TRP:NE1	2.28	0.48
1:B:113:THR:HB	1:D:104:TRP:NE1	2.27	0.48
1:A:134:ILE:O	1:A:177:VAL:HA	2.14	0.48
1:B:219:ALA:HB1	1:B:236:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ASN:HD22	1:A:111:ASN:N	2.10	0.47
1:A:130:ARG:NH1	1:A:173:ARG:HD2	2.30	0.47
1:B:147:PRO:HD3	1:D:168:GLN:OE1	2.13	0.47
1:B:113:THR:HB	1:D:104:TRP:HE1	1.80	0.47
1:B:237:HIS:HD2	2:B:263:HOH:O	1.97	0.47
1:B:133:ARG:HD3	1:B:176:THR:OG1	2.14	0.47
1:A:134:ILE:HB	1:A:177:VAL:HB	1.96	0.46
1:D:20:GLU:O	1:D:24:ARG:HG3	2.15	0.46
1:C:138:THR:HA	1:C:156:LYS:HD2	1.98	0.46
1:C:234:GLN:HB3	2:C:264:HOH:O	2.15	0.46
1:A:120:ARG:NH2	1:C:101:ASP:OD2	2.49	0.46
1:C:127:MET:HE2	1:C:127:MET:HB2	1.81	0.46
1:B:239:ASN:ND2	1:B:239:ASN:C	2.67	0.46
1:C:13:GLY:H	1:C:36:HIS:HD2	1.64	0.46
1:B:64:ARG:NE	1:B:117:ASN:HD21	2.12	0.45
1:D:64:ARG:HE	1:D:117:ASN:ND2	2.14	0.45
1:B:130:ARG:NH1	1:B:173:ARG:HD3	2.30	0.45
1:D:219:ALA:HB1	1:D:236:LEU:HD23	1.99	0.45
1:D:90:ILE:N	1:D:111:ASN:HD21	1.97	0.45
1:C:83:ILE:HG12	1:C:133:ARG:HB2	1.97	0.45
1:C:237:HIS:HD2	2:C:270:HOH:O	1.98	0.45
1:A:8:LYS:HD2	1:A:80:GLY:O	2.17	0.45
1:D:122:LEU:C	1:D:125:PRO:HD2	2.36	0.45
1:A:239:ASN:HD22	1:A:239:ASN:C	2.20	0.45
1:A:64:ARG:HE	1:A:117:ASN:ND2	2.13	0.45
1:B:101:ASP:OD1	1:D:120:ARG:NH2	2.50	0.45
1:B:64:ARG:HE	1:B:117:ASN:ND2	2.13	0.44
1:B:12:THR:O	1:B:87:ASN:HB3	2.18	0.44
1:B:137:ILE:HD12	1:B:137:ILE:N	2.33	0.44
1:C:167:ALA:HB2	1:C:177:VAL:HG13	1.99	0.44
1:C:184:PHE:HE1	2:C:271:HOH:O	2.01	0.44
1:C:183:GLY:O	1:C:184:PHE:CB	2.62	0.44
1:A:12:THR:HA	1:A:36:HIS:HB3	1.99	0.44
1:C:237:HIS:HE1	2:C:263:HOH:O	2.00	0.43
1:B:52:GLU:OE1	1:B:53:ARG:NE	2.35	0.43
1:C:84:LEU:HD11	1:C:118:LEU:HD13	2.00	0.43
1:C:124:HIS:HA	1:C:127:MET:HE2	1.99	0.43
1:D:140:ILE:HG23	1:D:141:VAL:N	2.34	0.43
1:C:123:THR:O	1:C:127:MET:HG3	2.19	0.43
1:C:64:ARG:HD3	1:C:117:ASN:ND2	2.33	0.43
1:D:111:ASN:N	1:D:111:ASN:HD22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:THR:O	1:C:87:ASN:HB3	2.19	0.43
1:D:167:ALA:HA	1:D:177:VAL:HG13	2.00	0.43
1:B:124:HIS:HA	1:B:127:MET:HE2	2.00	0.42
1:D:22:ILE:HG23	1:D:220:VAL:HG11	2.01	0.42
1:B:111:ASN:ND2	1:B:111:ASN:N	2.67	0.42
1:D:81:VAL:O	1:D:129:ARG:NH2	2.52	0.42
1:A:245:ILE:N	1:A:245:ILE:HD12	2.35	0.42
1:C:244:MET:HB3	1:D:164:LYS:HG2	2.02	0.41
1:C:12:THR:HA	1:C:36:HIS:HB3	2.03	0.41
1:B:8:LYS:HD2	1:B:80:GLY:O	2.20	0.41
1:A:36:HIS:CG	1:A:37:GLY:N	2.88	0.41
1:C:27:HIS:HE1	1:C:52:GLU:O	2.03	0.41
1:A:111:ASN:ND2	1:A:111:ASN:N	2.69	0.41
1:C:124:HIS:ND1	1:C:127:MET:CE	2.84	0.41
1:D:84:LEU:HD11	1:D:118:LEU:HD13	2.03	0.41
1:D:124:HIS:HA	1:D:127:MET:CE	2.51	0.41
1:A:204:ASN:O	1:A:206:PRO:HD3	2.20	0.41
1:C:233:GLY:O	1:D:244:MET:HB3	2.21	0.41
1:C:167:ALA:CA	1:C:177:VAL:HG13	2.51	0.41
1:B:99:MET:HE1	1:B:104:TRP:CE3	2.54	0.40
1:A:52:GLU:O	1:A:53:ARG:HB2	2.22	0.40
1:C:167:ALA:HA	1:C:177:VAL:HG13	2.02	0.40
1:C:140:ILE:HG23	1:C:141:VAL:N	2.36	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	237/246 (96%)	219 (92%)	16 (7%)	2 (1%)	24 41
1	B	226/246 (92%)	218 (96%)	8 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	232/246 (94%)	221 (95%)	9 (4%)	2 (1%)	21 37
1	D	234/246 (95%)	222 (95%)	12 (5%)	0	100 100
All	All	929/984 (94%)	880 (95%)	45 (5%)	4 (0%)	39 61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	196	LYS
1	A	188	ALA
1	C	51	GLY
1	A	47	ALA

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	183/187 (98%)	172 (94%)	11 (6%)	24 43
1	B	175/187 (94%)	159 (91%)	16 (9%)	12 22
1	C	179/187 (96%)	162 (90%)	17 (10%)	11 20
1	D	181/187 (97%)	165 (91%)	16 (9%)	12 23
All	All	718/748 (96%)	658 (92%)	60 (8%)	14 25

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLU
1	A	46	LEU
1	A	54	ILE
1	A	70	LEU
1	A	109	THR
1	A	113	THR
1	A	118	LEU
1	A	177	VAL

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Mol	Chain	Res	Type
1	A	208	LYS
1	A	210	MET
1	A	239	ASN
1	B	0	SER
1	B	39	ARG
1	B	40	GLU
1	B	46	LEU
1	B	54	ILE
1	B	67	VAL
1	B	70	LEU
1	B	97	VAL
1	B	98	ARG
1	B	113	THR
1	B	118	LEU
1	B	177	VAL
1	B	185	ILE
1	B	202	MET
1	B	216	ILE
1	B	239	ASN
1	C	38	THR
1	C	49	GLU
1	C	54	ILE
1	C	60	ASN
1	C	65	GLU
1	C	70	LEU
1	C	73	LYS
1	C	113	THR
1	C	118	LEU
1	C	130	ARG
1	C	141	VAL
1	C	177	VAL
1	C	184	PHE
1	C	196	LYS
1	C	208	LYS
1	C	210	MET
1	C	239	ASN
1	D	5	THR
1	D	7	ARG
1	D	40	GLU
1	D	46	LEU
1	D	60	ASN
1	D	70	LEU

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Mol	Chain	Res	Type
1	D	97	VAL
1	D	108	LEU
1	D	113	THR
1	D	118	LEU
1	D	130	ARG
1	D	173	ARG
1	D	177	VAL
1	D	208	LYS
1	D	209	ARG
1	D	239	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	29	GLN
1	A	36	HIS
1	A	111	ASN
1	A	117	ASN
1	A	124	HIS
1	A	234	GLN
1	A	237	HIS
1	A	239	ASN
1	B	27	HIS
1	B	36	HIS
1	B	111	ASN
1	B	117	ASN
1	B	204	ASN
1	B	234	GLN
1	B	237	HIS
1	B	239	ASN
1	C	27	HIS
1	C	36	HIS
1	C	60	ASN
1	C	111	ASN
1	C	117	ASN
1	C	131	ASN
1	C	174	ASN
1	C	234	GLN
1	C	237	HIS
1	C	239	ASN
1	D	27	HIS

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Mol	Chain	Res	Type
1	D	29	GLN
1	D	36	HIS
1	D	60	ASN
1	D	111	ASN
1	D	117	ASN
1	D	234	GLN
1	D	237	HIS
1	D	239	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	241/246 (97%)	-0.20	4 (1%)	73	76	25, 36, 55, 73	0
1	B	232/246 (94%)	-0.19	4 (1%)	73	76	27, 37, 51, 66	0
1	C	236/246 (95%)	-0.10	2 (0%)	87	89	25, 38, 62, 77	0
1	D	238/246 (96%)	-0.18	2 (0%)	87	89	26, 37, 55, 80	0
All	All	947/984 (96%)	-0.17	12 (1%)	79	82	25, 37, 59, 80	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	48	ALA	2.7
1	B	200	ALA	2.5
1	A	196	LYS	2.4
1	B	198	LYS	2.4
1	D	0	SER	2.4
1	B	201	ILE	2.3
1	A	189	MET	2.3
1	B	39	ARG	2.2
1	C	197	GLN	2.2
1	C	245	ILE	2.1
1	A	245	ILE	2.1
1	D	195	GLU	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.