Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:58 am BST

PDB ID	:	6DZX
Title	:	Crystal structure of the N. meningitides methionine-binding protein in its D-methionine bound conformation.
Authors	:	Nguyen, P.T.; Lai, J.Y.; Kaiser, J.T.; Rees, D.C.
Deposited on	:	2018-07-05
Resolution	:	1.68 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 ①) were used in the production of this report:

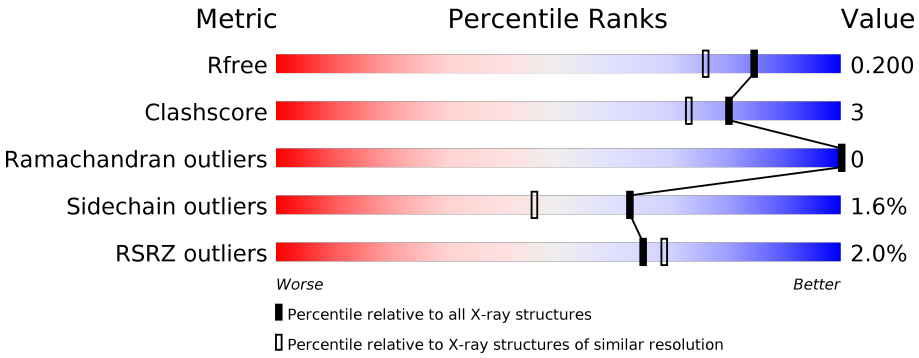
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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 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	247	91% 5%
1	B	247	% 93% 5%
1	C	247	5% 90% 6%
1	D	247	% 93%
1	E	247	3% 94%
1	F	247	% 87% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24101 atoms, of which 11260 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 Lipoprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	240	Total	C	H	N	O	S	0	0	0
			3754	1215	1860	307	369	3			
1	B	241	Total	C	H	N	O	S	0	0	0
			3775	1221	1872	309	370	3			
1	C	241	Total	C	H	N	O	S	0	0	0
			3760	1218	1861	308	370	3			
1	D	241	Total	C	H	N	O	S	0	0	0
			3775	1221	1872	309	370	3			
1	E	242	Total	C	H	N	O	S	0	0	0
			3782	1223	1875	310	371	3			
1	F	240	Total	C	H	N	O	S	0	0	0
			3754	1215	1860	307	369	3			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	LYS	-	expression tag	UNP C6S9R8
A	42	HIS	-	expression tag	UNP C6S9R8
A	64	ALA	PRO	conflict	UNP C6S9R8
B	41	LYS	-	expression tag	UNP C6S9R8
B	42	HIS	-	expression tag	UNP C6S9R8
B	64	ALA	PRO	conflict	UNP C6S9R8
C	41	LYS	-	expression tag	UNP C6S9R8
C	42	HIS	-	expression tag	UNP C6S9R8
C	64	ALA	PRO	conflict	UNP C6S9R8
D	41	LYS	-	expression tag	UNP C6S9R8
D	42	HIS	-	expression tag	UNP C6S9R8
D	64	ALA	PRO	conflict	UNP C6S9R8
E	41	LYS	-	expression tag	UNP C6S9R8
E	42	HIS	-	expression tag	UNP C6S9R8
E	64	ALA	PRO	conflict	UNP C6S9R8
F	41	LYS	-	expression tag	UNP C6S9R8
F	42	HIS	-	expression tag	UNP C6S9R8

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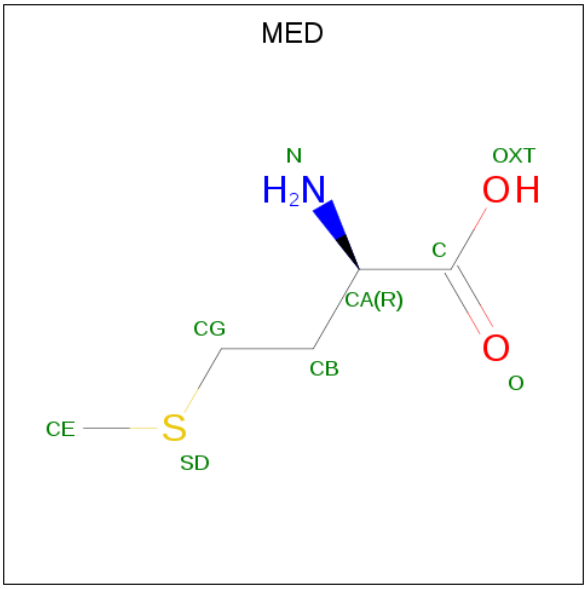
Chain	Residue	Modelled	Actual	Comment	Reference
F	64	ALA	PRO	conflict	UNP C6S9R8

- Molecule 2 is D-METHIONINE (three-letter code: MED) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			19	5	10	1	2	1		
2	B	1	Total	C	H	N	O	S	0	0
			19	5	10	1	2	1		
2	C	1	Total	C	H	N	O	S	0	0
			19	5	10	1	2	1		
2	D	1	Total	C	H	N	O	S	0	0
			19	5	10	1	2	1		
2	E	1	Total	C	H	N	O	S	0	0
			19	5	10	1	2	1		
2	F	1	Total	C	H	N	O	S	0	0
			19	5	10	1	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	251	Total	O	0	0
			251	251		
3	B	244	Total	O	0	0
			244	244		
3	C	207	Total	O	0	0
			207	207		

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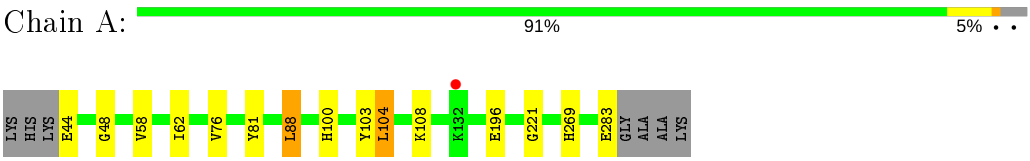
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	246	Total O 246 246	0	0
3	E	209	Total O 209 209	0	0
3	F	230	Total O 230 230	0	0

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 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.

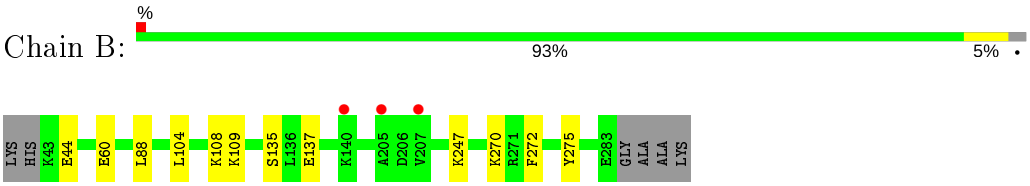
- Molecule 1: Lipoprotein

Chain A:



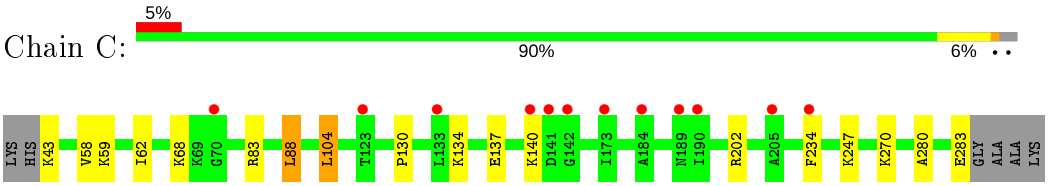
- Molecule 1: Lipoprotein

Chain B:



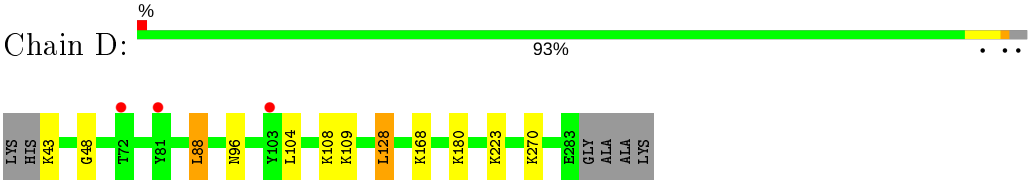
- Molecule 1: Lipoprotein

Chain C:



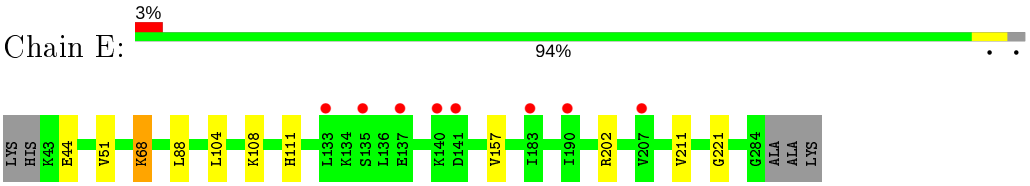
- Molecule 1: Lipoprotein

Chain D:



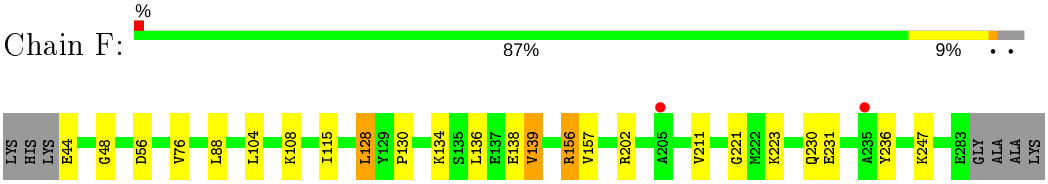
- Molecule 1: Lipoprotein

Chain E:



- Molecule 1: Lipoprotein

Chain F:


%
87%
9%
LYS
HIS
LYS
E44
G48
D56
V76
L88
L104
K108
I115
L128
Y129
P130
K134
S135
L136
E137
E138
V139
R156
V157
R202
A205
V211
G221
M222
K223
Q230
E231
A235
Y236
K247
E283
GLY
ALA
ALA
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	79.66Å 87.93Å 91.64Å 114.83° 104.12° 105.39°	Depositor
Resolution (Å)	39.67 – 1.68 39.67 – 1.68	Depositor EDS
% Data completeness (in resolution range)	96.0 (39.67-1.68) 96.4 (39.67-1.68)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 1.68Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.176 , 0.201 0.177 , 0.200	Depositor DCC
R_{free} test set	11107 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	26.3	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 49.7	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	0.97	EDS
Total number of atoms	24101	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MED

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	0.50	0/1936	0.65	2/2626 (0.1%)
1	B	0.52	0/1945	0.63	0/2637
1	C	0.50	0/1941	0.64	2/2633 (0.1%)
1	D	0.49	0/1945	0.66	2/2637 (0.1%)
1	E	0.49	0/1949	0.63	0/2642
1	F	0.51	0/1936	0.85	4/2626 (0.2%)
All	All	0.50	0/11652	0.68	10/15801 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	156	ARG	NE-CZ-NH2	-20.03	110.29	120.30
1	F	156	ARG	NE-CZ-NH1	17.93	129.26	120.30
1	F	128	LEU	CA-CB-CG	7.09	131.62	115.30
1	D	128	LEU	CA-CB-CG	6.80	130.95	115.30
1	D	88	LEU	CA-CB-CG	5.79	128.61	115.30
1	C	104	LEU	CA-CB-CG	5.47	127.89	115.30
1	A	88	LEU	CA-CB-CG	5.36	127.64	115.30
1	C	88	LEU	CA-CB-CG	5.36	127.63	115.30
1	A	81	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	F	156	ARG	CD-NE-CZ	5.02	130.63	123.60

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	1894	1860	1863	12	0
1	B	1903	1872	1876	8	0
1	C	1899	1861	1865	10	0
1	D	1903	1872	1876	9	0
1	E	1907	1875	1879	10	0
1	F	1894	1860	1863	18	0
2	A	9	10	10	0	0
2	B	9	10	10	0	0
2	C	9	10	10	0	0
2	D	9	10	10	0	0
2	E	9	10	10	0	0
2	F	9	10	10	0	0
3	A	251	0	0	6	1
3	B	244	0	0	2	0
3	C	207	0	0	6	0
3	D	246	0	0	5	0
3	E	209	0	0	4	0
3	F	230	0	0	7	1
All	All	12841	11260	11282	61	1

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 3.

All (61) 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:43:LYS:N	3:C:1101:HOH:O	2.03	0.90
1:F:156:ARG:HD2	1:F:231:GLU:OE2	1.71	0.90
1:F:44:GLU:N	3:F:1101:HOH:O	2.07	0.88
1:B:247:LYS:NZ	3:B:1102:HOH:O	2.06	0.87
1:B:44:GLU:OE2	3:B:1101:HOH:O	1.92	0.86
1:D:270:LYS:O	1:F:223:LYS:NZ	2.09	0.85
1:A:196:GLU:OE2	3:A:1101:HOH:O	2.02	0.77
1:D:180:LYS:NZ	3:D:1102:HOH:O	2.18	0.76
1:F:230:GLN:OE1	3:F:1102:HOH:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:247:LYS:NZ	3:F:1105:HOH:O	2.17	0.71
1:F:156:ARG:CD	1:F:231:GLU:OE2	2.43	0.66
1:A:44:GLU:OE2	3:A:1102:HOH:O	2.13	0.64
1:F:156:ARG:HD3	1:F:236:TYR:CD2	2.32	0.64
1:F:136:LEU:O	1:F:139:VAL:HG22	2.00	0.60
1:F:138:GLU:OE2	3:F:1103:HOH:O	2.16	0.60
1:C:137:GLU:OE2	3:C:1102:HOH:O	2.17	0.57
1:F:56:ASP:OD2	3:F:1104:HOH:O	2.17	0.56
1:D:223:LYS:CE	3:D:1101:HOH:O	2.52	0.56
1:A:221:GLY:O	1:C:270:LYS:HB3	2.11	0.51
1:D:168:LYS:HE3	3:D:1125:HOH:O	2.10	0.51
1:F:108:LYS:HD2	1:F:115:ILE:O	2.12	0.49
1:F:156:ARG:HD3	1:F:236:TYR:CE2	2.49	0.48
1:A:108:LYS:HD2	3:A:1104:HOH:O	2.12	0.48
1:C:247:LYS:HE2	3:C:1118:HOH:O	2.14	0.47
1:E:68:LYS:HD3	1:E:68:LYS:N	2.30	0.47
1:A:108:LYS:CD	3:A:1104:HOH:O	2.63	0.46
1:C:68:LYS:NZ	3:C:1104:HOH:O	2.29	0.46
1:E:157:VAL:HG22	1:E:211:VAL:HG11	1.96	0.46
1:E:111:HIS:HD2	3:F:1244:HOH:O	1.99	0.46
1:F:136:LEU:O	1:F:139:VAL:CG2	2.62	0.45
1:B:108:LYS:HG3	1:B:109:LYS:N	2.31	0.45
1:B:135:SER:OG	1:B:137:GLU:OE1	2.34	0.45
1:E:202:ARG:HG3	3:E:1221:HOH:O	2.16	0.45
1:E:108:LYS:CE	3:E:1103:HOH:O	2.65	0.45
1:D:168:LYS:CE	3:D:1125:HOH:O	2.64	0.44
1:B:60:GLU:HG2	1:E:51:VAL:CG1	2.48	0.44
1:C:280:ALA:O	1:C:283:GLU:HG3	2.17	0.44
1:A:269:HIS:HD2	3:A:1287:HOH:O	2.00	0.44
1:F:157:VAL:HG22	1:F:211:VAL:HG11	2.00	0.43
1:C:202:ARG:HG3	3:C:1165:HOH:O	2.18	0.43
1:E:108:LYS:NZ	3:E:1103:HOH:O	2.29	0.43
1:D:108:LYS:HG3	1:D:109:LYS:N	2.32	0.43
1:A:108:LYS:NZ	3:A:1104:HOH:O	2.23	0.43
1:C:83:ARG:NH2	3:C:1103:HOH:O	2.29	0.42
1:A:104:LEU:HD22	1:A:108:LYS:HE2	2.01	0.42
1:B:60:GLU:HG2	1:E:51:VAL:HG12	2.02	0.42
1:A:269:HIS:CE1	1:A:283:GLU:OE2	2.72	0.42
1:F:48:GLY:HA2	1:F:76:VAL:O	2.19	0.42
1:A:48:GLY:HA2	1:A:76:VAL:O	2.20	0.42
1:F:130:PRO:HB3	1:F:134:LYS:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:ARG:HG3	3:F:1192:HOH:O	2.20	0.42
1:E:44:GLU:OE2	3:E:1101:HOH:O	2.20	0.42
1:C:58:VAL:HA	1:C:62:ILE:HB	2.02	0.41
1:D:270:LYS:HB3	1:F:221:GLY:O	2.20	0.41
1:A:100:HIS:CE1	1:A:103:TYR:HB2	2.55	0.41
1:D:180:LYS:CE	3:D:1102:HOH:O	2.68	0.41
1:C:130:PRO:HB3	1:C:134:LYS:HA	2.02	0.41
1:D:48:GLY:O	1:D:96:ASN:HA	2.20	0.41
1:A:58:VAL:HA	1:A:62:ILE:HB	2.03	0.40
1:B:270:LYS:HB3	1:E:221:GLY:O	2.21	0.40
1:B:272:PHE:HB3	1:B:275:TYR:CG	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1264:HOH:O	3:F:1288:HOH:O[1_545]	2.09	0.11

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	238/247 (96%)	233 (98%)	5 (2%)	0	100	100
1	B	239/247 (97%)	234 (98%)	5 (2%)	0	100	100
1	C	239/247 (97%)	234 (98%)	5 (2%)	0	100	100
1	D	239/247 (97%)	234 (98%)	5 (2%)	0	100	100
1	E	240/247 (97%)	235 (98%)	5 (2%)	0	100	100
1	F	238/247 (96%)	233 (98%)	5 (2%)	0	100	100
All	All	1433/1482 (97%)	1403 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	203/207 (98%)	201 (99%)	2 (1%)	76 65
1	B	204/207 (99%)	202 (99%)	2 (1%)	76 65
1	C	203/207 (98%)	198 (98%)	5 (2%)	47 26
1	D	204/207 (99%)	200 (98%)	4 (2%)	55 36
1	E	204/207 (99%)	201 (98%)	3 (2%)	65 48
1	F	203/207 (98%)	199 (98%)	4 (2%)	55 36
All	All	1221/1242 (98%)	1201 (98%)	20 (2%)	62 46

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	LEU
1	A	104	LEU
1	B	88	LEU
1	B	104	LEU
1	C	59	LYS
1	C	88	LEU
1	C	104	LEU
1	C	140	LYS
1	C	234	PHE
1	D	43	LYS
1	D	88	LEU
1	D	104	LEU
1	D	128	LEU
1	E	68	LYS
1	E	88	LEU
1	E	104	LEU
1	F	88	LEU
1	F	104	LEU
1	F	128	LEU

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Mol	Chain	Res	Type
1	F	139	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	111	HIS

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

6 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	240/247 (97%)	-0.12	1 (0%) 92 93	22, 31, 51, 73	0
1	B	241/247 (97%)	-0.08	3 (1%) 79 82	22, 31, 51, 74	0
1	C	241/247 (97%)	0.14	12 (4%) 28 30	22, 32, 50, 84	0
1	D	241/247 (97%)	0.08	3 (1%) 79 82	23, 30, 48, 76	0
1	E	242/247 (97%)	0.04	8 (3%) 46 49	24, 33, 52, 90	0
1	F	240/247 (97%)	0.01	2 (0%) 86 88	23, 31, 51, 83	0
All	All	1445/1482 (97%)	0.01	29 (2%) 65 69	22, 31, 51, 90	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	190	ILE	3.8
1	E	140	LYS	3.0
1	E	190	ILE	2.8
1	E	133	LEU	2.7
1	F	205	ALA	2.7
1	C	140	LYS	2.7
1	B	207	VAL	2.7
1	C	184	ALA	2.5
1	B	205	ALA	2.5
1	C	205	ALA	2.5
1	C	142	GLY	2.5
1	C	234	PHE	2.4
1	C	141	ASP	2.4
1	D	81	TYR	2.3
1	A	132	LYS	2.3
1	E	141	ASP	2.3
1	E	183	ILE	2.3
1	C	133	LEU	2.2
1	D	72	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	137	GLU	2.2
1	D	103	TYR	2.2
1	C	70	GLY	2.2
1	F	235	ALA	2.2
1	E	207	VAL	2.2
1	C	173	ILE	2.2
1	E	135	SER	2.1
1	B	140	LYS	2.1
1	C	189	ASN	2.1
1	C	123	THR	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 (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MED	C	1001	9/9	0.86	0.20	26,32,38,47	0
2	MED	F	1001	9/9	0.98	0.13	24,30,37,37	0
2	MED	D	1001	9/9	0.98	0.17	24,29,35,35	0
2	MED	B	1001	9/9	0.99	0.11	23,27,39,39	0
2	MED	A	1001	9/9	0.99	0.10	20,32,38,38	0
2	MED	E	1001	9/9	0.99	0.10	22,29,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.