W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 11:50 PM GMT

PDB ID	:	5C8J
Title	:	A YidC-like protein in the archaeal plasma membrane
Authors	:	Borowska, M.T.; Dominik, P.K.; Anghel, S.A.; Kossiakoff, A.A.; Keenan, R.J.
Deposited on	:	2015-06-25
Resolution	:	3.50 Å(reported)

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

MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
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)	:	rb-20026982
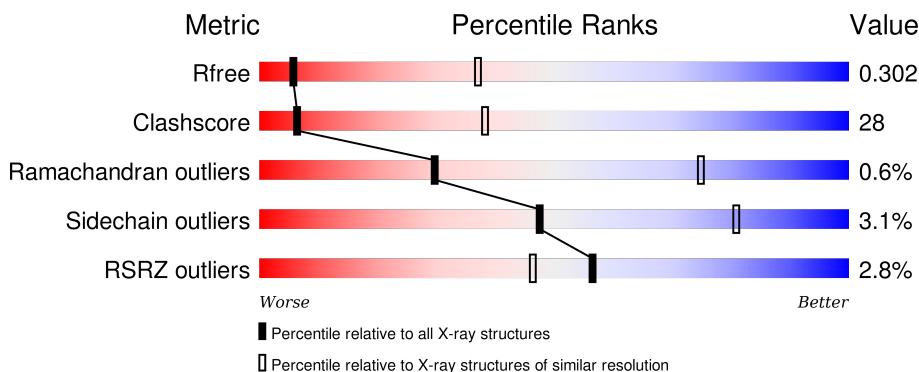
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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.
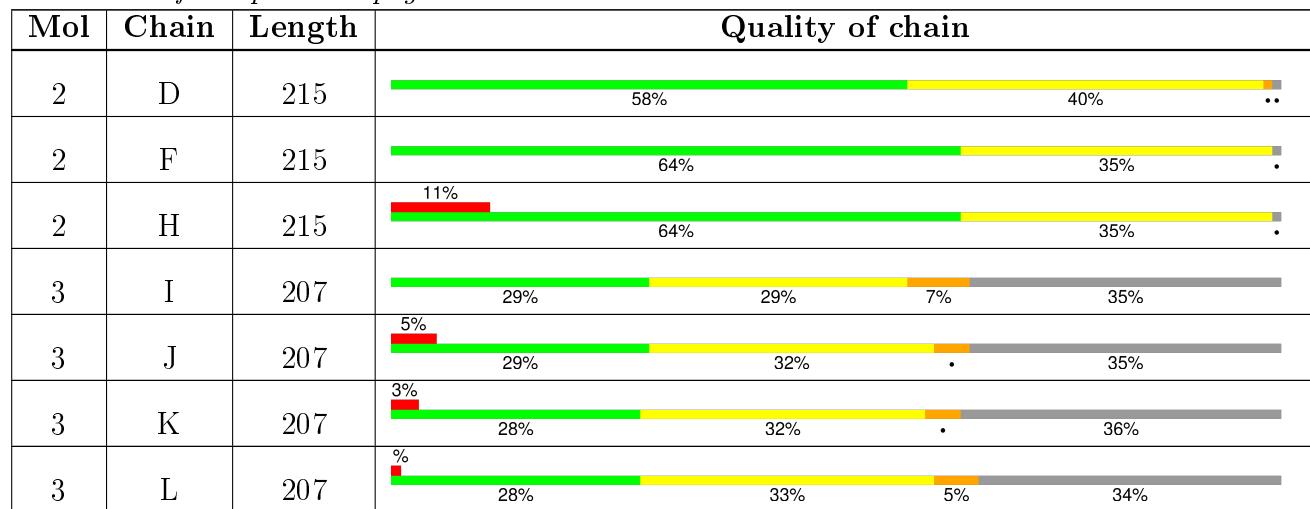
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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 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	239	
1	C	239	
1	E	239	
1	G	239	
2	B	215	

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Mol	Chain	Length	Quality of chain
2	D	215	58% 40%
2	F	215	64% 35%
2	H	215	11% 64% 35%
3	I	207	29% 29% 7% 35%
3	J	207	5% 29% 32% 35%
3	K	207	3% 28% 32% 36%
3	L	207	% 28% 33% 5% 34%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17889 atoms, of which 46 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 Antibody fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total 1725	C 1096	N 284	O 338	S 7	0	0	0
1	C	230	Total 1733	C 1100	N 285	O 340	S 8	0	0	0
1	E	230	Total 1731	C 1099	N 285	O 340	S 7	0	0	0
1	G	229	Total 1725	C 1096	N 284	O 338	S 7	0	0	0

- Molecule 2 is a protein called Antibody fragment, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total 1630	C 1013	N 277	O 334	S 6	0	0	0
2	D	212	Total 1620	C 1008	N 275	O 331	S 6	0	0	0
2	F	213	Total 1623	C 1010	N 276	O 332	S 5	0	0	0
2	H	213	Total 1623	C 1010	N 276	O 332	S 5	0	0	0
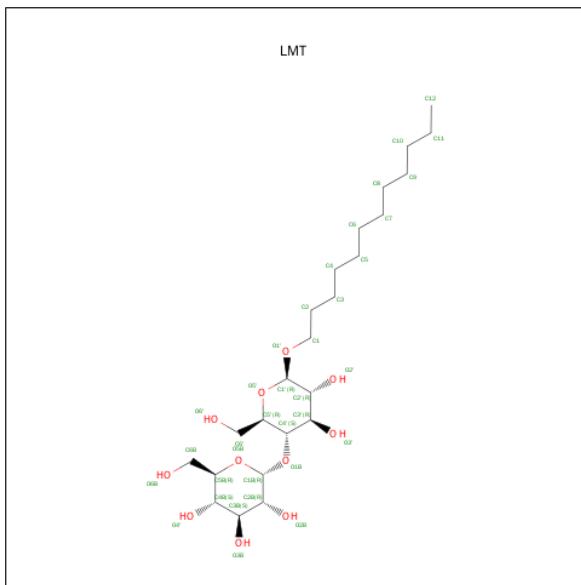
- Molecule 3 is a protein called Protein MJ0480.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	134	Total 1094	C 760	N 163	O 168	S 3	0	0	0
3	J	134	Total 1094	C 760	N 163	O 168	S 3	0	0	0
3	K	133	Total 1087	C 756	N 162	O 166	S 3	0	0	0
3	L	137	Total 1123	C 779	N 169	O 171	S 4	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	199	GLY	-	expression tag	UNP Q57904
I	200	SER	-	expression tag	UNP Q57904
I	201	SER	-	expression tag	UNP Q57904
I	202	HIS	-	expression tag	UNP Q57904
I	203	HIS	-	expression tag	UNP Q57904
I	204	HIS	-	expression tag	UNP Q57904
I	205	HIS	-	expression tag	UNP Q57904
I	206	HIS	-	expression tag	UNP Q57904
I	207	HIS	-	expression tag	UNP Q57904
J	199	GLY	-	expression tag	UNP Q57904
J	200	SER	-	expression tag	UNP Q57904
J	201	SER	-	expression tag	UNP Q57904
J	202	HIS	-	expression tag	UNP Q57904
J	203	HIS	-	expression tag	UNP Q57904
J	204	HIS	-	expression tag	UNP Q57904
J	205	HIS	-	expression tag	UNP Q57904
J	206	HIS	-	expression tag	UNP Q57904
J	207	HIS	-	expression tag	UNP Q57904
K	199	GLY	-	expression tag	UNP Q57904
K	200	SER	-	expression tag	UNP Q57904
K	201	SER	-	expression tag	UNP Q57904
K	202	HIS	-	expression tag	UNP Q57904
K	203	HIS	-	expression tag	UNP Q57904
K	204	HIS	-	expression tag	UNP Q57904
K	205	HIS	-	expression tag	UNP Q57904
K	206	HIS	-	expression tag	UNP Q57904
K	207	HIS	-	expression tag	UNP Q57904
L	199	GLY	-	expression tag	UNP Q57904
L	200	SER	-	expression tag	UNP Q57904
L	201	SER	-	expression tag	UNP Q57904
L	202	HIS	-	expression tag	UNP Q57904
L	203	HIS	-	expression tag	UNP Q57904
L	204	HIS	-	expression tag	UNP Q57904
L	205	HIS	-	expression tag	UNP Q57904
L	206	HIS	-	expression tag	UNP Q57904
L	207	HIS	-	expression tag	UNP Q57904

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).
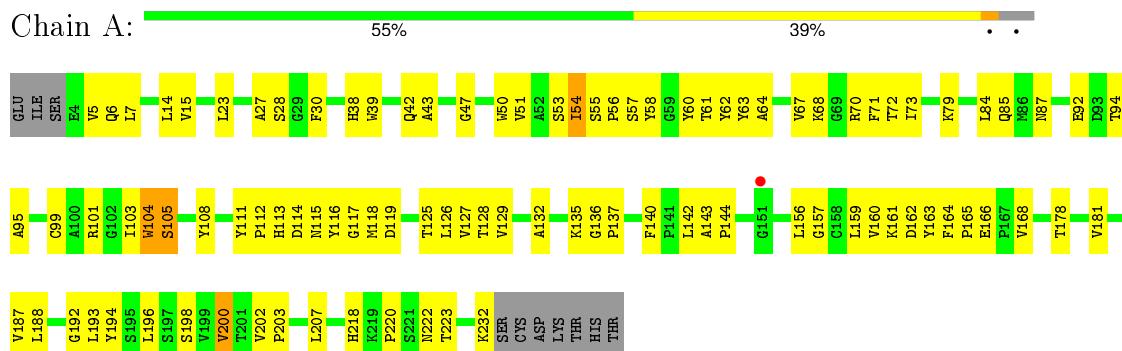
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	L	1	Total	C	H	O	0	0
			81	24	46	11		
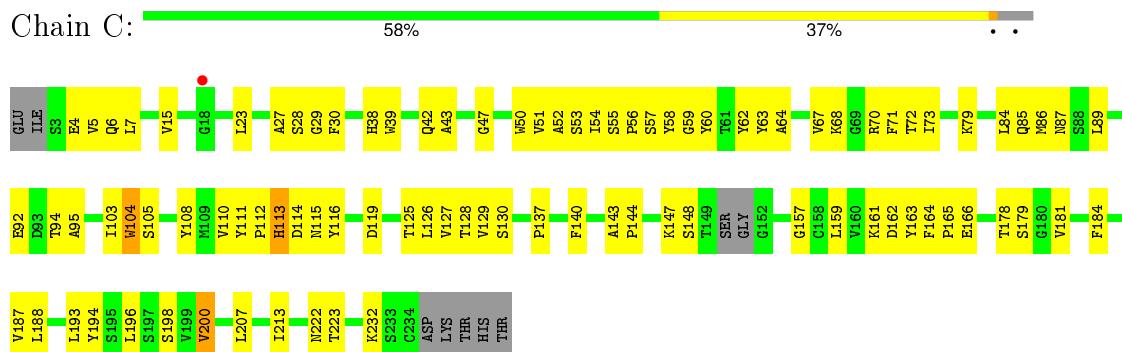
3 Residue-property plots ⓘ

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: Antibody fragment, heavy chain

- Molecule 1: Antibody fragment, heavy chain

- Molecule 1: Antibody fragment, heavy chain

• Molecule 1: Antibody fragment, heavy chain

Chain G:

• Molecule 2: Antibody fragment, light chain

Chain B:

• Molecule 2: Antibody fragment, light chain

Chain D:

• Molecule 2: Antibody fragment, light chain

Chain F:

V206 T207 K208 S209 F210 N211 E214 CYS

• Molecule 2: Antibody fragment, light chain

Chain H:

SER D2 I3 Q4 M5 T6 Q7 S15 D18 R19 V20 R25 Q28 S29 A33 V34 A35 W36 Y37 Q38 Q39 K40 P41 G42 K43 L48 I49 Y50 S51 A52 L55 V59 P60 S61 R62 S68 D71 L74 T75 I76 L79 Q80 P81 E82 D83 F84 A85 T86

Y87 Y88 C89 Q90 Q91 S92 S93 S94 R95 P96 V97 G102 T103 K104 I107 K108 P114 F119 P120 P121 S122 Q125 S128 G129 T130 A131 S132 V133 V134 C135 L136 F140 Y141 P142 R143 E144 A145 K146 V151 Q156 N159 S160 Q161 E162 E166 Q167 Y174 S175

L176 S177 S178 T179 L180 T181 L182 S183 K184 Y187 A194 H199 Q200 G201 L202 V206 S209 R212 G213 E214 CYS

• Molecule 3: Protein MJ0480

Chain I:

MET PHE GLY SER I5 Y9 K22 V23 L24 H25 P26 A27 I30 L31 I32 I36 V37 S38 L39 I40 I41 N42 I43 A44 T45 LYS LEU VAL ASP GLN LYS ARG VAL ALA GLU LEU LYS LYS GLU ILE GLN GLU GLN VAL LYS PHE LYS LYS MET SER LYS ASN PRO GLU

MET MET GLU LYS LEU GLN GLU GLN GLN ARG ILE MET GLN LEU ASN ALA GLU LEU MET LYS MET SER PHE ARG P102 M103 I104 Y105 T106 W107 V108 P109 I110 I111 L112 I113 F114 I115 Y116 L117 V120 I121 G122 F123 V126 Y127 L130 N131 W134 M135 G136 V137 V138 Y139 Y140

L141 P142 I143 I144 L145 S146 K147 I148 L149 F150 I151 D152 F153 W154 H155 W156 L157 I160 K163 F166 K167 I168 V169 S170 N171 T172 A173 L174 G175 W176 L177 G178 I181 F185 S188 L191 R192 K193 I194 LEU GLY ILE LYS GLY SER SER HIS HIS HIS HIS HIS

• Molecule 3: Protein MJ0480

Chain J:

MET PHE GLY SER I5 Y9 A15 I16 F17 M18 P19 I20 I21 K22 H25 P26 A27 I30 L31 I32 I36 V37 S38 L39 I40 I41 N42 I43 A44 T45 LYS LEU VAL ASP GLN LYS ARG VAL ALA GLU LEU LYS LYS GLU ILE GLN GLU GLN VAL LYS PHE LYS LYS

MET SER LYS ASN PRO GLU MET MET GLU LYS LEU GLN GLU GLN GLN ARG ILE MET GLN LEU ASN ALA GLU LEU MET LYS MET SER PHE ARG P102 M103 T106 W107 V108 P109 L112 I113 F114 I115 Y116 L117 V120 I121 G122 F123 G124 G125 V126 Y127 L130 N131 M135 G136

V137 V138 V139 Y140 L141 P142 I143 I144 L145 S146 K147 I148 L149 F150 F153 W154 H155 W156 L157 I160 F161 Y162 K163 G164 G165 F166 V169 S170 N171 T172 A173 L174 G175 W176 L177 G178 W179 Y180 I181 L182 C183 S184 F185 A186 T187 S188 L191 R192 K193 I194 LEU GLY ILE LYS GLY SER

SER HIS HIS HIS HIS HIS

• Molecule 3: Protein MJ0480

Chain K:

MET PHE GLY SER I5 F6 D7 I8 Y9 Y10 K11 D14 A15 I16 F17 M18 P19 I20 I21 K22 V23 L24 H25 P26 I32 I36 I40 I41 N42 I43 A44 THR LYS LEU LEU VAL ASP GLN LYS ARG VAL ALA GLU LEU LYS LYS GLU ILE GLN GLU PHE GLN VAL LYS PHE LYS

LYS MET SER LYS ASN PRO GLU MET MET GLU LYS LEU GLN GLN GLU GLU GLN GLN ARG ILE MET GLN GLN LEU ASN ALA GLU LEU MET LYS MET SER PHE ARG P102 M103 I104 Y105 T106 W107 V108 P109 I110 I111 L112 I113 F114 I115 Y116 L117 R118 H119 V120 Y121 V126 Y127 L130 N131 W134

N135 G136 V137 V138 V139 Y140 L141 P142 I143 I144 L145 I148 L149 F150 I151 W154 H155 W156 L157 I160 F161 Y162 K163 G164 G165 F166 K167 I168 V169 S170 N171 T172 A173 L174 G175 W176 L177 G178 W179 Y180 I181 L182 C183 S184 F185 A186 T187 L191 R192 K193 I194 LEU GLY ILE LYS GLY

SER SER HIS HIS HIS HIS HIS HIS

● Molecule 3: Protein MJ0480

Chain L: 28%   33%   5%   34%

MET PHE GLY SER I5 F6 D7 I8 Y9 Y10 K11 F17 I21 K22 V23 L24 H25 P26 I30 I31 I35 I36 I40 I41 N42 I43 A44 THR LYS LEU LEU VAL ASP GLN LYS ARG VAL ALA GLU LEU LYS LYS GLU ILE GLN GLU PHE GLN VAL LYS PHE LYS MET SER

LYS ASN PRO GLU MET MET GLU LYS LEU GLN GLU GLU GLN GLN ARG ILE MET GLN LEU ASN ALA GLU LEU MET LYS M98 S99 F100 R101 P102 M103 I104 Y105 T106 W107 V108 P109 I110 I111 L112 I113 F114 I115 Y116 L117 V120 Y121 V126 Y127 L130 W134 N135 G136 V137 V138 V139

Y140 L141 P142 I143 I144 L145 S146 K147 I148 L149 F150 I151 W154 H155 W156 L157 I160 F161 Y162 K163 G164 G165 F166 V169 S170 N171 T172 A173 L174 L177 G178 W179 Y180 I181 L182 F185 S188 L191 R192 K193 I194 LEU GLY ILE LYS GLY SER SER HIS HIS HIS HIS HIS HIS

HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	180.25Å 251.42Å 96.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.77 – 3.50 96.11 – 3.50	Depositor EDS
% Data completeness (in resolution range)	86.2 (89.77-3.50) 86.3 (96.11-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 3.49Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.253 , 0.302 0.252 , 0.302	Depositor DCC
R_{free} test set	2447 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	90.1	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 43.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.28$	Xtriage
Outliers	0 of 48191 reflections	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	17889	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.31% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0.26	0/1774	0.44	0/2422
1	C	0.27	0/1781	0.45	0/2430
1	E	0.26	0/1780	0.43	0/2430
1	G	0.26	0/1774	0.44	0/2422
2	B	0.25	0/1663	0.44	0/2255
2	D	0.24	0/1652	0.43	0/2239
2	F	0.25	0/1656	0.42	0/2247
2	H	0.25	0/1656	0.43	0/2247
3	I	0.25	0/1131	0.39	0/1546
3	J	0.26	0/1131	0.39	0/1546
3	K	0.24	0/1124	0.37	0/1536
3	L	0.25	0/1161	0.39	0/1585
All	All	0.25	0/18283	0.42	0/24905

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 (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	1725	0	1660	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1733	0	1665	88	0
1	E	1731	0	1665	83	0
1	G	1725	0	1660	96	0
2	B	1630	0	1590	82	0
2	D	1620	0	1580	82	0
2	F	1623	0	1585	66	0
2	H	1623	0	1585	69	0
3	I	1094	0	1150	113	0
3	J	1094	0	1150	97	0
3	K	1087	0	1143	99	0
3	L	1123	0	1178	108	0
4	L	35	46	44	1	0
All	All	17843	46	17655	983	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 28.

The worst 5 of 983 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)
3:L:41:ILE:HD11	3:L:106:THR:HB	1.34	1.06
1:E:103:ILE:HD13	1:E:119:ASP:HB2	1.34	1.05
1:G:137:PRO:HB3	1:G:163:TYR:HB3	1.37	1.03
1:A:135:LYS:HD2	1:A:193:LEU:HD11	1.44	0.99
3:I:148:ILE:HG23	3:L:150:PHE:HB3	1.46	0.97

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	227/239 (95%)	214 (94%)	13 (6%)	0	100	100
1	C	226/239 (95%)	216 (96%)	9 (4%)	1 (0%)	39	81
1	E	228/239 (95%)	214 (94%)	14 (6%)	0	100	100
1	G	227/239 (95%)	215 (95%)	11 (5%)	1 (0%)	39	81
2	B	212/215 (99%)	206 (97%)	6 (3%)	0	100	100
2	D	208/215 (97%)	201 (97%)	7 (3%)	0	100	100
2	F	211/215 (98%)	204 (97%)	7 (3%)	0	100	100
2	H	211/215 (98%)	203 (96%)	8 (4%)	0	100	100
3	I	130/207 (63%)	119 (92%)	7 (5%)	4 (3%)	5	41
3	J	130/207 (63%)	118 (91%)	10 (8%)	2 (2%)	13	56
3	K	129/207 (62%)	117 (91%)	9 (7%)	3 (2%)	8	48
3	L	133/207 (64%)	119 (90%)	12 (9%)	2 (2%)	13	56
All	All	2272/2644 (86%)	2146 (94%)	113 (5%)	13 (1%)	30	75

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	57	SER
3	I	137	VAL
3	I	169	VAL
3	J	137	VAL
3	J	169	VAL

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	191/201 (95%)	187 (98%)	4 (2%)	61	86
1	C	193/201 (96%)	190 (98%)	3 (2%)	70	89
1	E	192/201 (96%)	187 (97%)	5 (3%)	54	83
1	G	191/201 (95%)	187 (98%)	4 (2%)	61	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	189/190 (100%)	188 (100%)	1 (0%)	92	97
2	D	188/190 (99%)	186 (99%)	2 (1%)	80	92
2	F	188/190 (99%)	188 (100%)	0	100	100
2	H	188/190 (99%)	187 (100%)	1 (0%)	92	97
3	I	117/185 (63%)	105 (90%)	12 (10%)	9	40
3	J	117/185 (63%)	107 (92%)	10 (8%)	13	49
3	K	116/185 (63%)	108 (93%)	8 (7%)	19	59
3	L	120/185 (65%)	109 (91%)	11 (9%)	11	45
All	All	1990/2304 (86%)	1929 (97%)	61 (3%)	47	81

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	138	VAL
3	J	123	PHE
3	L	137	VAL
3	I	139	VAL
3	I	145	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	138	ASN
3	L	25	HIS
2	H	156	GLN
2	F	156	GLN
3	J	131	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
4	LMT	L	301	-	36,36,36	1.10	5 (13%)	47,47,47	1.07	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LMT	L	301	-	-	0/21/61/61	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	301	LMT	O3'-C3'	-2.71	1.36	1.43
4	L	301	LMT	O3B-C3B	-2.46	1.37	1.43
4	L	301	LMT	O2B-C2B	-2.25	1.37	1.43
4	L	301	LMT	O2'-C2'	-2.20	1.37	1.43
4	L	301	LMT	O4'-C4B	-2.15	1.37	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	301	LMT	C1-O1'-C1'	3.50	120.12	114.00
4	L	301	LMT	O1'-C1'-C2'	3.65	112.49	108.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	301	LMT	1	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	229/239 (95%)	-0.10	1 (0%)	93	90	65, 90, 131, 238	0
1	C	230/239 (96%)	-0.17	1 (0%)	93	90	51, 84, 131, 227	0
1	E	230/239 (96%)	-0.11	2 (0%)	85	78	64, 95, 178, 234	0
1	G	229/239 (95%)	0.18	12 (5%)	31	24	71, 114, 208, 242	0
2	B	214/215 (99%)	-0.23	1 (0%)	91	88	58, 95, 141, 184	0
2	D	212/215 (98%)	-0.27	0	100	100	68, 101, 139, 202	0
2	F	213/215 (99%)	-0.18	1 (0%)	91	88	69, 107, 148, 174	0
2	H	213/215 (99%)	0.28	24 (11%)	7	7	82, 135, 204, 239	0
3	I	134/207 (64%)	-0.15	1 (0%)	89	82	60, 112, 182, 229	0
3	J	134/207 (64%)	0.22	11 (8%)	14	12	81, 133, 220, 263	0
3	K	133/207 (64%)	0.40	7 (5%)	30	23	90, 145, 255, 279	0
3	L	137/207 (66%)	-0.09	3 (2%)	65	55	58, 107, 190, 256	0
All	All	2308/2644 (87%)	-0.04	64 (2%)	56	46	51, 105, 195, 279	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	42	ASN	6.5
2	H	178	SER	5.0
2	H	3	ILE	4.7
2	H	182	LEU	4.6
3	J	42	ASN	4.3

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors($Å^2$)	Q<0.9
4	LMT	L	301	35/35	0.64	0.21	-0.58	139,193,233,236	0

6.5 Other polymers (i)

There are no such residues in this entry.