wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 08:20 PM GMT

PDB ID	:	4XX1
Title	:	Low resolution structure of LCAT in complex with Fab1
Authors	:	Piper, D.E.; Walker, N.P.C.; Romanow, W.G.; Thibault, S.T.
Deposited on	:	2015-01-29
Resolution	:	3.60 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 3.60 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.
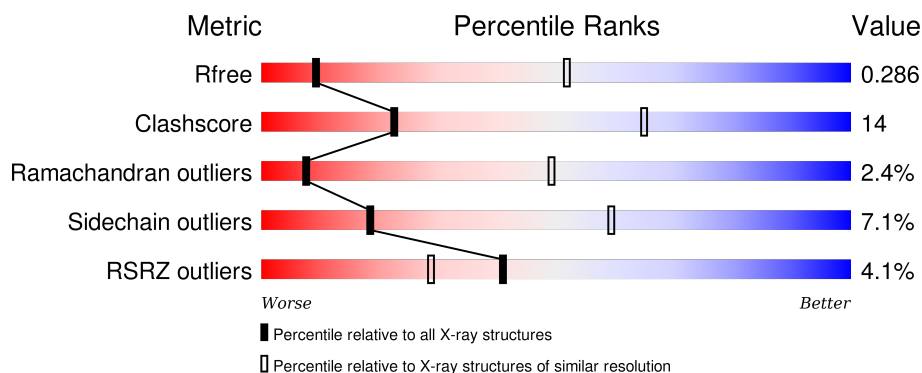
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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	G	213	5% / 67% 27% · ·
1	L	213	3% / 68% 27% · ·
1	O	213	14% / 24% 19% 5% 51%
2	E	238	2% / 66% 24% · 8%
2	H	238	7% / 68% 22% · 8%

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Mol	Chain	Length	Quality of chain
2	M	238	7% · · 17% · 26% · 8% · 48%
3	A	422	65% · 20% · 13%
3	B	422	66% · 19% · 13%
3	J	422	% · 54% · 28% · 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	J	502	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17233 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 Fab1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	210	Total 1577	C 990	N 259	O 323	S 5	0	0	0
1	G	210	Total 1577	C 990	N 259	O 323	S 5	0	0	0
1	O	105	Total 793	C 496	N 131	O 163	S 3	0	0	0

- Molecule 2 is a protein called Fab1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total 1668	C 1059	N 281	O 321	S 7	0	0	0
2	E	219	Total 1670	C 1060	N 281	O 322	S 7	0	0	0
2	M	124	Total 973	C 616	N 166	O 186	S 5	0	0	0

- Molecule 3 is a protein called Phosphatidylcholine-sterol acyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	369	Total 2970	C 1924	N 501	O 531	S 14	0	0	0
3	B	369	Total 2970	C 1924	N 501	O 531	S 14	0	0	0
3	J	361	Total 2909	C 1887	N 490	O 518	S 14	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	417	GLU	-	expression tag	UNP P04180
A	418	ASN	-	expression tag	UNP P04180

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Chain	Residue	Modelled	Actual	Comment	Reference
A	419	LEU	-	expression tag	UNP P04180
A	420	TYR	-	expression tag	UNP P04180
A	421	PHE	-	expression tag	UNP P04180
A	422	GLN	-	expression tag	UNP P04180
B	417	GLU	-	expression tag	UNP P04180
B	418	ASN	-	expression tag	UNP P04180
B	419	LEU	-	expression tag	UNP P04180
B	420	TYR	-	expression tag	UNP P04180
B	421	PHE	-	expression tag	UNP P04180
B	422	GLN	-	expression tag	UNP P04180
J	417	GLU	-	expression tag	UNP P04180
J	418	ASN	-	expression tag	UNP P04180
J	419	LEU	-	expression tag	UNP P04180
J	420	TYR	-	expression tag	UNP P04180
J	421	PHE	-	expression tag	UNP P04180
J	422	GLN	-	expression tag	UNP P04180

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
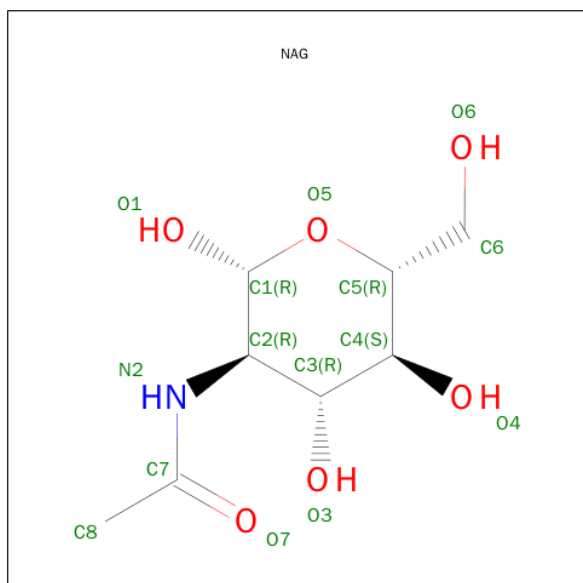
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	J	1	Total	C	N	O	0	0
			14	8	1	5		
4	J	1	Total	C	N	O	0	0
			14	8	1	5		
4	J	1	Total	C	N	O	0	0
			14	8	1	5		

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.
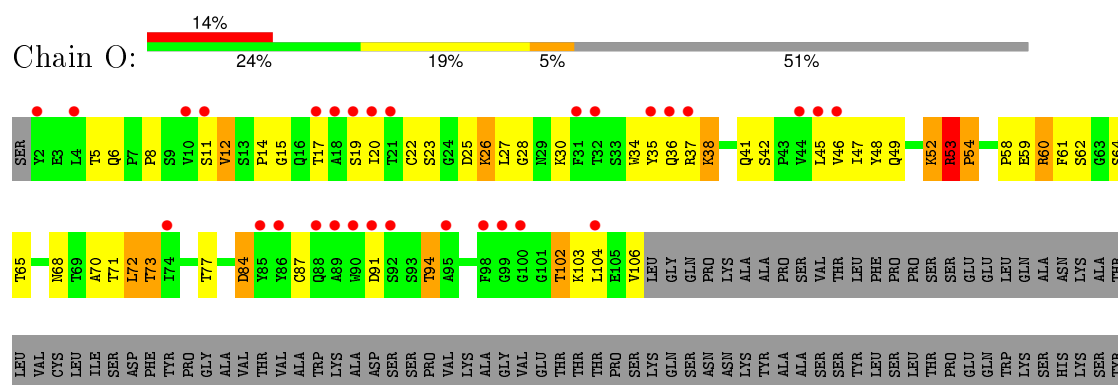
- Molecule 1: Fab1 light chain
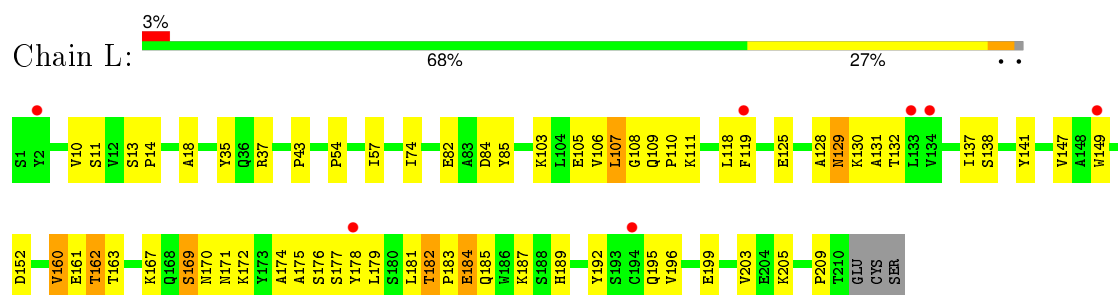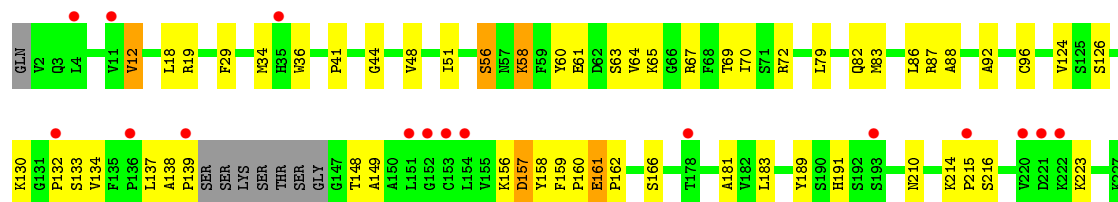

- Molecule 1: Fab1 light chain
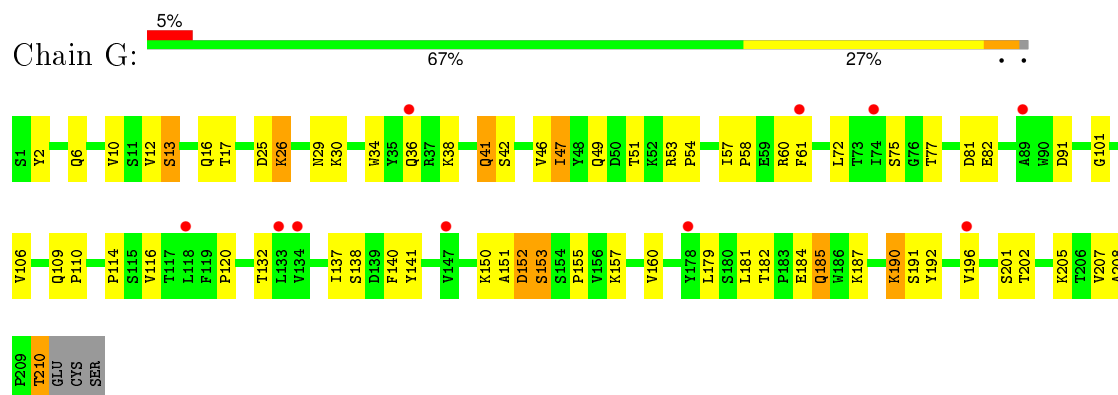
- Molecule 1: Fab1 light chain

SER CYS GLN VAL THR HIS GLY SER THR VAL GLU LYS THR VAL ALA PRO THR GLU CYS SER

● Molecule 2: Fab1 heavy chain
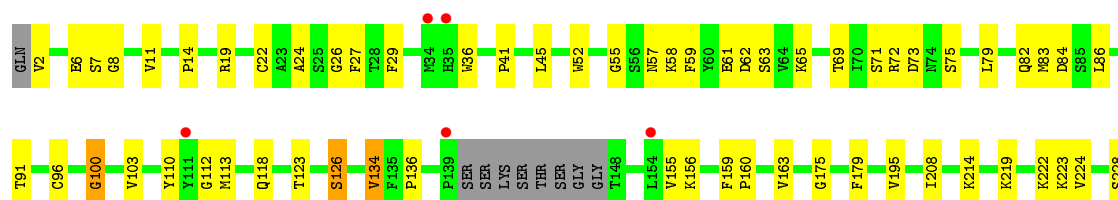
Chain H:

7%

68% 22% 8%

GLN V2 Q3 L4 V11 V12 L18 R19 F29 M34 H35 W36 P41 G44 V48 I51 S56 N57 K58 F59 Y60 E61 D62 S63 V64 K65 G66 R67 F68 T69 I70 S71 R72 L79 Q82 M83 L86 R87 A88 A92 C96 V124 S125 S126

K130 G131 P132 S133 V134 F135 P136 L137 A138 P139 SER SER LYS SER THR SER GLY G147 T148 A149 A150 L151 G152 C153 L154 V155 K156 D157 Y158 F159 P160 E161 P162 S166 T178 A181 V182 L183 Y189 S190 H191 S192 S193 N210 K214 P215 S216 V220 D221 K222 K223 K227

SER CYS ALA ALA ALA GLU ASN LEU TYR PHE GLN

● Molecule 2: Fab1 heavy chain

Chain E:

2%

66% 24% 8%

GLN V2 E6 S7 G8 V11 P14 R19 C22 A23 A24 S25 G26 F27 T28 F29 M34 H35 W36 P41 L45 W52 G55 S56 N57 K58 F59 Y60 E61 D62 S63 V64 K65 T69 I70 S71 R72 D73 N74 S75 L79 Q82 M83 D84 S85 L86

T91 C96 G100 V103 Y110 Y111 G112 M113 Q118 T123 S126 V134 F135 P136 P139 SER SER LYS SER THR SER GLY GLY T148 L154 V155 K156 F159 P160 V163 G175 F179 V195 I208 K214 K219 K222 K223 V224 S228

CYS ALA ALA ALA GLU ASN LEU TYR PHE GLN

● Molecule 2: Fab1 heavy chain

Chain M:

7%

17% 26% 8% 48%

GLN VAL Q3 L4 V5 E6 S7 G8 G9 G10 V11 V12 Q13 P14 G15 R16 S17 L18 R19 L20 S21 A24 F27 T28 F29 S30 S31 M34 H35 W36 V37 R38 Q39 A40 P41 G42 K43 G44 L45 E46 W47 V48 A49 V50 I51 W52 Y53 D54 G55 S56 N57 K58 D62 S63 V64

T69 I70 S71 R72 D73 N74 S75 K76 N77 T78 L79 Y80 L81 Q82 M83 D84 S85 L86 R87 A88 E89 D90 T91 A92 V93 Y94 Y95 C96 A97 R98 E99 G100 V103 R104 S105 Y108 S109 Y110 Y111 G112 M113 D114 V115 W116 G119 T120 T123 V124 S125 S126 ALA SER THR LYS GLY PRO

SER VAL PHE PRO LEU ALA PRO SER SER LYS SER THR SER GLY GLY THR ALA ALA LEU GLY CYS LEU VAL LYS ASP TYR PHE PRO GLU PRO VAL THR VAL SER TRP ASN SER GLY ALA LEU THR SER GLY VAL HIS THR PHE PRO ALA VAL LEU GLN SER SER GLY LEU TYR SER HIS SER

SER VAL VAL THR VAL PRO SER SER SER LEU GLY THR GLN THR TYR ILE CYS ASN VAL ASN HIS LYS PRO SER ASN THR LYS VAL ASP LYS LYS VAL GLU PRO LYS SER CYS ALA ALA ALA GLU ASN LEU TYR PHE GLN

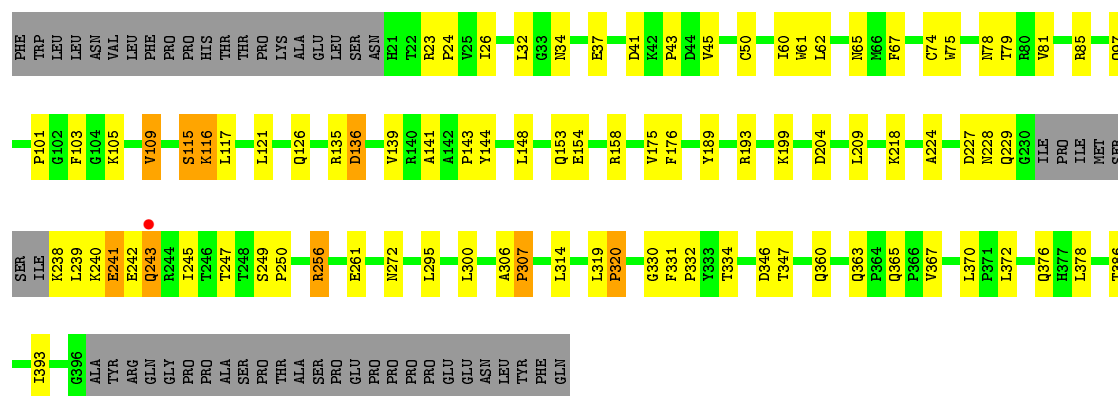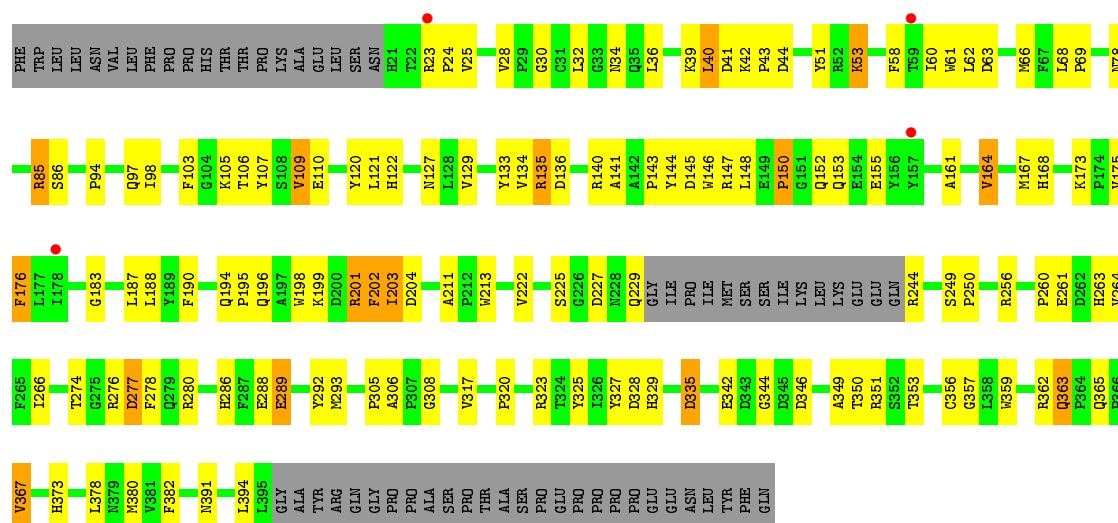● Molecule 3: Phosphatidylcholine-sterol acyltransferase

Chain A:

65% 20% 13%
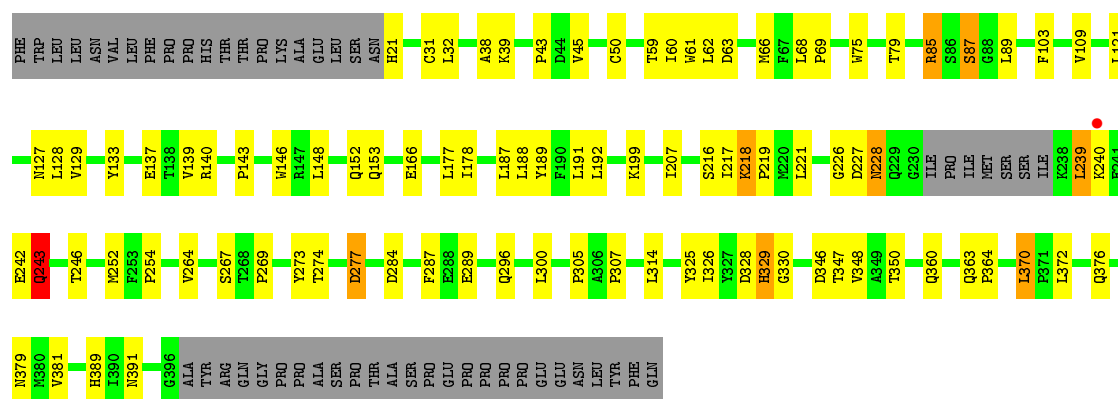
• Molecule 3: Phosphatidylcholine-sterol acyltransferase

Chain B:

• Molecule 3: Phosphatidylcholine-sterol acyltransferase

Chain J:

4   Data and refinement statistics   (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	166.42Å 166.42Å 97.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	72.06 – 3.60 80.85 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (72.06-3.60) 99.3 (80.85-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 3.58Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.196 , 0.280 0.215 , 0.286	Depositor DCC
R_{free} test set	1751 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	123.7	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 73.5	EDS
Estimated twinning fraction	0.045 for -h,-k,l 0.063 for h,-h-k,-l 0.047 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \lvert L \rvert > = 0.44, < L^2 > = 0.26$	Xtriage
Outliers	0 of 34814 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	17233	wwPDB-VP
Average B, all atoms (Å^2)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.29 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.9692e-03.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: NAG

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	G	0.30	0/1618	0.49	0/2211
1	L	0.32	0/1618	0.56	0/2211
1	O	0.35	0/813	0.61	0/1108
2	E	0.30	0/1714	0.48	0/2333
2	H	0.29	0/1712	0.46	0/2330
2	M	0.33	0/998	0.63	2/1351 (0.1%)
3	A	0.30	0/3063	0.48	0/4177
3	B	0.33	0/3063	0.50	0/4177
3	J	0.31	0/3002	0.51	0/4098
All	All	0.31	0/17601	0.51	2/23996 (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	L	0	2
1	O	0	2
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	20	LEU	CA-CB-CG	5.14	127.13	115.30
2	M	81	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	128	ALA	Peptide
1	L	184	GLU	Peptide
1	O	52	LYS	Peptide
1	O	53	ARG	Peptide

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	G	1577	0	1527	43	0
1	L	1577	0	1527	36	0
1	O	793	0	753	39	0
2	E	1670	0	1613	32	0
2	H	1668	0	1611	36	0
2	M	973	0	916	66	0
3	A	2970	0	2877	60	0
3	B	2970	0	2877	53	0
3	J	2909	0	2814	110	0
4	A	42	0	39	0	0
4	B	42	0	39	1	0
4	J	42	0	39	0	0
All	All	17233	0	16632	464	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 14.

The worst 5 of 464 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:A:216:SER:HG	3:A:218:LYS:HZ3	1.24	0.85
3:J:201:ARG:HG2	3:J:202:PHE:HD1	1.38	0.85
2:E:208:ILE:HG12	2:E:223:LYS:HB3	1.59	0.83
3:J:106:THR:HG23	3:J:135:ARG:HH12	1.41	0.83
2:M:8:GLY:HA3	2:M:20:LEU:HA	1.62	0.82

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	G	208/213 (98%)	185 (89%)	21 (10%)	2 (1%)	19	66
1	L	208/213 (98%)	184 (88%)	16 (8%)	8 (4%)	4	37
1	O	103/213 (48%)	79 (77%)	20 (19%)	4 (4%)	4	36
2	E	215/238 (90%)	193 (90%)	20 (9%)	2 (1%)	21	67
2	H	215/238 (90%)	185 (86%)	25 (12%)	5 (2%)	8	50
2	M	122/238 (51%)	88 (72%)	25 (20%)	9 (7%)	1	18
3	A	365/422 (86%)	329 (90%)	28 (8%)	8 (2%)	8	51
3	B	365/422 (86%)	331 (91%)	26 (7%)	8 (2%)	8	51
3	J	357/422 (85%)	321 (90%)	30 (8%)	6 (2%)	11	55
All	All	2158/2619 (82%)	1895 (88%)	211 (10%)	52 (2%)	7	49

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	107	LEU
1	L	160	VAL
1	L	170	ASN
1	L	209	PRO
3	A	239	LEU

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	G	178/181 (98%)	162 (91%)	16 (9%)	12	49
1	L	178/181 (98%)	172 (97%)	6 (3%)	44	80
1	O	88/181 (49%)	72 (82%)	16 (18%)	2	14
2	E	184/198 (93%)	177 (96%)	7 (4%)	40	77
2	H	183/198 (92%)	176 (96%)	7 (4%)	40	77
2	M	101/198 (51%)	79 (78%)	22 (22%)	1	9
3	A	319/367 (87%)	304 (95%)	15 (5%)	32	72
3	B	319/367 (87%)	302 (95%)	17 (5%)	28	69
3	J	313/367 (85%)	287 (92%)	26 (8%)	14	52
All	All	1863/2238 (83%)	1731 (93%)	132 (7%)	18	59

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	136	ASP
1	O	36	GLN
3	J	201	ARG
3	B	154	GLU
3	B	376	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	185	GLN
3	B	130	ASN
3	J	368	HIS
3	B	34	ASN
3	B	153	GLN

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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

9 ligands are 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	NAG	A	501	3	14,14,15	0.31	0	15,19,21	0.25	0
4	NAG	A	502	3	14,14,15	0.43	0	15,19,21	0.52	0
4	NAG	A	503	3	14,14,15	0.48	0	15,19,21	0.36	0
4	NAG	B	501	3	14,14,15	0.39	0	15,19,21	0.33	0
4	NAG	B	502	3	14,14,15	0.45	0	15,19,21	0.61	0
4	NAG	B	503	3	14,14,15	0.39	0	15,19,21	0.21	0
4	NAG	J	501	3	14,14,15	0.25	0	15,19,21	0.30	0
4	NAG	J	502	3	14,14,15	0.62	0	15,19,21	0.64	0
4	NAG	J	503	3	14,14,15	0.49	0	15,19,21	0.26	0

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	NAG	A	501	3	-	0/6/23/26	0/1/1/1
4	NAG	A	502	3	-	0/6/23/26	0/1/1/1
4	NAG	A	503	3	-	0/6/23/26	0/1/1/1
4	NAG	B	501	3	-	0/6/23/26	0/1/1/1
4	NAG	B	502	3	-	0/6/23/26	0/1/1/1
4	NAG	B	503	3	-	0/6/23/26	0/1/1/1
4	NAG	J	501	3	-	0/6/23/26	0/1/1/1
4	NAG	J	502	3	-	0/6/23/26	0/1/1/1
4	NAG	J	503	3	-	0/6/23/26	0/1/1/1

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	502	NAG	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(Å²)	Q<0.9
1	G	210/213 (98%)	0.14	10 (4%)	34	24	92, 144, 165, 174	0
1	L	210/213 (98%)	0.18	7 (3%)	50	36	79, 127, 171, 179	0
1	O	105/213 (49%)	1.36	30 (28%)	1	1	162, 187, 200, 202	0
2	E	219/238 (92%)	0.11	5 (2%)	64	48	89, 121, 140, 163	0
2	H	219/238 (92%)	0.44	16 (7%)	18	12	85, 134, 166, 173	0
2	M	124/238 (52%)	0.82	16 (12%)	5	4	146, 182, 192, 195	0
3	A	369/422 (87%)	0.06	1 (0%)	94	90	84, 106, 139, 165	0
3	B	369/422 (87%)	0.07	1 (0%)	94	90	69, 95, 126, 162	0
3	J	361/422 (85%)	0.09	4 (1%)	82	70	102, 133, 158, 179	0
All	All	2186/2619 (83%)	0.23	90 (4%)	41	29	69, 123, 184, 202	0

The worst 5 of 90 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	20	ILE	6.9
2	M	37	VAL	6.0
2	M	45	LEU	5.8
1	O	32	THR	5.4
1	O	89	ALA	5.4

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	NAG	J	502	14/15	0.90	0.35	2.37	102,134,141,142	0
4	NAG	B	502	14/15	0.92	0.36	1.40	96,111,124,124	0
4	NAG	A	502	14/15	0.91	0.23	0.03	100,122,132,136	0
4	NAG	B	501	14/15	0.93	0.22	-0.57	126,140,150,152	0
4	NAG	J	503	14/15	0.80	0.28	-	169,181,191,191	0
4	NAG	J	501	14/15	0.82	0.28	-	157,174,183,183	0
4	NAG	B	503	14/15	0.71	0.32	-	164,187,192,193	0
4	NAG	A	503	14/15	0.83	0.39	-	168,181,189,192	0
4	NAG	A	501	14/15	0.83	0.27	-	153,164,174,174	0

6.5 Other polymers (i)

There are no such residues in this entry.