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

Full wwPDB X-ray Structure Validation Report (i)

Aug 3, 2016 – 09:32 AM EDT

PDB ID	:	5KSD
Title	:	Crystal Structure of a Plasma Membrane Proton Pump
Authors	:	Croll, T.; Pedersen, B.P.; Nissen, P.
Deposited on	:	2016-07-08
Resolution	:	3.50 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 (i)) were used in the production of this report:

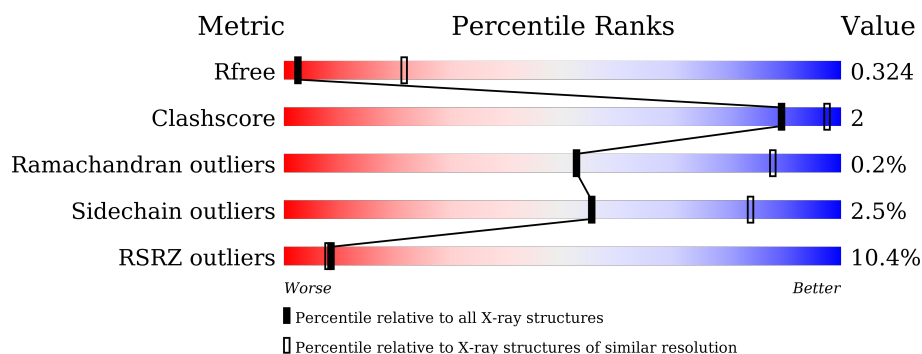|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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	Percentile Ranks	Value
Rfree		0.324
Clashscore		2
Ramachandran outliers		0.2%
Sidechain outliers		2.5%
RSRZ outliers		10.4%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

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	833	10% 91% 9%
1	B	833	11% 91% 9%

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
5	LMT	A	905	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12970 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 ATPase 2, plasma membrane-type.

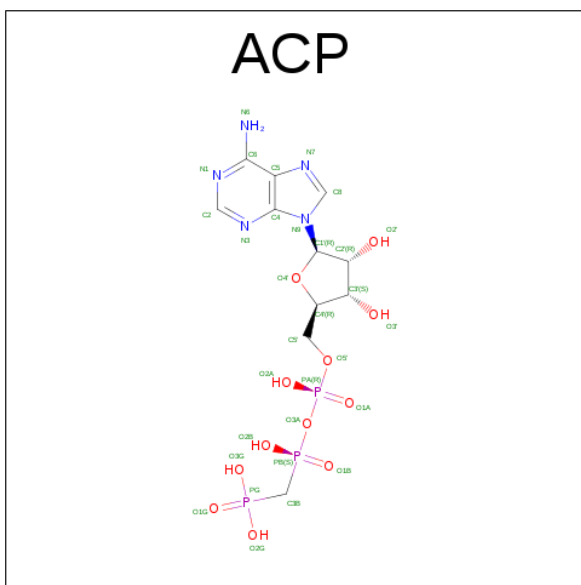| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	833	Total 6416	C 4132	N 1082	O 1169	S 33	0	0	0
1	B	833	Total 6416	C 4132	N 1082	O 1169	S 33	0	0	0

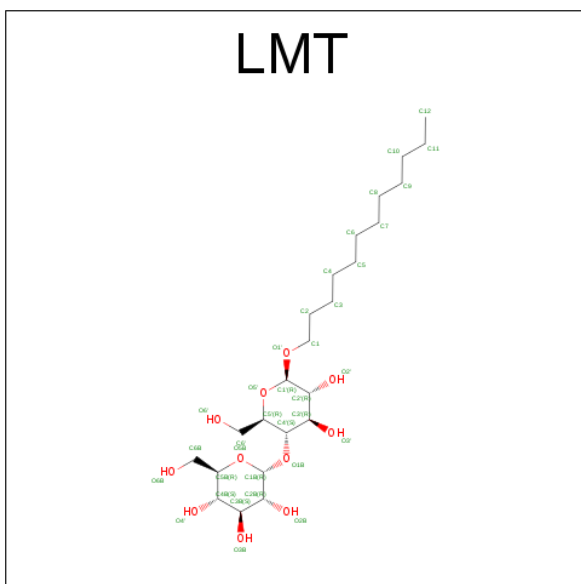- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Mg 2	0	0
2	A	2	Total 2	Mg 2	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	K 1	0	0
3	A	1	Total 1	K 1	0	0

- Molecule 4 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
4	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 5 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).

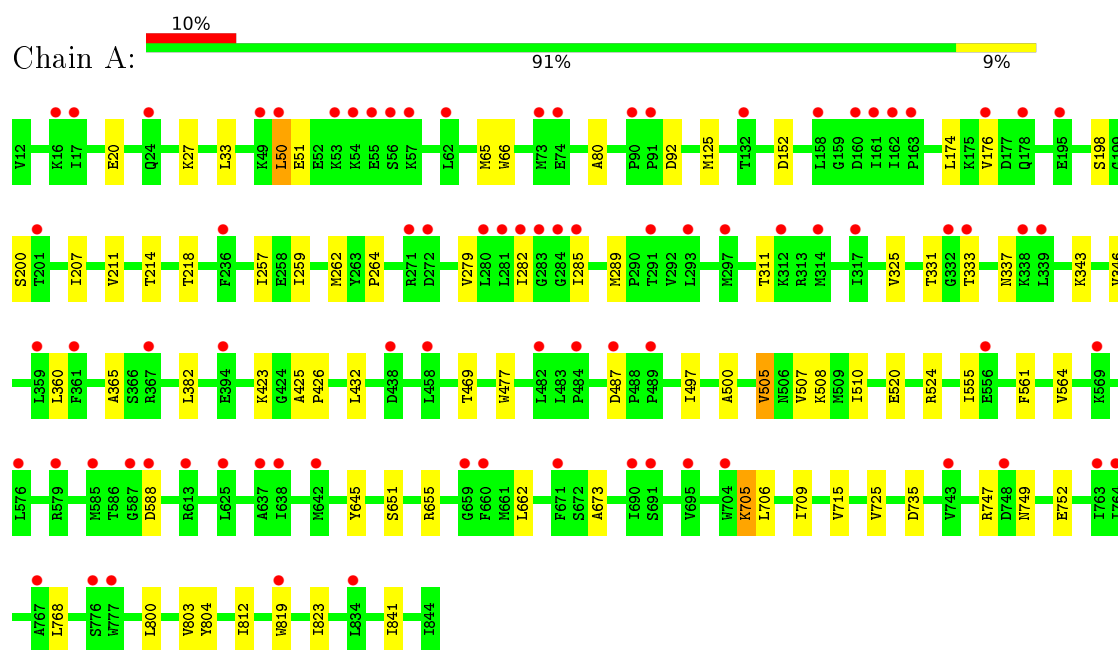| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			35	24	11		

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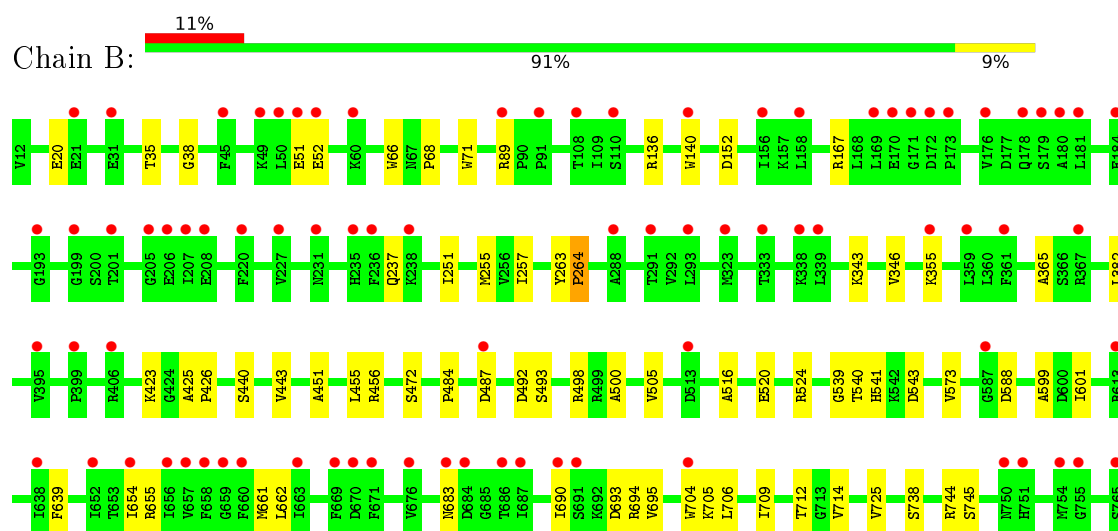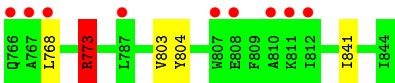| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	B	1	35	24	11	0	0

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: ATPase 2, plasma membrane-type

• Molecule 1: ATPase 2, plasma membrane-type

Q766 A767 L768 R773 L787 V803 Y804 W807 E808 F809 A810 K811 I812 I841 I844

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.29Å 144.42Å 312.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.02 – 3.50	Depositor
	84.41 – 3.50	EDS
% Data completeness	99.7 (52.02-3.50)	Depositor
(in resolution range)	99.7 (84.41-3.50)	EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.64 (at 3.49Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.287 , 0.324	Depositor
	0.287 , 0.324	DCC
R_{free} test set	1996 reflections (4.04%)	DCC
Wilson B-factor (Å^2)	109.6	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 35.7	EDS
L-test for twinning[2]	$<|L|> = 0.32, <L^2> = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.70	EDS
Total number of atoms	12970	wwPDB-VP
Average B, all atoms (Å^2)	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: K, ACP, LMT, MG

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	0.27	1/6542 (0.0%)	0.50	0/8865
1	B	0.26	0/6542	0.53	2/8865 (0.0%)
All	All	0.27	1/13084 (0.0%)	0.51	2/17730 (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	A	0	1
1	B	0	4
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	ILE	C-N	8.26	1.50	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	773	ARG	CD-NE-CZ	9.48	136.87	123.60
1	B	773	ARG	NE-CZ-NH1	-5.90	117.35	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	487	ASP	Peptide
1	B	456	ARG	Sidechain
1	B	472	SER	Peptide
1	B	487	ASP	Peptide
1	B	773	ARG	Sidechain

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	6416	0	6588	31	0
1	B	6416	0	6588	32	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	13	0	0
4	B	31	0	13	0	0
5	A	35	0	46	0	0
5	B	35	0	46	0	0
All	All	12970	0	13294	63	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 2.

All (63) 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:A:497:ILE:HD13	1:A:507:VAL:HB	1.83	0.60
1:B:662:LEU:HD23	1:B:725:VAL:HG21	1.85	0.57
1:A:520:GLU:HG3	1:A:524:ARG:HH12	1.70	0.57
1:A:500:ALA:HB1	1:A:505:VAL:HG23	1.87	0.56
1:A:651:SER:HB3	1:A:768:LEU:HD21	1.88	0.55
1:A:279:VAL:HA	1:A:282:ILE:HG22	1.89	0.54
1:A:331:THR:O	1:A:337:ASN:ND2	2.40	0.54
1:B:68:PRO:HA	1:B:71:TRP:CD1	2.43	0.54
1:B:451:ALA:HB1	1:B:516:ALA:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:712:THR:HA	1:B:841:ILE:HG12	1.90	0.53
1:A:365:ALA:HB3	1:A:423:LYS:HG3	1.91	0.53
1:B:520:GLU:HG3	1:B:524:ARG:HH12	1.76	0.51
1:A:80:ALA:HB1	1:A:92:ASP:HB3	1.92	0.51
1:B:500:ALA:HB1	1:B:505:VAL:HG13	1.93	0.50
1:B:573:VAL:HG21	1:B:599:ALA:HA	1.94	0.49
1:B:492:ASP:OD2	1:B:493:SER:N	2.46	0.49
1:A:662:LEU:HD23	1:A:725:VAL:HG21	1.95	0.48
1:A:432:LEU:HB3	1:A:477:TRP:CD1	2.49	0.48
1:B:343:LYS:HA	1:B:346:VAL:HG23	1.95	0.48
1:B:346:VAL:O	1:B:355:LYS:NZ	2.35	0.47
1:B:455:LEU:HD13	1:B:484:PRO:HB2	1.94	0.47
1:A:555:ILE:HG23	1:A:561:PHE:CZ	2.50	0.46
1:B:639:PHE:CE2	1:B:704:TRP:HB2	2.51	0.46
1:B:540:THR:HG23	1:B:541:HIS:H	1.81	0.46
1:B:639:PHE:CZ	1:B:704:TRP:HB2	2.52	0.46
1:A:555:ILE:HG23	1:A:561:PHE:HZ	1.80	0.45
1:A:800:LEU:HA	1:A:803:VAL:HG22	1.97	0.45
1:B:51:GLU:O	1:B:52:GLU:HB3	2.16	0.45
1:A:152:ASP:O	1:A:211:VAL:HG22	2.16	0.45
1:A:705:LYS:H	1:A:705:LYS:HD2	1.81	0.45
1:A:749:ASN:ND2	1:A:752:GLU:OE1	2.50	0.45
1:B:738:SER:HB3	1:B:745:SER:HA	1.99	0.45
1:A:289:MET:HA	1:A:645:TYR:HE2	1.81	0.45
1:B:690:ILE:HG23	1:B:773:ARG:NH1	2.33	0.44
1:B:263:TYR:HB3	1:B:264:PRO:HD3	2.00	0.44
1:A:50:LEU:HD13	1:A:51:GLU:H	1.82	0.44
1:B:539:GLY:HA2	1:B:543:ASP:HA	1.98	0.44
1:A:715:VAL:HG21	1:A:841:ILE:HB	1.99	0.44
1:A:343:LYS:HA	1:A:346:VAL:HG23	2.00	0.44
1:B:136:ARG:NH2	1:B:152:ASP:OD1	2.41	0.43
1:A:803:VAL:HG23	1:A:804:TYR:CG	2.53	0.43
1:A:259:ILE:HA	1:A:262:MET:HG2	2.00	0.43
1:A:706:LEU:HD23	1:A:709:ILE:HD11	2.00	0.43
1:A:735:ASP:CG	1:A:747:ARG:HH21	2.22	0.43
1:B:693:ASP:OD1	1:B:694:ARG:N	2.40	0.43
1:B:68:PRO:HA	1:B:71:TRP:HD1	1.83	0.43
1:A:176:VAL:HB	1:A:200:SER:OG	2.19	0.42
1:B:803:VAL:HG23	1:B:804:TYR:CG	2.54	0.42
1:A:510:ILE:HG23	1:A:564:VAL:HG21	2.01	0.42
1:B:35:THR:HG23	1:B:38:GLY:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ALA:HA	1:B:426:PRO:HD3	1.88	0.42
1:B:654:ILE:HG12	1:B:714:VAL:HA	2.02	0.42
1:A:279:VAL:HG12	1:A:673:ALA:HA	2.02	0.41
1:A:198:SER:OG	1:A:218:THR:HG21	2.20	0.41
1:B:365:ALA:HB3	1:B:423:LYS:HG3	2.01	0.41
1:A:325:VAL:HG21	1:A:508:LYS:HE2	2.03	0.41
1:B:251:ILE:O	1:B:255:MET:HG2	2.21	0.41
1:A:425:ALA:HA	1:A:426:PRO:HD3	1.92	0.41
1:B:20:GLU:HG3	1:B:167:ARG:HH22	1.86	0.41
1:B:601:ILE:N	1:B:601:ILE:HD12	2.35	0.41
1:A:819:TRP:CD1	1:A:823:ILE:HD11	2.56	0.40
1:B:706:LEU:HD23	1:B:709:ILE:HD11	2.02	0.40
1:B:440:SER:HA	1:B:443:VAL:HG22	2.03	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	831/833 (100%)	785 (94%)	44 (5%)	2 (0%)	52	88
1	B	831/833 (100%)	777 (94%)	52 (6%)	2 (0%)	52	88
All	All	1662/1666 (100%)	1562 (94%)	96 (6%)	4 (0%)	52	88

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	ILE
1	B	257	ILE
1	A	264	PRO
1	B	264	PRO

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	685/685 (100%)	665 (97%)	20 (3%)	50	81
1	B	685/685 (100%)	671 (98%)	14 (2%)	63	87
All	All	1370/1370 (100%)	1336 (98%)	34 (2%)	55	84

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	27	LYS
1	A	33	LEU
1	A	50	LEU
1	A	65	MET
1	A	66	TRP
1	A	125	MET
1	A	174	LEU
1	A	207	ILE
1	A	214	THR
1	A	311	THR
1	A	333	THR
1	A	360	LEU
1	A	382	LEU
1	A	469	THR
1	A	505	VAL
1	A	588	ASP
1	A	655	ARG
1	A	705	LYS
1	A	812	ILE
1	B	66	TRP
1	B	89	ARG
1	B	140	TRP
1	B	237	GLN
1	B	382	LEU
1	B	498	ARG
1	B	588	ASP

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Mol	Chain	Res	Type
1	B	655	ARG
1	B	661	MET
1	B	683	ASN
1	B	695	VAL
1	B	705	LYS
1	B	744	ARG
1	B	768	LEU

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

Mol	Chain	Res	Type
1	B	720	GLN

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)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

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	ACP	A	904	2	29,33,33	4.52	11 (37%)	29,52,52	2.79	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	LMT	A	905	-	36,36,36	1.20	4 (11%)	47,47,47	0.94	1 (2%)
4	ACP	B	904	2	29,33,33	4.56	11 (37%)	29,52,52	2.78	2 (6%)
5	LMT	B	905	-	36,36,36	1.21	4 (11%)	47,47,47	1.03	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	ACP	A	904	2	-	0/15/38/38	0/3/3/3
5	LMT	A	905	-	-	0/21/61/61	0/2/2/2
4	ACP	B	904	2	-	0/15/38/38	0/3/3/3
5	LMT	B	905	-	-	0/21/61/61	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	904	ACP	C2'-C1'	-13.53	1.32	1.53
4	A	904	ACP	C2'-C1'	-13.34	1.32	1.53
4	A	904	ACP	O4'-C4'	-6.56	1.30	1.45
4	B	904	ACP	O4'-C4'	-6.47	1.30	1.45
4	A	904	ACP	PB-O2B	-3.08	1.49	1.56
4	A	904	ACP	O3'-C3'	-2.75	1.36	1.43
4	B	904	ACP	O3'-C3'	-2.73	1.36	1.43
4	B	904	ACP	PB-O2B	-2.57	1.50	1.56
5	A	905	LMT	O3B-C3B	2.15	1.48	1.43
5	B	905	LMT	O3B-C3B	2.19	1.48	1.43
5	B	905	LMT	C2-C1	2.33	1.61	1.51
5	A	905	LMT	C2-C1	2.39	1.61	1.51
5	A	905	LMT	O5B-C1B	2.64	1.48	1.41
5	B	905	LMT	O5B-C1B	2.80	1.49	1.41
5	A	905	LMT	O5'-C1'	3.01	1.49	1.41
5	B	905	LMT	O5'-C1'	3.03	1.49	1.41
4	A	904	ACP	C2-N3	3.04	1.37	1.32
4	B	904	ACP	C2-N3	3.04	1.37	1.32
4	A	904	ACP	PG-C3B	3.45	1.83	1.80
4	B	904	ACP	PG-C3B	3.48	1.83	1.80
4	B	904	ACP	O2'-C2'	3.79	1.51	1.43
4	A	904	ACP	O2'-C2'	3.84	1.52	1.43
4	B	904	ACP	C6-N6	4.46	1.52	1.34
4	A	904	ACP	C6-N6	4.47	1.52	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	904	ACP	PB-C3B	4.78	1.85	1.80
4	B	904	ACP	PB-C3B	5.29	1.85	1.80
4	A	904	ACP	PB-O3A	6.93	1.66	1.58
4	B	904	ACP	PB-O3A	7.16	1.66	1.58
4	A	904	ACP	O4'-C1'	14.22	1.61	1.41
4	B	904	ACP	O4'-C1'	14.24	1.61	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	904	ACP	N3-C2-N1	-11.61	119.75	128.87
4	B	904	ACP	N3-C2-N1	-11.61	119.75	128.87
4	B	904	ACP	N6-C6-N1	-8.26	104.66	118.52
4	A	904	ACP	N6-C6-N1	-8.14	104.86	118.52
5	B	905	LMT	C1B-O1B-C4'	-3.00	110.02	118.00
5	A	905	LMT	C1B-O1B-C4'	-2.78	110.60	118.00
4	A	904	ACP	C5'-C4'-C3'	-2.04	107.31	115.20
5	B	905	LMT	O1'-C1'-C2'	2.85	111.50	108.00

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 (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	A	833/833 (100%)	0.47	82 (9%)	10	9	69, 129, 195, 256	0
1	B	833/833 (100%)	0.54	91 (10%)	7	7	65, 136, 227, 311	0
All	All	1666/1666 (100%)	0.51	173 (10%)	8	8	65, 133, 215, 311	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	54	LYS	8.5
1	A	283	GLY	8.2
1	B	170	GLU	7.7
1	B	50	LEU	7.4
1	B	181	LEU	7.2
1	B	49	LYS	6.3
1	B	180	ALA	6.0
1	A	284	GLY	6.0
1	B	487	ASP	5.4
1	B	660	PHE	5.0
1	B	206	GLU	4.7
1	B	808	GLU	4.7
1	B	658	PHE	4.6
1	A	55	GLU	4.5
1	A	161	ILE	4.5
1	A	49	LYS	4.3
1	A	50	LEU	4.3
1	B	338	LYS	4.3
1	B	207	ILE	4.3
1	A	282	ILE	4.3
1	B	227	VAL	4.2
1	B	52	GLU	4.2
1	A	588	ASP	4.2
1	B	750	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	748	ASP	4.1
1	B	687	ILE	4.1
1	A	56	SER	4.1
1	A	487	ASP	4.1
1	B	21	GLU	4.0
1	B	205	GLY	4.0
1	A	613	ARG	3.9
1	B	671	PHE	3.9
1	A	660	PHE	3.9
1	B	683	ASN	3.8
1	B	235	HIS	3.7
1	B	323	MET	3.7
1	B	659	GLY	3.7
1	B	178	GLN	3.7
1	B	768	LEU	3.7
1	A	458	LEU	3.7
1	B	669	PHE	3.6
1	B	339	LEU	3.6
1	A	17	ILE	3.5
1	A	271	ARG	3.5
1	B	810	ALA	3.5
1	B	670	ASP	3.5
1	B	176	VAL	3.5
1	A	704	TRP	3.5
1	A	90	PRO	3.4
1	B	31	GLU	3.4
1	B	686	THR	3.3
1	A	556	GLU	3.3
1	B	201	THR	3.3
1	B	690	ILE	3.3
1	B	293	LEU	3.3
1	A	638	ILE	3.3
1	A	587	GLY	3.3
1	A	359	LEU	3.2
1	A	484	PRO	3.2
1	B	184	GLU	3.2
1	B	754	MET	3.2
1	B	751	HIS	3.2
1	B	169	LEU	3.1
1	A	438	ASP	3.1
1	A	62	LEU	3.1
1	B	811	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	156	ILE	2.9
1	A	291	THR	2.9
1	A	280	LEU	2.9
1	B	89	ARG	2.9
1	A	579	ARG	2.9
1	B	236	PHE	2.9
1	A	293	LEU	2.8
1	B	787	LEU	2.8
1	A	236	PHE	2.8
1	B	367	ARG	2.8
1	A	763	ILE	2.8
1	A	819	TRP	2.8
1	B	755	GLY	2.7
1	A	312	LYS	2.7
1	B	333	THR	2.7
1	B	231	ASN	2.7
1	A	201	THR	2.7
1	A	332	GLY	2.7
1	B	587	GLY	2.7
1	A	777	TRP	2.6
1	A	743	VAL	2.6
1	B	691	SER	2.6
1	A	482	LEU	2.6
1	A	297	MET	2.6
1	B	684	ASP	2.6
1	B	807	TRP	2.6
1	B	220	PHE	2.6
1	A	338	LYS	2.6
1	A	776	SER	2.6
1	A	695	VAL	2.6
1	A	691	SER	2.6
1	B	765	SER	2.6
1	A	160	ASP	2.6
1	A	394	GLU	2.6
1	A	178	GLN	2.6
1	B	208	GLU	2.5
1	A	16	LYS	2.5
1	A	285	ILE	2.5
1	B	654	ILE	2.5
1	B	513	ASP	2.5
1	B	812	ILE	2.5
1	A	176	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	663	ILE	2.5
1	A	272	ASP	2.5
1	A	625	LEU	2.5
1	A	767	ALA	2.5
1	A	569	LYS	2.4
1	B	399	PRO	2.4
1	B	173	PRO	2.4
1	B	652	ILE	2.4
1	A	361	PHE	2.4
1	B	179	SER	2.4
1	A	73	MET	2.4
1	A	74	GLU	2.4
1	B	291	THR	2.4
1	A	576	LEU	2.4
1	B	51	GLU	2.4
1	A	57	LYS	2.3
1	B	613	ARG	2.3
1	A	91	PRO	2.3
1	B	406	ARG	2.3
1	B	359	LEU	2.3
1	A	637	ALA	2.3
1	B	60	LYS	2.3
1	B	45	PHE	2.3
1	A	585	MET	2.3
1	A	367	ARG	2.3
1	A	163	PRO	2.3
1	B	395	VAL	2.3
1	A	195	GLU	2.2
1	B	288	ALA	2.2
1	B	638	ILE	2.2
1	A	53	LYS	2.2
1	A	642	MET	2.2
1	A	671	PHE	2.2
1	B	193	GLY	2.2
1	B	171	GLY	2.2
1	B	676	VAL	2.2
1	B	355	LYS	2.2
1	B	108	THR	2.2
1	A	339	LEU	2.2
1	A	24	GLN	2.2
1	B	361	PHE	2.2
1	B	158	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	656	ILE	2.2
1	A	314	MET	2.1
1	B	91	PRO	2.1
1	B	657	VAL	2.1
1	B	110	SER	2.1
1	A	659	GLY	2.1
1	B	140	TRP	2.1
1	B	238	LYS	2.1
1	A	132	THR	2.1
1	B	766	GLN	2.1
1	A	489	PRO	2.1
1	B	199	GLY	2.1
1	B	704	TRP	2.1
1	A	162	ILE	2.1
1	A	764	ILE	2.1
1	A	158	LEU	2.1
1	A	333	THR	2.1
1	A	317	ILE	2.0
1	B	767	ALA	2.0
1	A	690	ILE	2.0
1	A	834	LEU	2.0
1	B	172	ASP	2.0
1	A	281	LEU	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. 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
5	LMT	A	905	35/35	0.74	0.65	1.65	98,158,193,193	0
4	ACP	A	904	31/31	0.89	0.34	-0.40	85,106,143,161	0
4	ACP	B	904	31/31	0.85	0.31	-0.52	74,132,160,193	0
5	LMT	B	905	35/35	0.86	0.21	-1.14	79,106,134,153	0
3	K	B	903	1/1	0.91	0.17	-1.16	117,117,117,117	0
3	K	A	903	1/1	0.92	0.09	-2.56	108,108,108,108	0
2	MG	A	901	1/1	0.71	0.57	-	140,140,140,140	0
2	MG	B	902	1/1	0.90	0.61	-	111,111,111,111	0
2	MG	B	901	1/1	0.74	0.27	-	104,104,104,104	0
2	MG	A	902	1/1	0.92	0.38	-	105,105,105,105	0

6.5 Other polymers (i)

There are no such residues in this entry.