wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 05:21 PM GMT

PDB ID	:	4HYT
Title	:	Na,K-ATPase in the E2P state with bound ouabain and Mg2+ in the cation-binding site
Authors	:	Laursen, M.; Yatime, L.; Nissen, P.; Fedosova, N.U.
Deposited on	:	2012-11-14
Resolution	:	3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

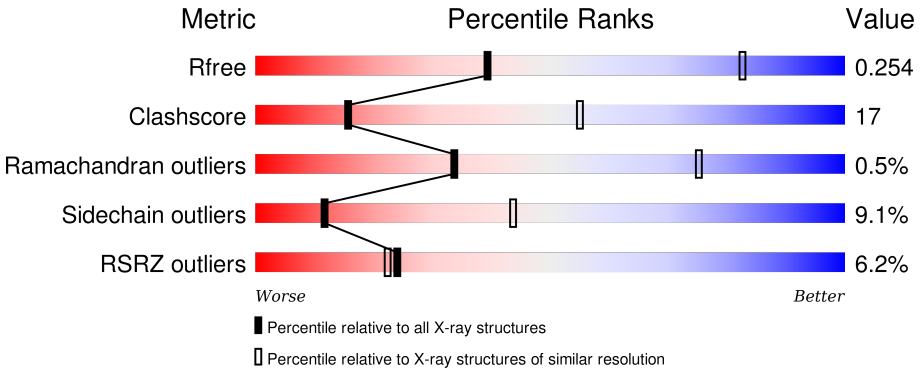
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	1021	4% 66% 28%
1	C	1021	8% 67% 27%
2	B	303	5% 51% 37% 7% 5%
2	D	303	7% 50% 38% 6% 5%
3	E	65	32% 15% 51%

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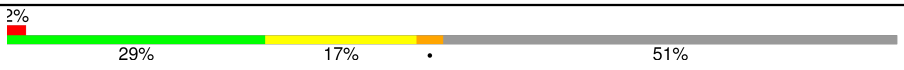
Mol	Chain	Length	Quality of chain
3	G	65	

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
10	CE1	A	1110	-	-	-	X
10	CE1	E	2002	-	-	-	X
4	MG	A	1102	-	-	-	X
4	MG	C	2002	-	-	-	X
6	CLR	C	2005	-	-	-	X
9	17F	A	1108	-	-	-	X
9	17F	A	1109	-	-	-	X
9	17F	B	1005	-	-	-	X
9	17F	D	2004	-	-	-	X
9	17F	G	1002	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 21220 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 Sodium/potassium-transporting ATPase subunit alpha-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	996	Total	C	N	O	P	S	0	0	0
			7730	4922	1301	1459	1	47			
1	C	996	Total	C	N	O	P	S	0	0	0
			7730	4922	1301	1459	1	47			

- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	289	Total	C	N	O	S	0	0	0
			2368	1534	386	435	13			
2	D	287	Total	C	N	O	S	0	0	0
			2349	1519	384	433	13			

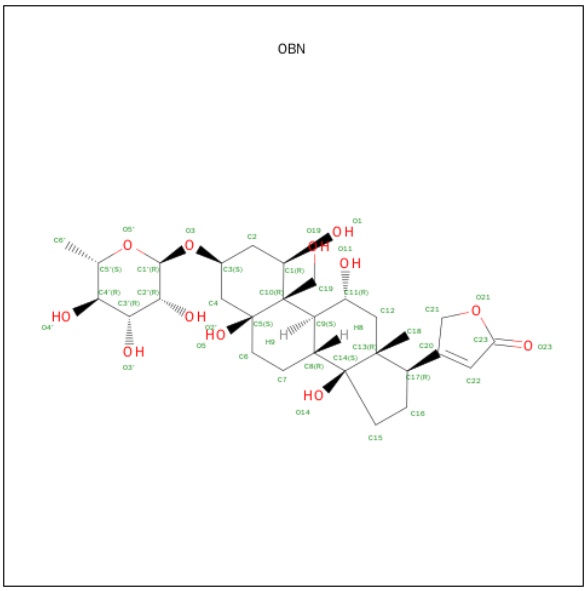
- Molecule 3 is a protein called Na+/K+ ATPase gamma subunit transcript variant a.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	32	Total	C	N	O	0	0	0
			255	174	37	44			
3	E	32	Total	C	N	O	0	0	0
			255	174	37	44			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

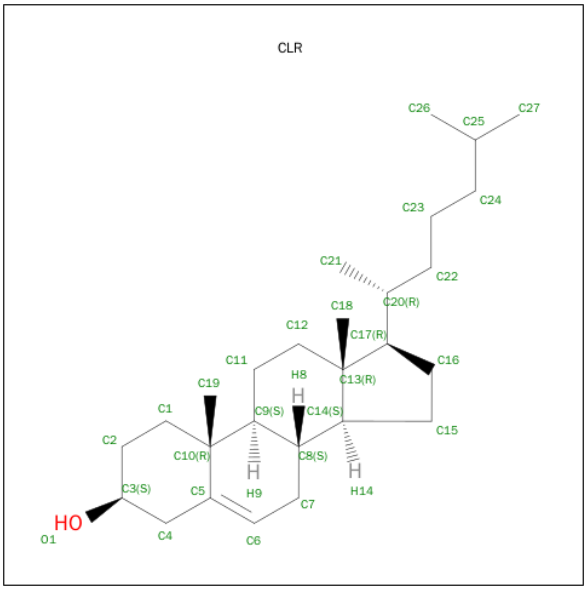
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Mg	0	0
			3	3		
4	C	3	Total	Mg	0	0
			3	3		

- Molecule 5 is OUABAIN (three-letter code: OBN) (formula: $C_{29}H_{44}O_{12}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 41 29 12	0	0
5	C	1	Total C O 41 29 12	0	0

- Molecule 6 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 28 27 1	0	0
6	G	1	Total C O 28 27 1	0	0

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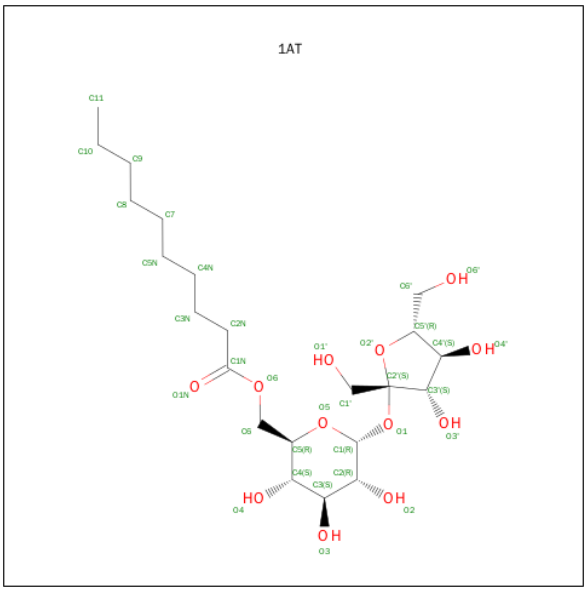
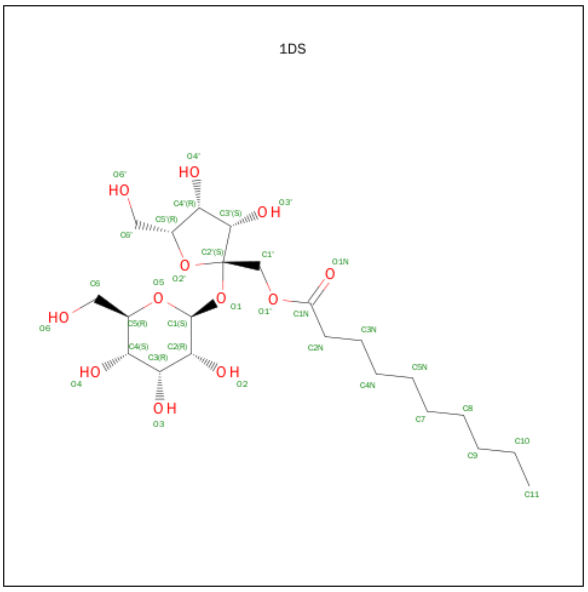
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 28 27 1	0	0
6	E	1	Total C O 28 27 1	0	0

- Molecule 7 is BETA-D-FRUCTOFURANOSYL 6-O-DECANOYL-ALPHA-D-GLUCOPYRANOSIDE (three-letter code: 1AT) (formula: $C_{22}H_{40}O_{12}$).



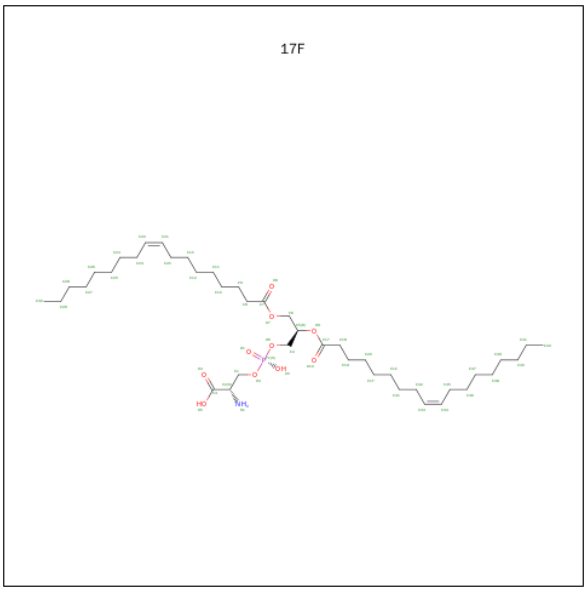
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 29 17 12	0	0

- Molecule 8 is 1-O-DECANOYL-BETA-D-TAGATOFURANOSYL BETA-D-ALLOPYRANOSIDE (three-letter code: 1DS) (formula: $C_{22}H_{40}O_{12}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 29 17 12	0	0

- Molecule 9 is O-[(S)-({(2R)-2,3-BIS[(9Z)-OCTADEC-9-ENOYLOXY]PROPYL}OXY)(HYDROXY)PHOSPHORYL]-L-SERINE (three-letter code: 17F) (formula: $C_{42}H_{78}NO_{10}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N O P 18 8 1 8 1	0	0
9	A	1	Total C N O P 18 8 1 8 1	0	0

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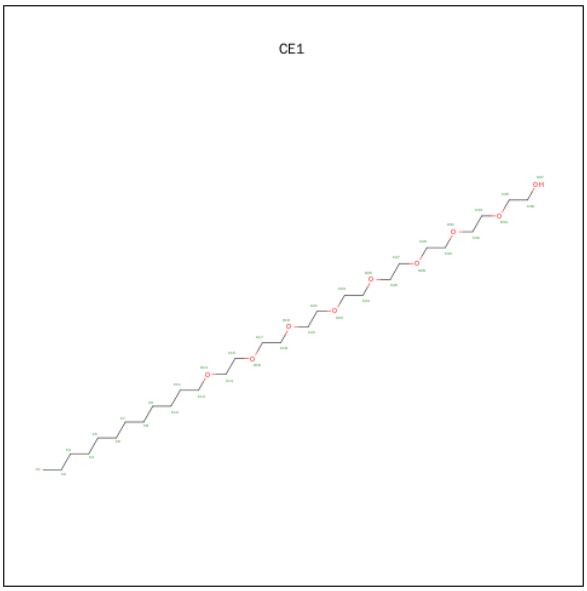
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			24	14	1	8	1		
9	G	1	Total	C	N	O	P	0	0
			27	15	1	10	1		
9	D	1	Total	C	N	O	P	0	0
			28	16	1	10	1		

- Molecule 10 is O-DODECANYL OCTAETHYLENE GLYCOL (three-letter code: CE1) (formula: $C_{28}H_{58}O_9$).

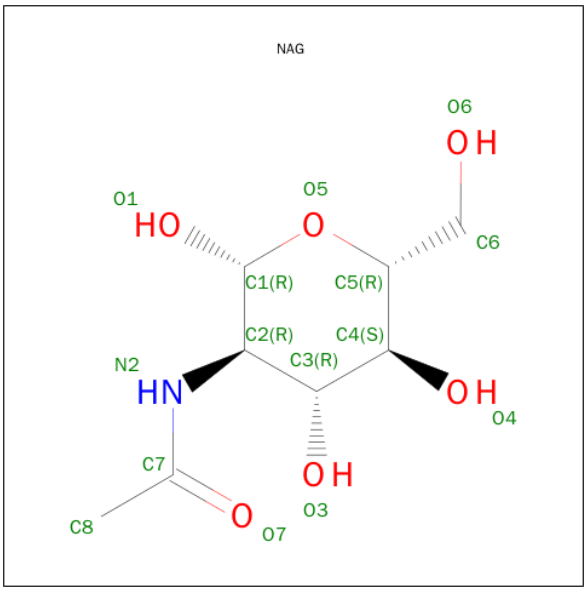


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			34	26	8		
10	E	1	Total	C	O	0	0
			22	18	4		

- Molecule 11 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 12 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total C N O 14 8 1 5	0	0
12	B	1	Total C N O 14 8 1 5	0	0
12	D	1	Total C N O 14 8 1 5	0	0
12	D	1	Total C N O 14 8 1 5	0	0
12	D	1	Total C N O 14 8 1 5	0	0

- Molecule 13 is water.

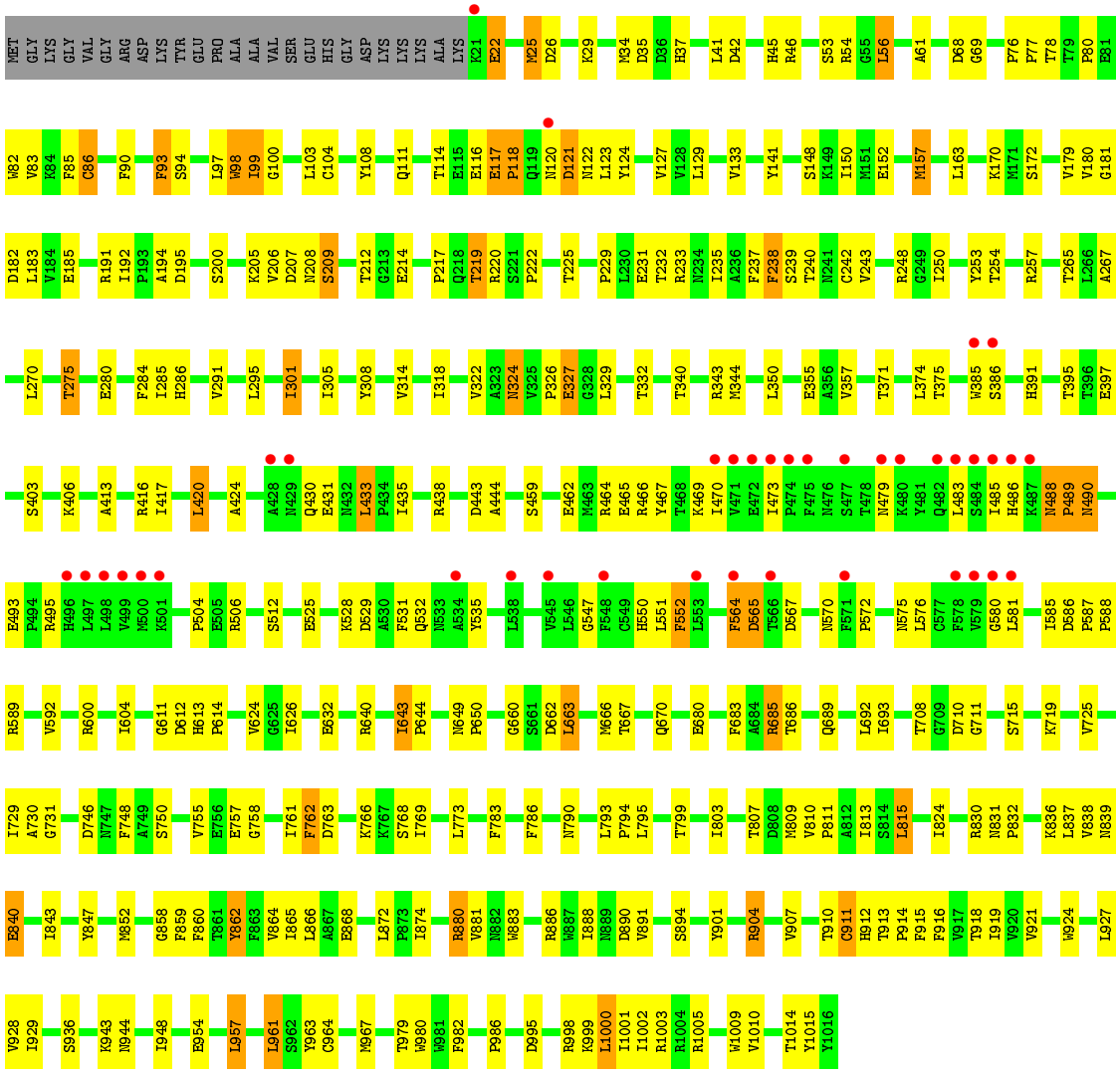
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	3	Total O 3 3	0	0
13	C	3	Total O 3 3	0	0

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 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.

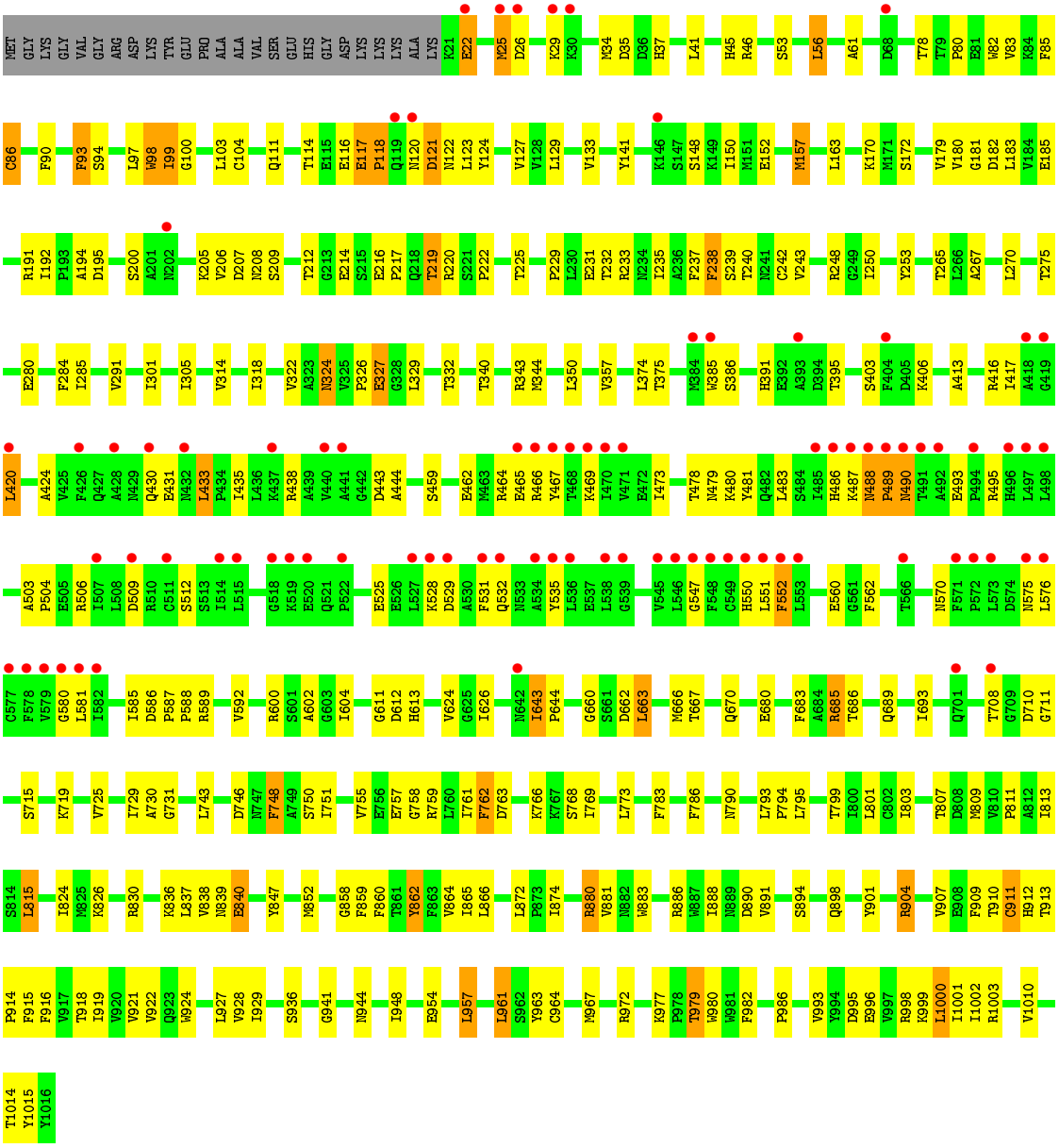
- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

Chain A:



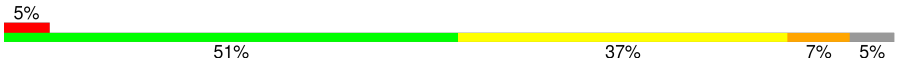
- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

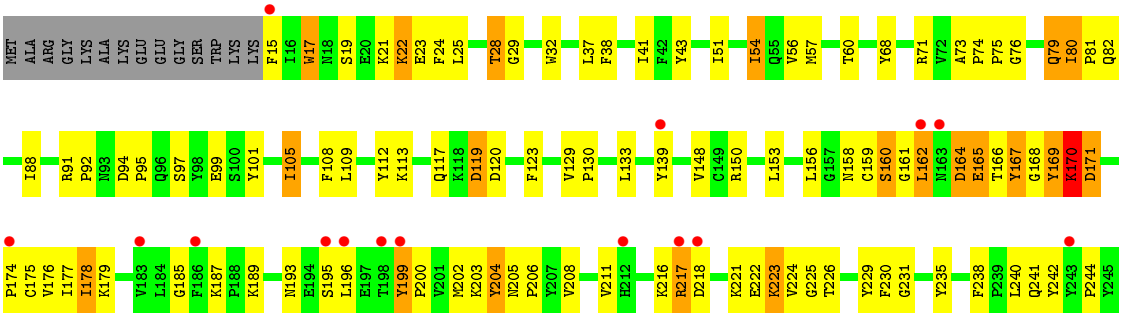
Chain C:

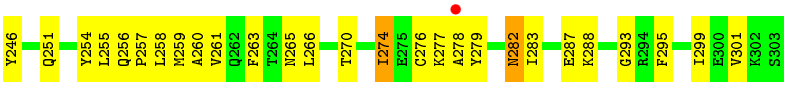


• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

Chain B:

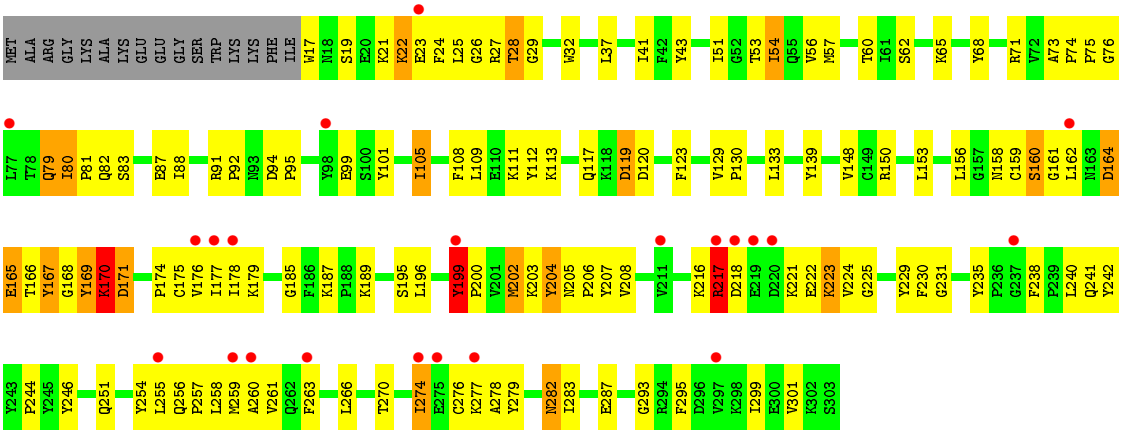






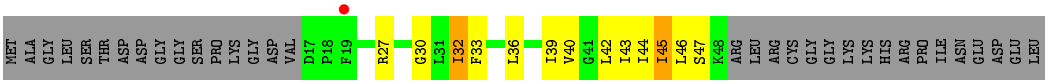
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

Chain D:



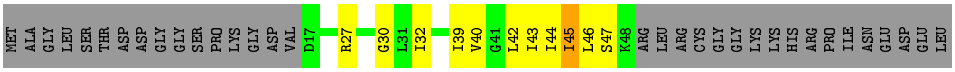
• Molecule 3: Na+/K+ ATPase gamma subunit transcript variant a

Chain G:



• Molecule 3: Na+/K+ ATPase gamma subunit transcript variant a

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.47Å 118.08Å 494.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.83 – 3.40 53.88 – 3.40	Depositor EDS
% Data completeness (in resolution range)	75.7 (49.83-3.40) 75.7 (53.88-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.226 , 0.244 0.232 , 0.254	Depositor DCC
R_{free} test set	3603 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	111.6	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 70.0	EDS
Estimated twinning fraction	0.037 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	1 of 72261 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	21220	wwPDB-VP
Average B, all atoms (Å^2)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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

Bond lengths and bond angles in the following residue types are not validated in this section: OBN, 1AT, MG, NAG, 17F, PHD, 1DS, CE1, CLR

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	0.31	0/7867	0.53	0/10674
1	C	0.30	0/7867	0.53	0/10674
2	B	0.32	0/2431	0.59	0/3279
2	D	0.34	0/2411	0.59	2/3252 (0.1%)
3	E	0.38	0/261	0.54	0/354
3	G	0.39	0/261	0.55	0/354
All	All	0.31	0/21098	0.54	2/28587 (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
2	B	0	2
2	D	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	D	217	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	D	199	TYR	CB-CG-CD2	-5.15	117.91	121.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	160	SER	Peptide
2	B	165	GLU	Peptide
2	D	160	SER	Peptide
2	D	165	GLU	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	A	7730	0	7777	243	0
1	C	7730	0	7777	226	0
2	B	2368	0	2335	116	0
2	D	2349	0	2315	119	0
3	E	255	0	259	7	0
3	G	255	0	259	9	0
4	A	3	0	0	0	0
4	C	3	0	0	0	0
5	A	41	0	44	10	0
5	C	41	0	44	6	0
6	A	28	0	46	5	0
6	C	28	0	46	2	0
6	E	28	0	46	4	0
6	G	28	0	46	4	0
7	A	29	0	27	6	0
8	A	29	0	27	6	0
9	A	36	0	16	7	0
9	B	24	0	20	2	0
9	D	28	0	22	0	0
9	G	27	0	20	4	0
10	A	34	0	53	18	0
10	E	22	0	37	1	0
11	B	28	0	25	0	0
12	B	28	0	26	0	0
12	D	42	0	39	0	0
13	A	3	0	0	1	0
13	C	3	0	0	0	0
All	All	21220	0	21306	726	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 17.

The worst 5 of 726 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:68:ASP:OD1	1:A:69:GLY:N	1.78	1.15
1:C:794:PRO:HG3	1:C:862:TYR:HE2	1.17	1.07
1:A:794:PRO:HG3	1:A:862:TYR:HE2	1.15	1.07
1:C:794:PRO:HG3	1:C:862:TYR:CE2	1.95	1.00
1:A:794:PRO:HG3	1:A:862:TYR:CE2	1.95	1.00

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	993/1021 (97%)	940 (95%)	51 (5%)	2 (0%)	52 87
1	C	993/1021 (97%)	947 (95%)	44 (4%)	2 (0%)	52 87
2	B	287/303 (95%)	255 (89%)	28 (10%)	4 (1%)	14 55
2	D	285/303 (94%)	255 (90%)	26 (9%)	4 (1%)	14 55
3	E	30/65 (46%)	28 (93%)	2 (7%)	0	100 100
3	G	30/65 (46%)	28 (93%)	2 (7%)	0	100 100
All	All	2618/2778 (94%)	2453 (94%)	153 (6%)	12 (0%)	34 75

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	199	TYR
2	D	199	TYR
2	B	161	GLY
2	D	161	GLY
2	B	170	LYS

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	846/864 (98%)	777 (92%)	69 (8%)	14 50
1	C	846/864 (98%)	780 (92%)	66 (8%)	16 52
2	B	259/269 (96%)	225 (87%)	34 (13%)	5 25
2	D	257/269 (96%)	226 (88%)	31 (12%)	6 28
3	E	26/52 (50%)	23 (88%)	3 (12%)	7 31
3	G	26/52 (50%)	23 (88%)	3 (12%)	7 31
All	All	2260/2370 (95%)	2054 (91%)	206 (9%)	12 44

5 of 206 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	203	LYS
1	C	85	PHE
2	D	178	ILE
2	B	217	ARG
3	G	45	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	486	HIS
2	B	241	GLN
1	C	486	HIS
2	D	241	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)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	PHD	A	369	1,4	8,11,12	1.13	1 (12%)	9,15,17	1.65	3 (33%)
1	PHD	C	369	1,4	8,11,12	1.12	1 (12%)	9,15,17	1.61	3 (33%)

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
1	PHD	A	369	1,4	-	0/7/11/13	0/0/0/0
1	PHD	C	369	1,4	-	0/7/11/13	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	369	PHD	CB-CA	-2.21	1.49	1.53
1	A	369	PHD	CB-CA	-2.08	1.49	1.53

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	369	PHD	OD2-CG-CB	-2.83	118.19	124.69
1	C	369	PHD	OD2-CG-CB	-2.58	118.77	124.69
1	A	369	PHD	O-C-CA	-2.53	118.91	125.49
1	C	369	PHD	O-C-CA	-2.43	119.16	125.49
1	C	369	PHD	CA-CB-CG	2.19	116.86	113.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

2 carbohydrates 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	$\#\|Z\| > 2$
11	NAG	B	1001	11,2	14,14,15	0.33	0	15,19,21	0.38	0
11	NAG	B	1002	11	14,14,15	0.23	0	15,19,21	0.23	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
11	NAG	B	1001	11,2	-	0/6/23/26	0/1/1/1
11	NAG	B	1002	11	-	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.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 6 are monoatomic - leaving 20 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	$\#\|Z\| > 2$
5	OBN	A	1104	-	44,46,46	0.79	1 (2%)	65,76,76	1.80	15 (23%)
6	CLR	A	1105	-	31,31,31	2.29	7 (22%)	48,48,48	2.63	16 (33%)
7	1AT	A	1106	-	30,30,35	1.41	3 (10%)	43,43,48	2.38	15 (34%)
8	1DS	A	1107	-	30,30,35	1.26	4 (13%)	42,43,48	2.23	15 (35%)
9	17F	A	1108	-	14,17,53	1.35	2 (14%)	13,23,60	3.29	4 (30%)
9	17F	A	1109	-	14,17,53	1.21	2 (14%)	13,23,60	3.46	6 (46%)
10	CE1	A	1110	-	33,33,36	0.57	0	32,32,35	0.95	1 (3%)
12	NAG	B	1003	2	14,14,15	0.31	0	15,19,21	0.47	0
12	NAG	B	1004	2	14,14,15	0.47	0	15,19,21	0.23	0
9	17F	B	1005	-	20,23,53	1.21	2 (10%)	20,29,60	3.01	7 (35%)
5	OBN	C	2004	-	44,46,46	0.74	1 (2%)	65,76,76	1.70	14 (21%)
6	CLR	C	2005	-	31,31,31	2.26	8 (25%)	48,48,48	2.61	17 (35%)
12	NAG	D	2001	2	14,14,15	0.34	0	15,19,21	0.38	0
12	NAG	D	2002	2	14,14,15	0.58	0	15,19,21	0.53	0
12	NAG	D	2003	2	14,14,15	0.54	0	15,19,21	0.49	0
9	17F	D	2004	-	24,27,53	1.10	3 (12%)	24,34,60	2.03	7 (29%)
6	CLR	E	2001	-	31,31,31	2.23	8 (25%)	48,48,48	2.52	17 (35%)
10	CE1	E	2002	-	21,21,36	0.71	0	20,20,35	1.18	3 (15%)
6	CLR	G	1001	-	31,31,31	2.25	8 (25%)	48,48,48	2.52	17 (35%)
9	17F	G	1002	-	23,26,53	1.11	2 (8%)	23,33,60	2.94	7 (30%)

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
5	OBN	A	1104	-	-	0/11/116/116	0/6/6/6
6	CLR	A	1105	-	-	0/10/68/68	0/4/4/4
7	1AT	A	1106	-	-	0/19/58/63	0/2/2/2
8	1DS	A	1107	-	-	0/19/58/63	0/2/2/2
9	17F	A	1108	-	-	0/16/20/59	0/0/0/0
9	17F	A	1109	-	-	1/16/20/59	0/0/0/0
10	CE1	A	1110	-	-	0/31/31/34	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	B	1003	2	-	0/6/23/26	0/1/1/1
12	NAG	B	1004	2	-	0/6/23/26	0/1/1/1
9	17F	B	1005	-	-	0/23/27/59	0/0/0/0
5	OBN	C	2004	-	-	0/11/116/116	0/6/6/6
6	CLR	C	2005	-	-	0/10/68/68	0/4/4/4
12	NAG	D	2001	2	-	0/6/23/26	0/1/1/1
12	NAG	D	2002	2	-	0/6/23/26	0/1/1/1
12	NAG	D	2003	2	-	0/6/23/26	0/1/1/1
9	17F	D	2004	-	-	0/29/33/59	0/0/0/0
6	CLR	E	2001	-	-	0/10/68/68	0/4/4/4
10	CE1	E	2002	-	-	0/19/19/34	0/0/0/0
6	CLR	G	1001	-	-	0/10/68/68	0/4/4/4
9	17F	G	1002	-	-	0/27/31/59	0/0/0/0

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	1002	17F	O9-C5	-3.32	1.38	1.46
9	B	1005	17F	O9-C5	-3.27	1.41	1.47
9	A	1108	17F	O9-C5	-2.98	1.41	1.47
6	E	2001	CLR	C20-C17	-2.92	1.48	1.54
6	G	1001	CLR	C20-C17	-2.88	1.49	1.54

The worst 5 of 161 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1105	CLR	C4-C5-C6	-7.02	108.65	120.57
7	A	1106	1AT	O2-C2-C3	-7.00	94.58	110.34
6	A	1105	CLR	C7-C6-C5	-6.52	110.99	125.01
6	G	1001	CLR	C7-C6-C5	-6.26	111.56	125.01
6	E	2001	CLR	C7-C6-C5	-6.14	111.82	125.01

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1109	17F	C17-O9-C5-C6

There are no ring outliers.

14 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1104	OBN	10	0
6	A	1105	CLR	5	0
7	A	1106	1AT	6	0
8	A	1107	1DS	6	0
9	A	1108	17F	6	0
9	A	1109	17F	2	0
10	A	1110	CE1	18	0
9	B	1005	17F	2	0
5	C	2004	OBN	6	0
6	C	2005	CLR	2	0
6	E	2001	CLR	4	0
10	E	2002	CE1	1	0
6	G	1001	CLR	4	0
9	G	1002	17F	4	0

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	995/1021 (97%)	0.04	39 (3%) 43 38	51, 91, 218, 288	0
1	C	995/1021 (97%)	0.26	86 (8%) 13 13	58, 126, 273, 342	0
2	B	289/303 (95%)	0.12	16 (5%) 29 26	67, 151, 221, 258	0
2	D	287/303 (94%)	0.35	22 (7%) 16 16	63, 136, 210, 241	0
3	E	32/65 (49%)	-0.47	0 100 100	72, 81, 120, 147	0
3	G	32/65 (49%)	-0.12	1 (3%) 52 48	64, 83, 134, 141	0
All	All	2630/2778 (94%)	0.16	164 (6%) 24 22	51, 116, 242, 342	0

The worst 5 of 164 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	217	ARG	15.0
2	D	218	ASP	10.8
1	C	491	THR	8.5
1	C	545	VAL	8.3
1	A	471	VAL	7.7

6.2 Non-standard residues in protein, DNA, RNA chains

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, 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	LLDF	B-factors(Å^2)	Q<0.9
1	PHD	C	369	12/13	0.98	0.18	-	107,112,123,124	0
1	PHD	A	369	12/13	0.98	0.17	-	66,71,74,75	0

6.3 Carbohydrates (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, 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	LLDF	B-factors(Å^2)	Q<0.9
11	NAG	B	1001	14/15	0.82	0.18	-	179,192,203,207	0
11	NAG	B	1002	14/15	0.72	0.41	-	205,218,224,229	0

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, 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	LLDF	B-factors(Å^2)	Q<0.9
4	MG	A	1102	1/1	0.97	0.41	14.72	82,82,82,82	0
6	CLR	C	2005	28/28	0.84	0.49	5.32	93,104,113,231	0
9	17F	D	2004	28/54	0.82	0.47	4.78	154,172,243,246	0
9	17F	G	1002	27/54	0.71	0.39	4.15	83,124,256,258	0
10	CE1	E	2002	22/37	0.86	0.36	3.82	67,109,155,157	0
9	17F	A	1109	18/54	0.84	0.32	3.25	96,114,166,169	0
10	CE1	A	1110	34/37	0.87	0.30	2.84	79,110,144,146	0
9	17F	A	1108	18/54	0.84	0.32	2.74	80,155,188,197	0
9	17F	B	1005	24/54	0.78	0.28	2.64	74,128,199,208	0
4	MG	C	2002	1/1	0.97	0.34	2.60	124,124,124,124	0
6	CLR	E	2001	28/28	0.96	0.25	0.81	64,71,73,73	0
6	CLR	A	1105	28/28	0.93	0.26	0.27	74,112,143,159	0
6	CLR	G	1001	28/28	0.97	0.20	0.00	57,66,79,83	0
5	OBN	A	1104	41/41	0.95	0.19	-0.33	72,81,85,88	0
5	OBN	C	2004	41/41	0.94	0.19	-0.41	84,92,99,104	0
4	MG	A	1101	1/1	0.96	0.19	-0.61	113,113,113,113	0
4	MG	C	2001	1/1	0.98	0.20	-0.70	147,147,147,147	0
7	1AT	A	1106	29/34	0.94	0.19	-0.81	85,99,116,118	0
8	1DS	A	1107	29/34	0.93	0.20	-0.99	56,123,141,170	0
4	MG	A	1103	1/1	0.95	0.22	-1.10	58,58,58,58	0
4	MG	C	2003	1/1	0.92	0.20	-1.61	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
12	NAG	D	2001	14/15	0.85	0.22	-	138,159,173,175	0
12	NAG	D	2003	14/15	0.80	0.32	-	191,198,211,218	0
12	NAG	B	1003	14/15	0.71	0.22	-	197,209,221,225	0
12	NAG	D	2002	14/15	0.79	0.14	-	142,150,163,169	0
12	NAG	B	1004	14/15	0.74	0.45	-	199,203,212,213	0

6.5 Other polymers

There are no such residues in this entry.