



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:13 PM GMT

PDB ID : 3WGU  
Title : Crystal structure of a Na<sup>+</sup>-bound Na<sup>+</sup>,K<sup>+</sup>-ATPase preceding the E1P state without oligomycin  
Authors : Kanai, R.; Ogawa, H.; Vilsen, B.; Cornelius, F.; Toyoshima, C.  
Deposited on : 2013-08-09  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

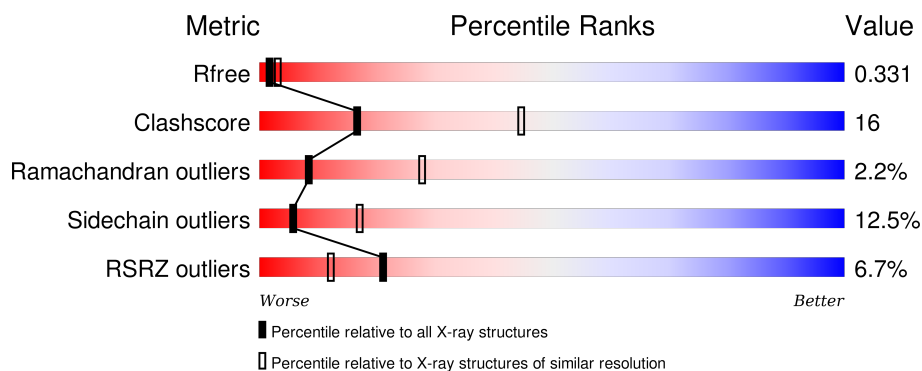
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	1016	<div> <div>3%</div> <div>58%</div> <div>34%</div> <div>6%</div> <div>.</div> </div>
1	C	1016	<div> <div>4%</div> <div>60%</div> <div>34%</div> <div>.</div> <div>.</div> </div>
2	B	303	<div> <div>15%</div> <div>51%</div> <div>42%</div> <div>6%</div> <div>.</div> </div>
2	D	303	<div> <div>17%</div> <div>56%</div> <div>37%</div> <div>6%</div> <div>.</div> </div>
3	E	65	<div> <div>8%</div> <div>28%</div> <div>23%</div> <div>.</div> <div>46%</div> </div>

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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
5	ALF	A	2002	-	-	-	X
5	ALF	C	2002	-	-	X	-
7	NA	A	2005	-	-	-	X
7	NA	A	2006	-	-	-	X
7	NA	A	2007	-	-	-	X
7	NA	C	2007	-	-	-	X
8	CLR	A	2009	-	-	-	X
8	CLR	A	2010	-	-	-	X
8	CLR	B	3001	-	-	-	X
8	CLR	C	2010	-	-	-	X
9	PC1	A	2012	-	-	-	X
9	PC1	A	2013	-	-	-	X
9	PC1	B	3002	-	-	-	X
9	PC1	C	2013	-	-	-	X
9	PC1	C	2014	-	-	-	X
9	PC1	C	2015	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21807 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	994	Total	C	N	O	S	0	0	0
			7714	4918	1300	1449	47			
1	C	994	Total	C	N	O	S	0	0	0
			7714	4918	1300	1449	47			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	303	Total	C	N	O	S	0	0	0
			2479	1603	408	454	14			
2	D	303	Total	C	N	O	S	0	0	0
			2479	1603	408	454	14			

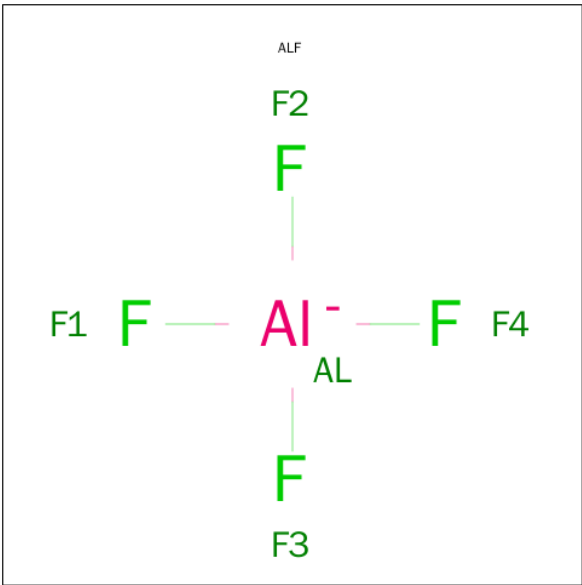
- Molecule 3 is a protein called Na<sup>+</sup>/K<sup>+</sup> ATPase gamma subunit transcript variant a.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	34	Total	C	N	O	0	0	0
			270	183	39	48			
3	E	35	Total	C	N	O	0	0	0
			281	189	43	49			

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

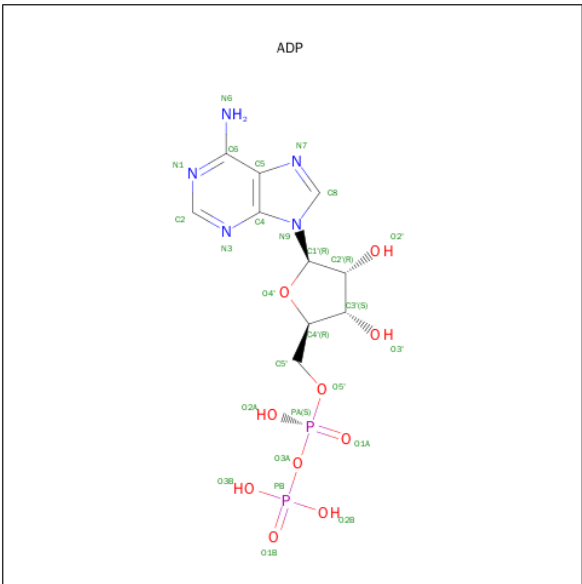
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		

- Molecule 5 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Al	F	0	0
			5	1	4		
5	C	1	Total	Al	F	0	0
			5	1	4		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			27	10	5	10		

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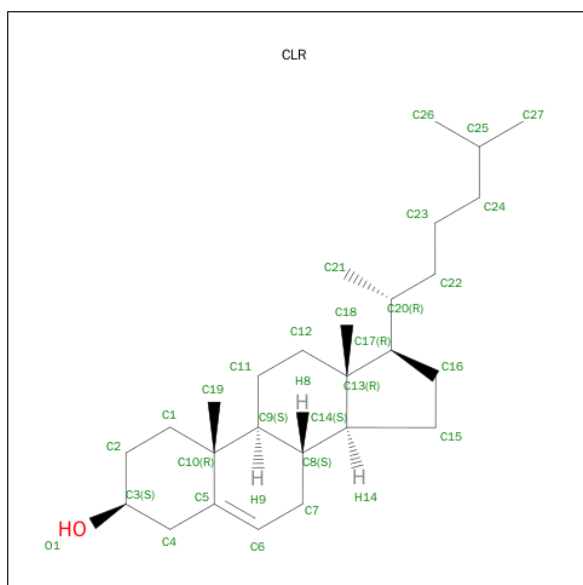
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

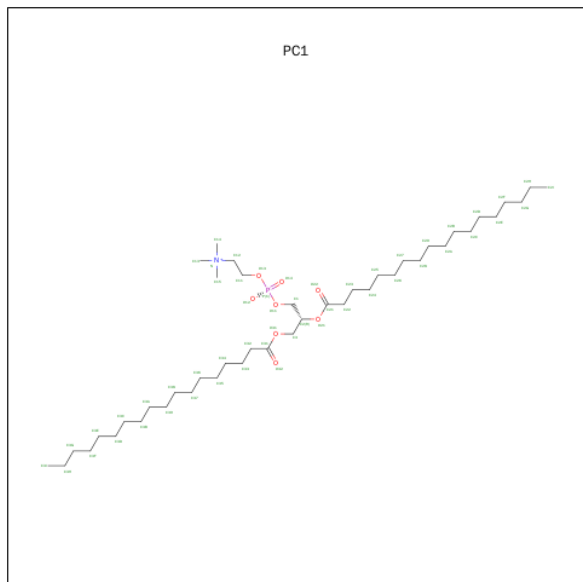
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	Na	0	0
			4	4		
7	C	4	Total	Na	0	0
			4	4		

- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



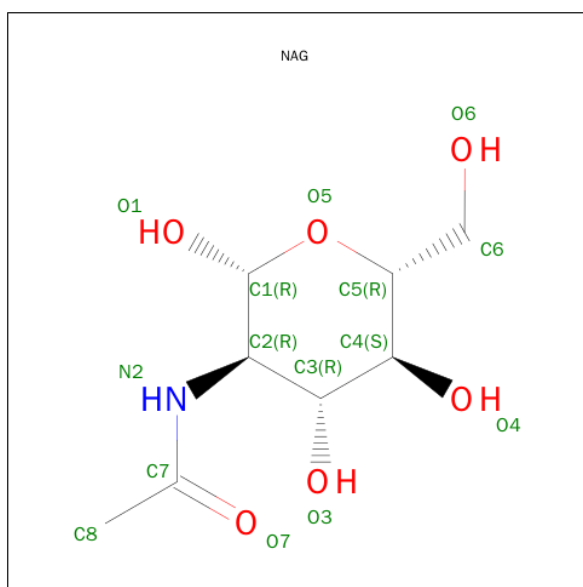
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			28	27	1		
8	A	1	Total	C	O	0	0
			28	27	1		
8	B	1	Total	C	O	0	0
			28	27	1		
8	C	1	Total	C	O	0	0
			28	27	1		
8	C	1	Total	C	O	0	0
			28	27	1		
8	C	1	Total	C	O	0	0
			28	27	1		

- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	D	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 10 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

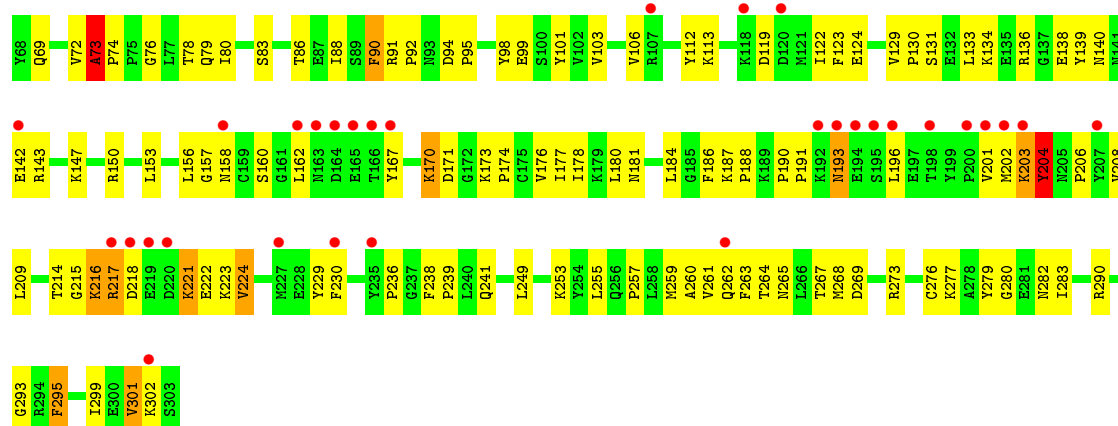
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	30	Total	O	0	0
			30	30		
11	B	2	Total	O	0	0
			2	2		
11	C	23	Total	O	0	0
			23	23		
11	D	3	Total	O	0	0
			3	3		

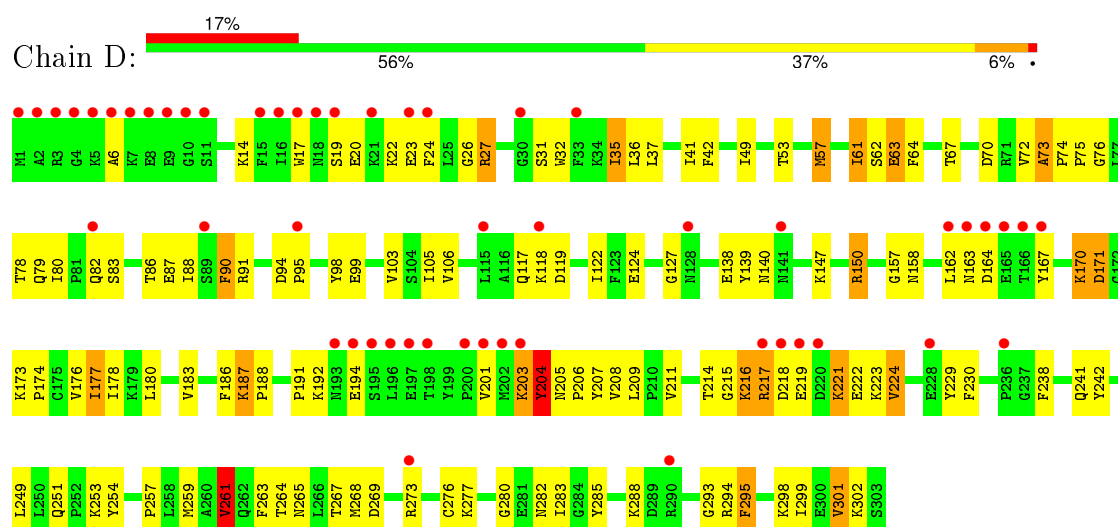




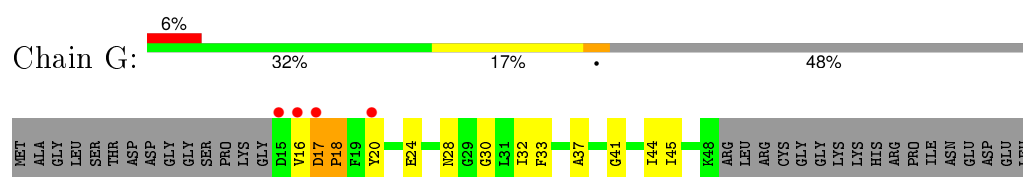




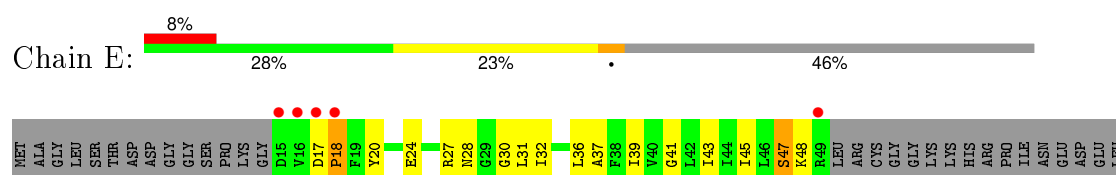
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.38Å 211.60Å 257.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.99 – 2.80 15.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.9 (15.99-2.80) 88.9 (15.99-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.68 (at 2.82Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.265 , 0.299 0.318 , 0.331	Depositor DCC
$R_{free}$ test set	6460 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.1	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.13 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.18$	Xtriage
Outliers	0 of 126511 reflections	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	21807	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: MG, NAG, ADP, ALF, NA, PC1, 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	0.48	1/7864 (0.0%)	0.65	5/10671 (0.0%)
1	C	0.41	0/7864	0.58	1/10671 (0.0%)
2	B	0.33	0/2544	0.53	1/3426 (0.0%)
2	D	0.34	0/2544	0.51	0/3426
3	E	0.59	1/287 (0.3%)	0.87	3/389 (0.8%)
3	G	0.43	0/276	0.57	0/375
All	All	0.43	2/21379 (0.0%)	0.60	10/28958 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	18	PRO	N-CD	7.79	1.58	1.47
1	A	511	CYS	CB-SG	-5.39	1.73	1.81

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	17	ASP	C-N-CD	-10.59	97.31	120.60
1	C	495	ARG	CB-CA-C	-8.16	94.09	110.40
1	A	495	ARG	CB-CA-C	-7.90	94.59	110.40
1	A	600	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	369	ASP	CB-CG-OD2	6.80	124.42	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	7714	0	7769	262	0
1	C	7714	0	7768	248	0
2	B	2479	0	2458	92	0
2	D	2479	0	2458	80	0
3	E	281	0	285	9	0
3	G	270	0	272	12	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
5	A	5	0	0	1	0
5	C	5	0	0	2	0
6	A	27	0	12	5	0
6	C	27	0	12	6	0
7	A	4	0	0	0	0
7	C	4	0	0	0	0
8	A	56	0	87	12	0
8	B	28	0	44	4	0
8	C	84	0	131	23	0
9	A	216	0	352	14	0
9	B	54	0	88	0	0
9	C	216	0	352	21	0
9	D	54	0	88	3	0
10	B	14	0	13	0	0
10	D	14	0	13	0	0
11	A	30	0	0	0	0
11	B	2	0	0	0	0
11	C	23	0	0	3	0
11	D	3	0	0	1	0
All	All	21807	0	22202	724	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 16.

The worst 5 of 724 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:ARG:HG3	1:C:495:ARG:O	1.61	0.97
1:C:57:THR:HG23	1:C:60:ARG:HB2	1.52	0.90
2:B:221:LYS:HE3	2:B:223:LYS:HB2	1.54	0.90
8:C:2010:CLR:H272	9:C:2014:PC1:H2I2	1.54	0.88
1:A:494:PRO:HG2	1:A:552:PHE:HB3	1.56	0.87

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	992/1016 (98%)	882 (89%)	97 (10%)	13 (1%)	15	44
1	C	992/1016 (98%)	890 (90%)	88 (9%)	14 (1%)	14	42
2	B	301/303 (99%)	234 (78%)	55 (18%)	12 (4%)	4	12
2	D	301/303 (99%)	231 (77%)	55 (18%)	15 (5%)	3	8
3	E	33/65 (51%)	32 (97%)	0	1 (3%)	5	18
3	G	32/65 (49%)	27 (84%)	3 (9%)	2 (6%)	2	4
All	All	2651/2768 (96%)	2296 (87%)	298 (11%)	57 (2%)	8	28

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	388	ASN
1	A	402	VAL
2	B	139	TYR
3	G	17	ASP
3	G	18	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	844/861 (98%)	723 (86%)	121 (14%)	4	12
1	C	844/861 (98%)	751 (89%)	93 (11%)	8	23
2	B	269/269 (100%)	234 (87%)	35 (13%)	5	15
2	D	269/269 (100%)	238 (88%)	31 (12%)	7	21
3	E	29/52 (56%)	24 (83%)	5 (17%)	2	7
3	G	28/52 (54%)	27 (96%)	1 (4%)	42	76
All	All	2283/2364 (97%)	1997 (88%)	286 (12%)	6	17

5 of 286 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	57	MET
1	C	56	LEU
2	D	171	ASP
2	B	78	THR
2	B	216	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	292	GLN
1	C	156	ASN
2	D	69	GLN
3	G	28	ASN
1	C	119	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 34 ligands modelled in this entry, 12 are monoatomic - leaving 22 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	ALF	A	2002	-	0,4,4	0.00	-	0,6,6	0.00	-
6	ADP	A	2004	4	22,29,29	1.27	2 (9%)	27,45,45	1.88	6 (22%)
8	CLR	A	2009	-	31,31,31	4.38	14 (45%)	48,48,48	2.45	16 (33%)
8	CLR	A	2010	-	31,31,31	4.41	14 (45%)	48,48,48	2.96	20 (41%)
9	PC1	A	2011	-	53,53,53	0.86	3 (5%)	57,61,61	1.18	5 (8%)
9	PC1	A	2012	-	53,53,53	0.88	3 (5%)	57,61,61	1.30	6 (10%)
9	PC1	A	2013	-	53,53,53	0.87	3 (5%)	57,61,61	1.16	4 (7%)
9	PC1	A	2014	-	53,53,53	0.88	4 (7%)	57,61,61	1.30	4 (7%)
8	CLR	B	3001	-	31,31,31	4.38	13 (41%)	48,48,48	2.35	16 (33%)
9	PC1	B	3002	-	53,53,53	0.85	3 (5%)	57,61,61	1.17	4 (7%)
10	NAG	B	3003	-	14,14,15	0.40	0	15,19,21	0.75	0
5	ALF	C	2002	-	0,4,4	0.00	-	0,6,6	0.00	-
6	ADP	C	2004	-	22,29,29	0.98	2 (9%)	27,45,45	1.78	5 (18%)
8	CLR	C	2009	-	31,31,31	4.31	14 (45%)	48,48,48	2.38	16 (33%)
8	CLR	C	2010	-	31,31,31	4.40	13 (41%)	48,48,48	2.43	19 (39%)
8	CLR	C	2011	-	31,31,31	4.50	13 (41%)	48,48,48	2.46	19 (39%)
9	PC1	C	2012	-	53,53,53	0.87	4 (7%)	57,61,61	1.25	5 (8%)
9	PC1	C	2013	-	53,53,53	0.88	3 (5%)	57,61,61	1.30	5 (8%)
9	PC1	C	2014	-	53,53,53	0.91	4 (7%)	57,61,61	1.28	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	PC1	C	2015	-	53,53,53	0.86	3 (5%)	57,61,61	1.26	5 (8%)
9	PC1	D	401	-	53,53,53	0.88	3 (5%)	57,61,61	1.21	4 (7%)
10	NAG	D	402	-	14,14,15	0.44	0	15,19,21	0.74	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
5	ALF	A	2002	-	-	0/0/0/0	0/0/0/0
6	ADP	A	2004	4	-	0/12/32/32	0/3/3/3
8	CLR	A	2009	-	-	0/10/68/68	0/4/4/4
8	CLR	A	2010	-	-	0/10/68/68	0/4/4/4
9	PC1	A	2011	-	-	0/57/57/57	0/0/0/0
9	PC1	A	2012	-	-	0/57/57/57	0/0/0/0
9	PC1	A	2013	-	-	0/57/57/57	0/0/0/0
9	PC1	A	2014	-	-	0/57/57/57	0/0/0/0
8	CLR	B	3001	-	-	0/10/68/68	0/4/4/4
9	PC1	B	3002	-	-	0/57/57/57	0/0/0/0
10	NAG	B	3003	-	-	0/6/23/26	0/1/1/1
5	ALF	C	2002	-	-	0/0/0/0	0/0/0/0
6	ADP	C	2004	-	-	0/12/32/32	0/3/3/3
8	CLR	C	2009	-	-	0/10/68/68	0/4/4/4
8	CLR	C	2010	-	-	0/10/68/68	0/4/4/4
8	CLR	C	2011	-	-	0/10/68/68	0/4/4/4
9	PC1	C	2012	-	-	0/57/57/57	0/0/0/0
9	PC1	C	2013	-	-	0/57/57/57	0/0/0/0
9	PC1	C	2014	-	-	0/57/57/57	0/0/0/0
9	PC1	C	2015	-	-	2/57/57/57	0/0/0/0
9	PC1	D	401	-	-	0/57/57/57	0/0/0/0
10	NAG	D	402	-	-	0/6/23/26	0/1/1/1

The worst 5 of 118 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	2011	CLR	C10-C9	-12.49	1.33	1.56
8	A	2010	CLR	C10-C9	-12.40	1.33	1.56
8	A	2009	CLR	C10-C9	-12.19	1.34	1.56
8	C	2010	CLR	C10-C9	-11.95	1.34	1.56
8	B	3001	CLR	C10-C9	-11.93	1.34	1.56

The worst 5 of 165 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2010	CLR	C21-C20-C22	-10.07	93.56	110.35
8	A	2010	CLR	C21-C20-C17	-7.74	100.07	112.96
6	C	2004	ADP	N3-C2-N1	-5.97	124.32	128.89
6	A	2004	ADP	N3-C2-N1	-5.59	124.61	128.89
8	C	2010	CLR	C10-C5-C6	-4.55	114.50	122.92

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	2015	PC1	C2-O21-C21-O22
9	C	2015	PC1	C2-O21-C21-C22

There are no ring outliers.

19 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2002	ALF	1	0
6	A	2004	ADP	5	0
8	A	2009	CLR	4	0
8	A	2010	CLR	8	0
9	A	2011	PC1	4	0
9	A	2012	PC1	4	0
9	A	2013	PC1	3	0
9	A	2014	PC1	4	0
8	B	3001	CLR	4	0
5	C	2002	ALF	2	0
6	C	2004	ADP	6	0
8	C	2009	CLR	4	0
8	C	2010	CLR	12	0
8	C	2011	CLR	7	0
9	C	2012	PC1	3	0
9	C	2013	PC1	3	0
9	C	2014	PC1	11	0
9	C	2015	PC1	6	0
9	D	401	PC1	3	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	994/1016 (97%)	-0.16	29 (2%)	55	43	25, 73, 140, 201	0
1	C	994/1016 (97%)	0.07	43 (4%)	39	27	47, 84, 159, 204	0
2	B	303/303 (100%)	0.83	46 (15%)	3	1	71, 147, 222, 240	0
2	D	303/303 (100%)	0.84	52 (17%)	2	1	71, 136, 214, 240	0
3	E	35/65 (53%)	0.63	5 (14%)	4	2	76, 95, 189, 199	0
3	G	34/65 (52%)	0.92	4 (11%)	6	3	78, 101, 174, 199	0
All	All	2663/2768 (96%)	0.18	179 (6%)	21	12	25, 89, 176, 240	0

The worst 5 of 179 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	15	ASP	15.1
2	D	218	ASP	14.2
2	D	166	THR	13.0
2	B	1	MET	11.9
1	C	396	THR	10.5

### 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 ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	NA	A	2005	1/1	0.93	0.44	13.00	159,159,159,159	0
7	NA	A	2007	1/1	0.84	0.43	5.41	127,127,127,127	0
7	NA	C	2007	1/1	0.92	0.35	5.26	179,179,179,179	0
9	PC1	C	2015	54/54	0.75	0.45	4.83	119,145,185,228	0
8	CLR	A	2009	28/28	0.87	0.40	4.69	115,125,157,163	0
9	PC1	C	2014	54/54	0.77	0.51	3.41	93,138,188,199	0
7	NA	A	2006	1/1	0.72	0.27	3.38	86,86,86,86	0
9	PC1	A	2012	54/54	0.81	0.40	3.30	70,138,173,177	0
8	CLR	A	2010	28/28	0.91	0.26	2.78	91,115,123,156	0
9	PC1	C	2013	54/54	0.79	0.36	2.67	76,124,159,196	0
8	CLR	B	3001	28/28	0.85	0.29	2.32	55,124,129,156	0
8	CLR	C	2010	28/28	0.88	0.29	2.28	42,104,166,180	0
9	PC1	A	2013	54/54	0.87	0.33	2.25	88,124,142,168	0
9	PC1	B	3002	54/54	0.80	0.29	2.13	76,116,145,193	0
5	ALF	A	2002	5/5	0.98	0.24	2.02	9,16,42,141	0
7	NA	C	2006	1/1	0.89	0.27	1.96	113,113,113,113	0
9	PC1	D	401	54/54	0.87	0.26	1.60	68,94,169,191	0
9	PC1	A	2011	54/54	0.90	0.30	0.80	81,119,150,155	0
8	CLR	C	2009	28/28	0.89	0.24	0.73	56,113,136,137	0
9	PC1	C	2012	54/54	0.89	0.30	0.63	93,118,156,159	0
7	NA	C	2005	1/1	0.91	0.20	0.53	84,84,84,84	0
9	PC1	A	2014	54/54	0.81	0.38	0.49	105,138,172,233	0
4	MG	A	2003	1/1	0.94	0.18	0.46	24,24,24,24	0
5	ALF	C	2002	5/5	0.95	0.16	-0.58	38,48,56,67	0
6	ADP	C	2004	27/27	0.95	0.15	-0.69	8,62,69,86	0
8	CLR	C	2011	28/28	0.94	0.12	-0.97	45,98,125,139	0
6	ADP	A	2004	27/27	0.97	0.11	-1.05	6,35,51,60	0
4	MG	C	2003	1/1	0.99	0.08	-2.50	48,48,48,48	0
10	NAG	B	3003	14/15	0.80	0.51	-	145,151,160,164	0
7	NA	A	2008	1/1	0.76	0.26	-	100,100,100,100	0
7	NA	C	2008	1/1	0.88	0.39	-	62,62,62,62	0
4	MG	C	2001	1/1	0.85	0.28	-	96,96,96,96	0
10	NAG	D	402	14/15	0.84	0.26	-	114,138,143,143	0
4	MG	A	2001	1/1	0.88	0.41	-	67,67,67,67	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.