



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:50 AM GMT

PDB ID : 3N23  
Title : Crystal structure of the high affinity complex between ouabain and the E2P form of the sodium-potassium pump  
Authors : Yatime, L.; Laursen, M.; Morth, J.P.; Esmann, M.; Nissen, P.; Fedosova, N.U.  
Deposited on : 2010-05-17  
Resolution : 4.60 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

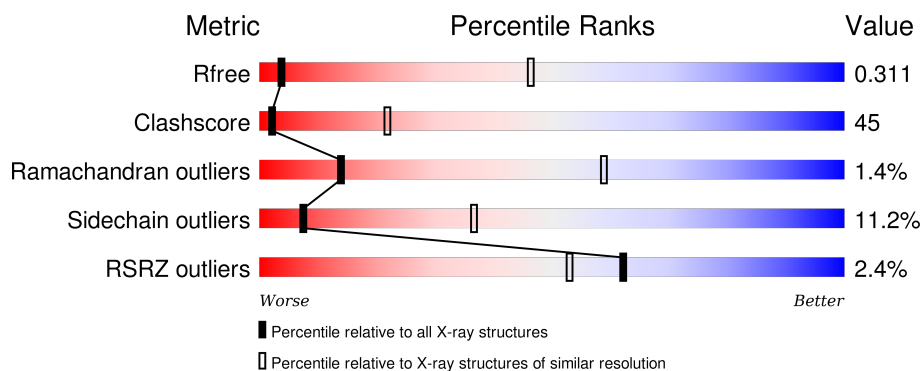
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.60 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	1089 (5.52-3.60)
Clashscore	102246	1004 (5.52-3.64)
Ramachandran outliers	100387	1131 (5.52-3.60)
Sidechain outliers	100360	1112 (5.50-3.60)
RSRZ outliers	91569	1092 (5.52-3.60)

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	992	<div> <div>45%</div> <div>49%</div> <div>6%</div> </div>
1	C	992	<div> <div>3%</div> <div>44%</div> <div>49%</div> <div>6%</div> </div>
2	B	277	<div> <div>4%</div> <div>31%</div> <div>52%</div> <div>12%</div> <div>5%</div> </div>
2	D	277	<div> <div>2%</div> <div>29%</div> <div>55%</div> <div>12%</div> <div>5%</div> </div>
3	E	31	<div> <div>52%</div> <div>48%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	31	

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
1	PHD	A	369	-	-	X	-
4	OBN	A	1	-	-	X	-
4	OBN	C	1	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20272 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	992	Total	C	N	O	P	S	0	0	0
			7693	4901	1293	1451	1	47			
1	C	992	Total	C	N	O	P	S	0	0	0
			7693	4901	1293	1451	1	47			

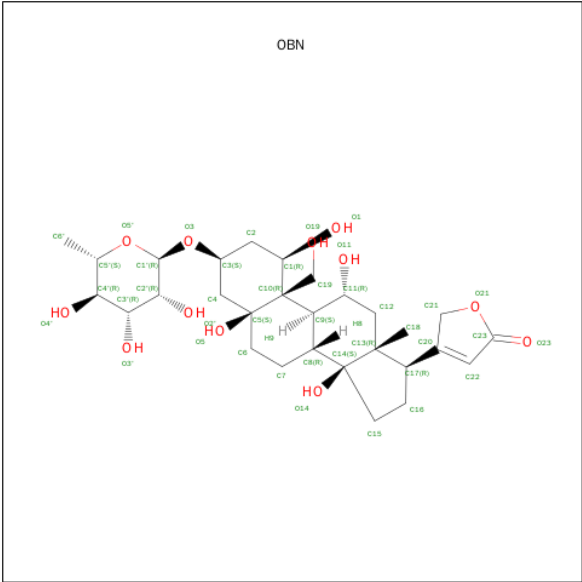
- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	264	Total	C	N	O	S	0	0	0
			2155	1400	352	390	13			
2	D	264	Total	C	N	O	S	0	0	0
			2155	1400	352	390	13			

- 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	31	Total	C	N	O	0	0	0
			246	168	35	43			
3	E	31	Total	C	N	O	0	0	0
			246	168	35	43			

- Molecule 4 is OUABAIN (three-letter code: OBN) (formula: C<sub>29</sub>H<sub>44</sub>O<sub>12</sub>).



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

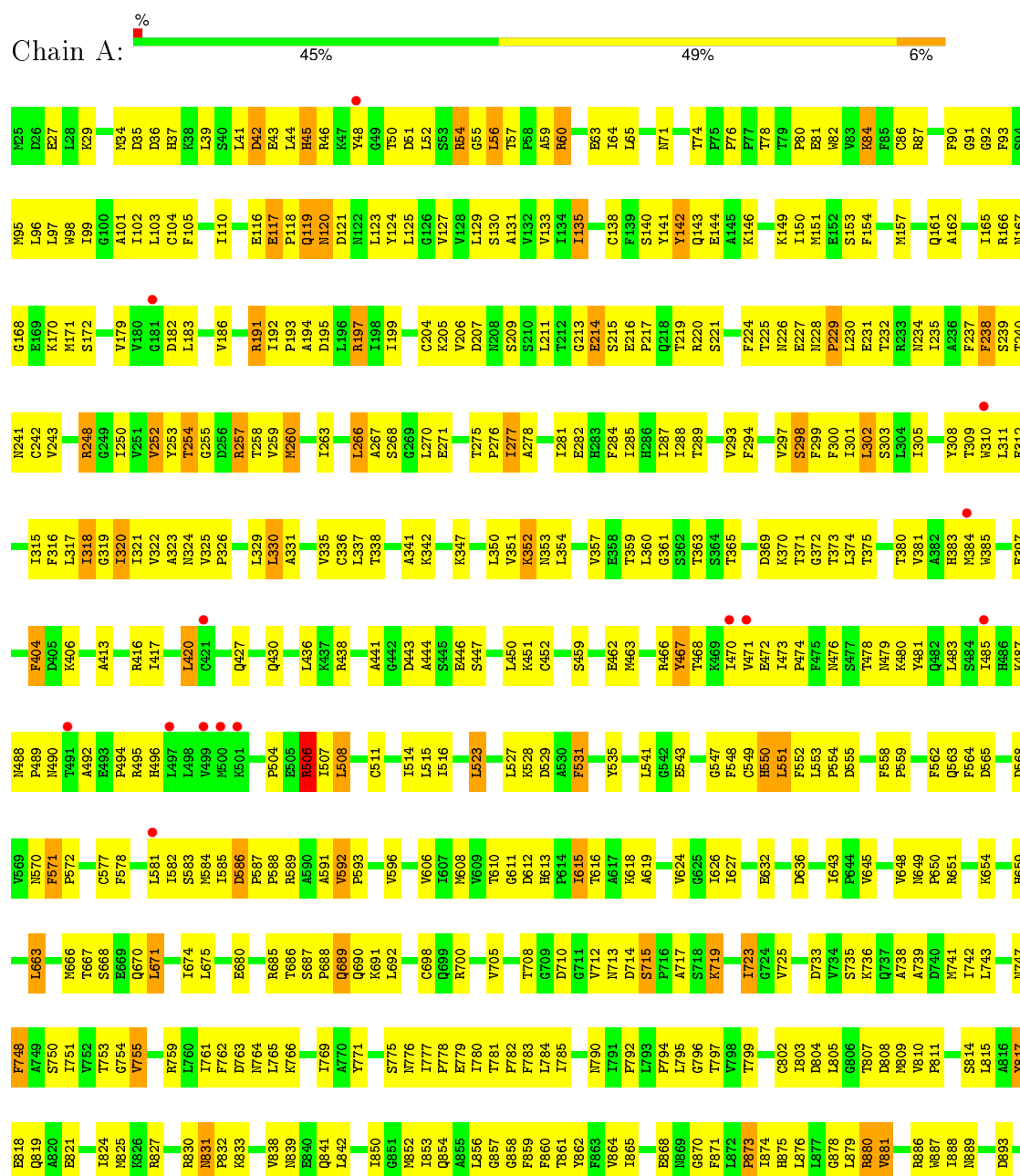
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

### 3 Residue-property plots

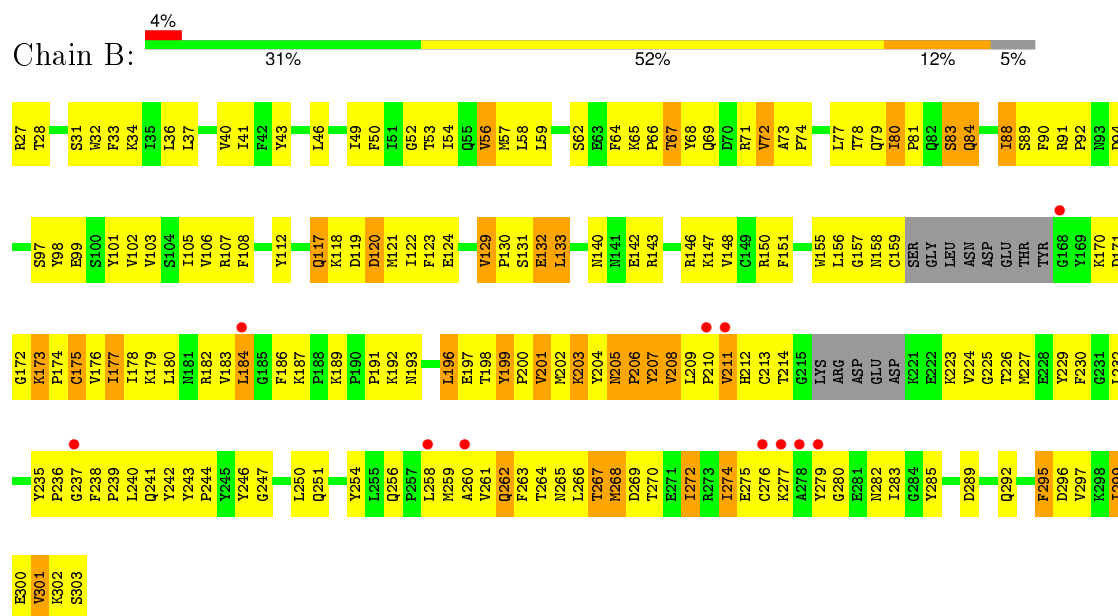
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Sodium/potassium-transporting ATPase subunit alpha-1

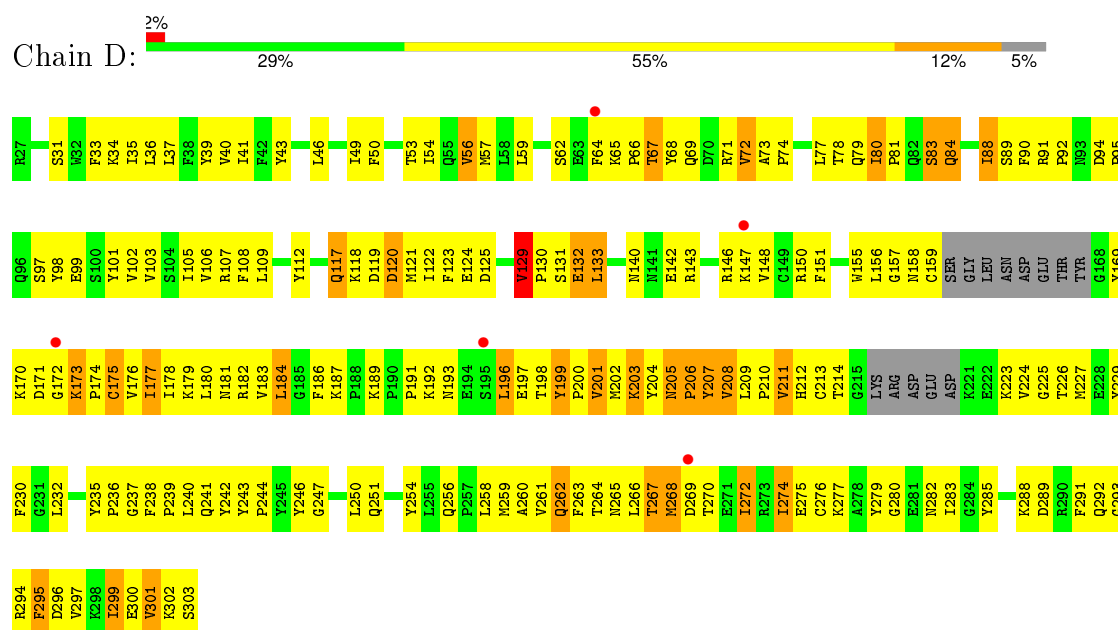




- Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



- 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





D17	F18	F19	Y20	Y21	D22	Y23	E24	T25	L31	L32	L36	L39	V40	G41	L42	L43	L44	L45	L46	S47
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.16Å 118.93Å 494.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.55 – 4.60 49.65 – 4.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.55-4.60) 99.9 (49.65-4.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 4.64Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6 _289)	Depositor
R, $R_{free}$	0.272 , 0.302 0.284 , 0.311	Depositor DCC
$R_{free}$ test set	1976 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	186.0	Xtriage
Anisotropy	0.689	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 189.0	EDS
Estimated twinning fraction	0.056 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 39348 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	20272	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	277.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OBN, MG, PHD

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	0.34	1/7830 (0.0%)	0.52	6/10626 (0.1%)
1	C	0.35	1/7830 (0.0%)	0.53	5/10626 (0.0%)
2	B	0.35	0/2211	0.50	0/2981
2	D	0.35	0/2211	0.49	0/2981
3	E	0.42	0/252	0.52	0/343
3	G	0.41	0/252	0.50	0/343
All	All	0.35	2/20586 (0.0%)	0.52	11/27900 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	551	LEU	CG-CD2	-7.22	1.25	1.51
1	A	551	LEU	CG-CD2	-5.95	1.29	1.51

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	248	ARG	NE-CZ-NH1	12.22	126.41	120.30
1	C	551	LEU	CB-CG-CD2	-10.02	93.97	111.00
1	A	551	LEU	CB-CG-CD2	-9.79	94.36	111.00
1	C	551	LEU	CB-CG-CD1	9.77	127.61	111.00
1	A	551	LEU	CB-CG-CD1	9.74	127.55	111.00

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	7693	0	7740	605	1
1	C	7693	0	7741	656	0
2	B	2155	0	2143	291	0
2	D	2155	0	2143	295	1
3	E	246	0	246	13	0
3	G	246	0	246	11	0
4	A	41	0	44	23	0
4	C	41	0	44	23	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
All	All	20272	0	20347	1820	1

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 45.

The worst 5 of 1820 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:48:TYR:OH	1:A:252:VAL:HG12	1.32	1.25
2:B:130:PRO:HG2	2:B:204:TYR:CZ	1.73	1.24
2:D:204:TYR:C	2:D:206:PRO:HD2	1.60	1.21
2:D:129:VAL:HG22	2:D:130:PRO:CD	1.73	1.19
2:B:204:TYR:C	2:B:206:PRO:HD2	1.65	1.16

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ARG:NH2	2:D:132:GLU:O[4_545]	2.05	0.15

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	989/992 (100%)	807 (82%)	171 (17%)	11 (1%)	17	64
1	C	989/992 (100%)	809 (82%)	168 (17%)	12 (1%)	16	62
2	B	258/277 (93%)	197 (76%)	56 (22%)	5 (2%)	10	53
2	D	258/277 (93%)	195 (76%)	56 (22%)	7 (3%)	6	47
3	E	29/31 (94%)	25 (86%)	4 (14%)	0	100	100
3	G	29/31 (94%)	25 (86%)	4 (14%)	0	100	100
All	All	2552/2600 (98%)	2058 (81%)	459 (18%)	35 (1%)	14	59

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	158	ASN
2	B	206	PRO
2	D	158	ASN
2	D	206	PRO
2	B	120	ASP

### 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	842/842 (100%)	747 (89%)	95 (11%)	7	36
1	C	842/842 (100%)	760 (90%)	82 (10%)	10	43
2	B	236/248 (95%)	202 (86%)	34 (14%)	4	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	236/248 (95%)	202 (86%)	34 (14%)	4	27
3	E	25/25 (100%)	24 (96%)	1 (4%)	38	73
3	G	25/25 (100%)	23 (92%)	2 (8%)	15	53
All	All	2206/2230 (99%)	1958 (89%)	248 (11%)	7	37

5 of 248 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	192	LYS
1	C	60	ARG
2	D	184	LEU
2	B	201	VAL
2	B	285	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	212	HIS
1	C	161	GLN
2	D	117	GLN
2	B	262	GLN
1	C	37	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	1,5	8,11,12	2.12	1 (12%)	9,15,17	2.68	4 (44%)
1	PHD	C	369	1,5	8,11,12	2.15	1 (12%)	9,15,17	2.61	4 (44%)

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	1,5	-	0/7/11/13	0/0/0/0
1	PHD	C	369	1,5	-	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	A	369	PHD	OD2-CG	5.15	1.38	1.22
1	C	369	PHD	OD2-CG	5.23	1.38	1.22

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	369	PHD	OD2-CG-CB	-4.48	114.40	124.69
1	C	369	PHD	OD1-CG-OD2	-4.24	112.72	121.67
1	A	369	PHD	OD2-CG-CB	-4.07	115.34	124.69
1	A	369	PHD	OD1-CG-OD2	-3.82	113.62	121.67
1	A	369	PHD	O-C-CA	-2.28	119.55	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	369	PHD	7	0
1	C	369	PHD	5	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	OBN	A	1	-	44,46,46	0.75	1 (2%)	65,76,76	2.03	14 (21%)
4	OBN	C	1	-	44,46,46	0.83	1 (2%)	65,76,76	2.21	18 (27%)

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	OBN	A	1	-	-	0/11/116/116	0/6/6/6
4	OBN	C	1	-	-	0/11/116/116	0/6/6/6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	OBN	O21-C23	3.12	1.44	1.36
4	C	1	OBN	O21-C23	3.43	1.45	1.36

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	OBN	C16-C17-C20	-5.12	104.18	113.36
4	C	1	OBN	C15-C14-C8	-4.76	108.96	116.02
4	A	1	OBN	C15-C14-C8	-4.58	109.23	116.02
4	C	1	OBN	C18-C13-C12	-4.46	104.96	111.14
4	C	1	OBN	C16-C17-C20	-4.12	105.99	113.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



2 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	OBN	23	0
4	C	1	OBN	23	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 ⓘ

### 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<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	991/992 (99%)	-0.20	14 (1%) 78 70	158, 252, 353, 457	0
1	C	991/992 (99%)	-0.08	33 (3%) 50 40	175, 274, 412, 550	0
2	B	264/277 (95%)	0.06	11 (4%) 40 32	207, 280, 383, 469	0
2	D	264/277 (95%)	-0.04	5 (1%) 70 61	207, 280, 383, 469	0
3	E	31/31 (100%)	-0.43	0 100 100	177, 249, 313, 421	0
3	G	31/31 (100%)	-0.35	0 100 100	158, 247, 330, 396	0
All	All	2572/2600 (98%)	-0.11	63 (2%) 62 53	158, 266, 391, 550	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	573	LEU	4.7
1	C	488	ASN	4.7
1	C	574	ASP	4.6
1	C	572	PRO	4.1
1	C	491	THR	3.9

### 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<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
1	PHD	A	369	12/13	0.95	0.23	-	249,249,377,377	0
1	PHD	C	369	12/13	0.95	0.24	-	288,288,461,461	0

### 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, 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( $\text{\AA}^2$ )	Q<0.9
5	MG	C	1017	1/1	0.99	0.31	1.29	274,274,274,274	0
5	MG	A	1017	1/1	0.96	0.28	0.63	274,274,274,274	0
4	OBN	A	1	41/41	0.92	0.28	0.30	274,274,274,274	0
4	OBN	C	1	41/41	0.90	0.27	0.11	274,274,274,274	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.