



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:13 PM GMT

PDB ID : 2C1W  
Title : THE STRUCTURE OF XENDOU: A SPLICING INDEPENDENT SNORNA  
PROCESSING ENDORIBONUCLEASE  
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Deposited on : 2005-09-21  
Resolution : 2.20 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

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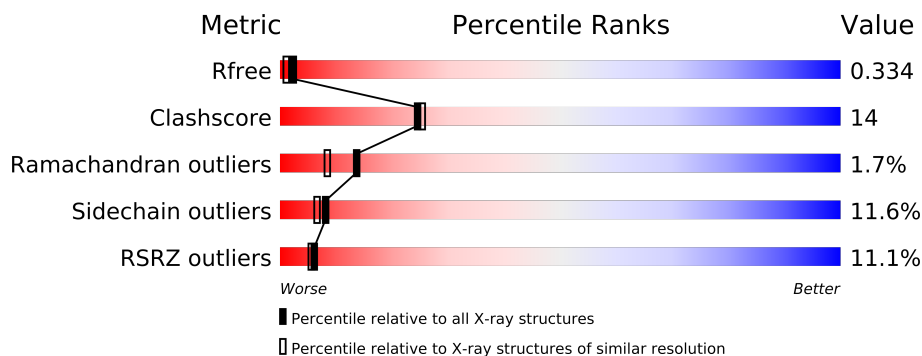
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 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))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	292	
1	B	292	
1	C	292	

## 2 Entry composition

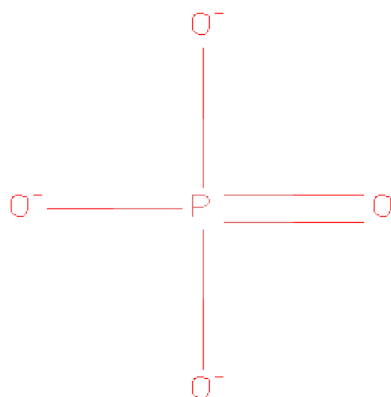
There are 3 unique types of molecules in this entry. The entry contains 7368 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ENDOU PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	7	0
			2293	1466	396	421	10			
1	B	276	Total	C	N	O	S	0	7	0
			2317	1479	401	428	9			
1	C	271	Total	C	N	O	S	0	12	0
			2305	1475	396	425	9			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

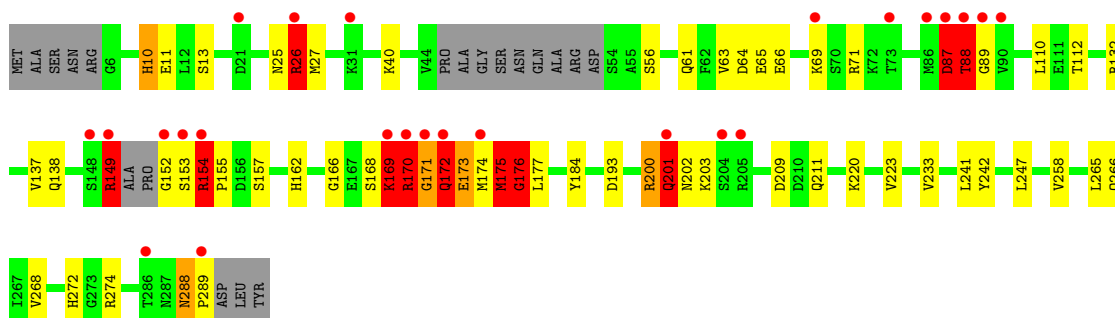
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	161	Total 161	O 161	0	0
3	B	167	Total 167	O 167	0	0
3	C	110	Total 110	O 110	0	0

### 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.

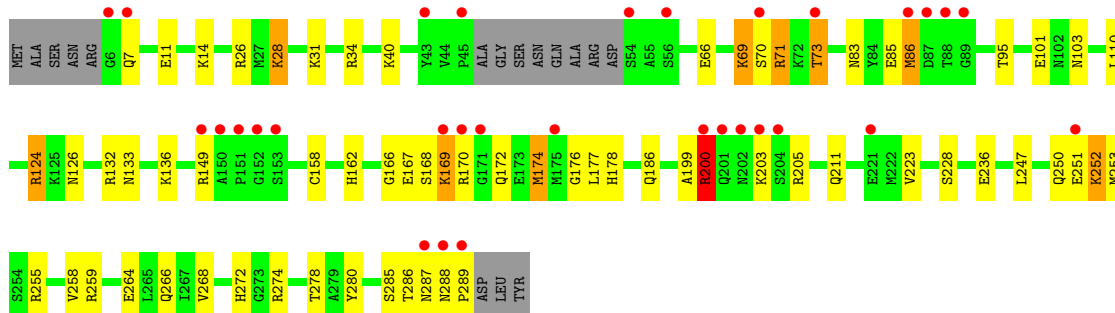
#### • Molecule 1: ENDOU PROTEIN

Chain A: 



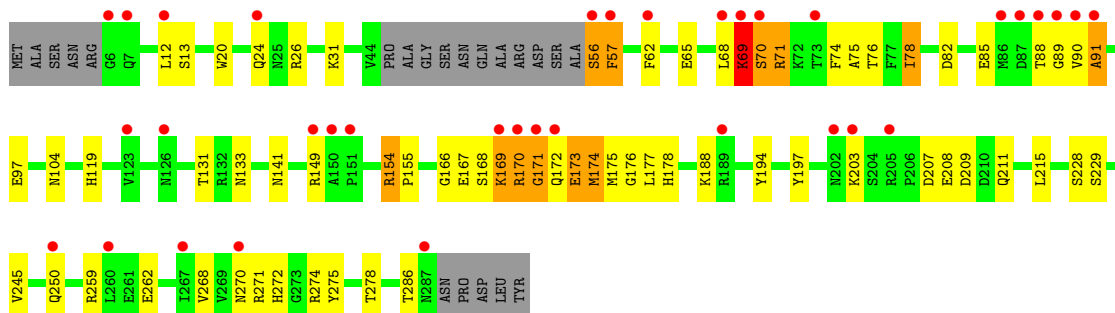
#### • Molecule 1: ENDOU PROTEIN

Chain B: 



#### • Molecule 1: ENDOU PROTEIN

Chain C: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.45Å 53.20Å 133.47Å 90.00° 121.86° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.90 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (20.00-2.20) 96.9 (19.90-2.20)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.42 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.274 , 0.277 0.270 , 0.334	Depositor DCC
$R_{free}$ test set	2466 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.5	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 50.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 48653 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7368	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.85	6/2363 (0.3%)	1.00	16/3176 (0.5%)
1	B	0.74	0/2388	0.87	3/3218 (0.1%)
1	C	0.74	2/2391 (0.1%)	0.86	6/3219 (0.2%)
All	All	0.78	8/7142 (0.1%)	0.91	25/9613 (0.3%)

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	16
1	B	0	2
1	C	1	9
All	All	1	27

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170[A]	ARG	CA-C	11.41	1.82	1.52
1	A	170[B]	ARG	CA-C	11.41	1.82	1.52
1	C	133[A]	ASN	C-N	-9.91	1.11	1.34
1	C	133[B]	ASN	C-N	-9.91	1.11	1.34
1	A	149[A]	ARG	CA-C	8.35	1.74	1.52
1	A	149[B]	ARG	CA-C	8.35	1.74	1.52
1	A	242	TYR	CD1-CE1	7.97	1.51	1.39
1	A	89	GLY	N-CA	6.37	1.55	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	LYS	CB-CA-C	-14.67	81.07	110.40
1	C	70	SER	N-CA-CB	-14.22	89.17	110.50
1	B	69	LYS	CB-CA-C	-11.91	86.58	110.40
1	C	70	SER	N-CA-C	10.74	139.99	111.00
1	B	70	SER	CB-CA-C	-10.22	90.69	110.10
1	A	172	GLN	CB-CA-C	-10.07	90.25	110.40
1	A	170[A]	ARG	N-CA-C	-9.83	84.45	111.00
1	A	170[B]	ARG	N-CA-C	-9.83	84.45	111.00
1	A	170[A]	ARG	CA-C-N	-8.42	99.36	116.20
1	A	170[B]	ARG	CA-C-N	-8.42	99.36	116.20
1	B	71	ARG	N-CA-C	-8.19	88.90	111.00
1	A	169	LYS	N-CA-C	7.92	132.39	111.00
1	A	173	GLU	N-CA-CB	-7.88	96.41	110.60
1	A	170[A]	ARG	CA-C-O	7.74	136.36	120.10
1	A	170[B]	ARG	CA-C-O	7.74	136.36	120.10
1	A	176	GLY	N-CA-C	7.68	132.29	113.10
1	A	88	THR	N-CA-C	-7.54	90.63	111.00
1	C	69	LYS	CB-CA-C	7.46	125.32	110.40
1	A	89	GLY	N-CA-C	6.98	130.55	113.10
1	A	56	SER	CB-CA-C	6.92	123.24	110.10
1	C	133[A]	ASN	O-C-N	-6.87	111.71	122.70
1	C	133[B]	ASN	O-C-N	-6.87	111.71	122.70
1	C	57	PHE	N-CA-C	-5.33	96.60	111.00
1	A	173	GLU	N-CA-C	-5.12	97.17	111.00
1	A	193	ASP	CB-CG-OD2	5.06	122.85	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	69	LYS	CA

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	GLY	Peptide
1	A	168	SER	Peptide
1	A	169	LYS	Peptide
1	A	170[A]	ARG	Peptide
1	A	170[B]	ARG	Peptide
1	A	171	GLY	Peptide
1	A	173	GLU	Peptide
1	A	175	MET	Peptide
1	A	176	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	A	201[A]	GLN	Peptide
1	A	201[B]	GLN	Peptide
1	A	25	ASN	Peptide
1	A	26	ARG	Peptide
1	A	87	ASP	Peptide
1	B	174	MET	Peptide
1	B	200	ARG	Peptide
1	C	169[A]	LYS	Peptide
1	C	169[B]	LYS	Peptide
1	C	171	GLY	Peptide
1	C	286	THR	Peptide
1	C	56	SER	Peptide
1	C	68	LEU	Peptide
1	C	69	LYS	Peptide
1	C	91	ALA	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2293	0	14	32	0
1	B	2317	0	0	41	0
1	C	2305	0	0	30	0
2	A	5	0	0	2	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	161	0	0	5	0
3	B	167	0	0	10	0
3	C	110	0	0	3	0
All	All	7368	0	14	97	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (97) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:201[A]:GLN:HG2	1:B:274:ARG:NE	1.73	1.02
1:C:170:ARG:CG	1:C:171:GLY:N	2.28	0.94
1:A:201[A]:GLN:CG	1:B:274:ARG:NE	2.33	0.90
1:C:278:THR:CG2	3:C:2051:HOH:O	2.29	0.80
1:B:170[B]:ARG:CG	1:B:170[B]:ARG:NH1	2.46	0.79
1:B:288:ASN:CB	1:B:289:PRO:CD	2.61	0.78
1:A:170[A]:ARG:CA	1:A:171:GLY:N	2.42	0.77
1:C:194:TYR:CD2	3:C:2063:HOH:O	2.38	0.76
1:B:169:LYS:CG	1:B:172:GLN:CG	2.64	0.76
1:A:201[B]:GLN:HA	1:A:201[B]:GLN:OE1	1.89	0.73
1:B:34:ARG:NH2	3:B:2030:HOH:O	2.24	0.70
1:B:255:ARG:NH2	1:C:91:ALA:O	2.25	0.69
1:C:166:GLY:O	1:C:176:GLY:N	2.24	0.69
1:B:199:ALA:O	1:C:274:ARG:NH2	2.25	0.69
1:C:91:ALA:CB	1:C:154:ARG:NE	2.56	0.68
1:B:83:ASN:ND2	1:B:101:GLU:OE1	2.26	0.68
1:A:157:SER:OG	1:A:162:HIS:CE1	2.48	0.67
1:B:85:GLU:OE2	1:B:186:GLN:NE2	2.28	0.66
1:A:201[A]:GLN:HG3	1:B:274:ARG:NE	2.11	0.65
1:B:31:LYS:NZ	3:B:2027:HOH:O	2.30	0.64
1:C:167:GLU:OE2	1:C:173:GLU:N	2.31	0.64
1:B:169:LYS:CG	1:B:172:GLN:CB	2.76	0.63
1:A:10[B]:HIS:CD2	3:A:2007:HOH:O	2.50	0.63
1:B:126:ASN:ND2	3:B:2086:HOH:O	2.33	0.62
1:B:103:ASN:OD1	1:B:136:LYS:NZ	2.33	0.61
1:B:166:GLY:O	1:B:176:GLY:N	2.35	0.59
1:C:228:SER:N	3:C:2082:HOH:O	2.35	0.59
1:B:26:ARG:NH1	3:B:2021:HOH:O	2.35	0.58
1:B:158:CYS:O	1:B:162:HIS:CD2	2.58	0.57
1:A:153:SER:O	1:A:154:ARG:CB	2.53	0.56
1:B:236:GLU:OE1	1:B:236:GLU:N	2.38	0.56
1:A:87:ASP:O	1:A:88:THR:C	2.44	0.55
1:C:168:SER:OG	1:C:173:GLU:OE1	2.25	0.55
1:B:251[B]:GLU:CB	3:B:2147:HOH:O	2.55	0.55
1:A:26:ARG:NH2	3:A:2021:HOH:O	2.40	0.54
1:B:251[A]:GLU:CB	3:B:2147:HOH:O	2.56	0.54
1:A:223:VAL:CG1	1:B:136:LYS:NZ	2.72	0.53
1:B:287:ASN:ND2	3:B:2167:HOH:O	2.41	0.52
1:B:73:THR:OG1	1:B:73:THR:O	2.27	0.51
1:B:203:LYS:CB	3:B:2167:HOH:O	2.59	0.50
1:A:65:GLU:OE1	1:A:184:TYR:OH	2.29	0.50
1:A:200:ARG:O	1:A:202:ASN:O	2.30	0.49
1:C:245:VAL:O	1:C:271:ARG:NH2	2.44	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:149[B]:ARG:NH2	1:A:272:HIS:CE1	2.81	0.49
1:B:167:GLU:OE2	1:B:168:SER:N	2.46	0.48
1:B:168:SER:OG	1:B:169:LYS:CE	2.61	0.48
1:A:172:GLN:NE2	1:A:220:LYS:NZ	2.62	0.47
1:C:74:PHE:O	1:C:78:ILE:CG2	2.62	0.47
1:A:266:GLN:NE2	3:A:2152:HOH:O	2.47	0.47
1:C:174:MET:O	1:C:175:MET:CG	2.63	0.47
1:A:162:HIS:CD2	2:A:1290:PO4:O2	2.68	0.47
1:C:209:ASP:O	1:C:211:GLN:NE2	2.48	0.46
1:B:178:HIS:ND1	1:B:228:SER:O	2.49	0.46
1:A:166:GLY:O	1:A:176:GLY:CA	2.63	0.46
1:B:66:GLU:O	1:B:69:LYS:O	2.34	0.46
1:B:167:GLU:OE1	1:B:174:MET:O	2.33	0.46
1:A:132:ARG:CZ	3:A:2081:HOH:O	2.64	0.46
1:B:149[B]:ARG:CG	1:B:272:HIS:ND1	2.80	0.45
1:C:149[B]:ARG:NH2	1:C:168:SER:OG	2.50	0.45
1:C:20:TRP:O	1:C:26:ARG:NH2	2.50	0.45
1:A:63:VAL:CG1	1:A:184:TYR:CZ	3.01	0.44
1:B:200:ARG:NH1	1:B:203:LYS:CB	2.81	0.44
1:A:288:ASN:N	1:A:289:PRO:CD	2.81	0.44
1:A:149[B]:ARG:NH2	2:A:1290:PO4:O4	2.50	0.44
1:B:255:ARG:NH2	3:B:2154:HOH:O	2.50	0.44
1:B:178:HIS:CD2	1:B:280:TYR:CB	3.02	0.43
1:B:28[A]:LYS:CB	1:B:28[A]:LYS:NZ	2.80	0.43
1:A:258:VAL:O	1:A:265:LEU:N	2.52	0.43
1:B:11:GLU:OE2	1:B:124:ARG:NH2	2.52	0.43
1:C:69:LYS:O	1:C:69:LYS:CD	2.67	0.42
1:C:70:SER:O	1:C:71:ARG:C	2.57	0.42
1:B:278:THR:CG2	3:B:2105:HOH:O	2.67	0.42
1:B:162:HIS:N	1:B:162:HIS:CD2	2.88	0.42
1:B:86:MET:O	1:B:170[B]:ARG:NH2	2.53	0.42
1:B:286:THR:CG2	1:B:287:ASN:ND2	2.83	0.42
1:A:174[B]:MET:CE	3:A:2058:HOH:O	2.67	0.42
1:C:65[B]:GLU:OE2	1:C:188:LYS:NZ	2.53	0.41
1:C:272:HIS:N	1:C:275:TYR:O	2.53	0.41
1:C:197:TYR:C	1:C:197:TYR:CD2	2.94	0.41
1:C:178:HIS:O	1:C:229:SER:OG	2.39	0.41
1:A:137:VAL:O	1:A:138:GLN:C	2.59	0.41
1:C:69:LYS:O	1:C:75:ALA:CB	2.69	0.40
1:A:65:GLU:O	1:A:69:LYS:N	2.54	0.40

There are no symmetry-related clashes.

## 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	273/292 (94%)	231 (85%)	32 (12%)	10 (4%)	5	2
1	B	279/292 (96%)	245 (88%)	32 (12%)	2 (1%)	30	28
1	C	279/292 (96%)	250 (90%)	25 (9%)	4 (1%)	16	12
All	All	831/876 (95%)	726 (87%)	89 (11%)	16 (2%)	14	7

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	ARG
1	A	175	MET
1	A	203[A]	LYS
1	A	203[B]	LYS
1	A	10[A]	HIS
1	A	10[B]	HIS
1	A	64	ASP
1	B	73	THR
1	C	90	VAL
1	B	200	ARG
1	C	173	GLU
1	A	154	ARG
1	C	89	GLY
1	A	288	ASN
1	C	155	PRO
1	A	155	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	252/259 (97%)	220 (87%)	32 (13%)	6	5
1	B	254/259 (98%)	226 (89%)	28 (11%)	9	8
1	C	255/259 (98%)	220 (86%)	35 (14%)	5	4
All	All	761/777 (98%)	666 (88%)	95 (12%)	8	5

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	13	SER
1	A	26	ARG
1	A	27	MET
1	A	40[A]	LYS
1	A	40[B]	LYS
1	A	61	GLN
1	A	66	GLU
1	A	71	ARG
1	A	87	ASP
1	A	88	THR
1	A	110	LEU
1	A	112	THR
1	A	149[A]	ARG
1	A	149[B]	ARG
1	A	154	ARG
1	A	169	LYS
1	A	170[A]	ARG
1	A	170[B]	ARG
1	A	172	GLN
1	A	175	MET
1	A	177	LEU
1	A	200	ARG
1	A	201[A]	GLN
1	A	201[B]	GLN
1	A	209	ASP
1	A	211	GLN
1	A	233	VAL
1	A	241	LEU
1	A	247	LEU
1	A	268	VAL
1	A	274	ARG
1	B	7	GLN
1	B	14	LYS

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Mol	Chain	Res	Type
1	B	28[A]	LYS
1	B	28[B]	LYS
1	B	40	LYS
1	B	71	ARG
1	B	86	MET
1	B	95	THR
1	B	110	LEU
1	B	124	ARG
1	B	132	ARG
1	B	133	ASN
1	B	169	LYS
1	B	177	LEU
1	B	200	ARG
1	B	205	ARG
1	B	211	GLN
1	B	223	VAL
1	B	247	LEU
1	B	250	GLN
1	B	252	LYS
1	B	253	MET
1	B	258	VAL
1	B	259	ARG
1	B	264	GLU
1	B	266	GLN
1	B	268	VAL
1	B	285	SER
1	C	12	LEU
1	C	13	SER
1	C	24	GLN
1	C	31	LYS
1	C	56	SER
1	C	57	PHE
1	C	62	PHE
1	C	71	ARG
1	C	76	THR
1	C	78	ILE
1	C	82[A]	ASP
1	C	82[B]	ASP
1	C	88	THR
1	C	97	GLU
1	C	104[A]	ASN
1	C	104[B]	ASN

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Mol	Chain	Res	Type
1	C	131	THR
1	C	141	ASN
1	C	154	ARG
1	C	169[A]	LYS
1	C	169[B]	LYS
1	C	170	ARG
1	C	172[A]	GLN
1	C	172[B]	GLN
1	C	174	MET
1	C	177	LEU
1	C	203	LYS
1	C	207	ASP
1	C	208	GLU
1	C	215	LEU
1	C	259	ARG
1	C	262	GLU
1	C	268	VAL
1	C	270[A]	ASN
1	C	270[B]	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PO4	A	1290	-	4,4,4	0.59	0	6,6,6	0.34	0
2	PO4	B	1290	-	4,4,4	0.18	0	6,6,6	0.32	0
2	PO4	C	1288	-	4,4,4	0.49	0	6,6,6	0.29	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
2	PO4	A	1290	-	-	0/0/0/0	0/0/0/0
2	PO4	B	1290	-	-	0/0/0/0	0/0/0/0
2	PO4	C	1288	-	-	0/0/0/0	0/0/0/0

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.

## 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<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	273/292 (93%)	0.58	25 (9%) 9 8	17, 32, 67, 83	2 (0%)
1	B	276/292 (94%)	0.60	31 (11%) 6 5	17, 30, 75, 89	2 (0%)
1	C	271/292 (92%)	0.85	35 (12%) 4 4	22, 41, 76, 100	1 (0%)
All	All	820/876 (93%)	0.68	91 (11%) 6 5	17, 34, 75, 100	5 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	90	VAL	7.1
1	B	89	GLY	7.0
1	B	202	ASN	7.0
1	B	152	GLY	6.5
1	B	88	THR	6.5
1	C	70	SER	6.4
1	B	70	SER	5.9
1	A	152	GLY	5.8
1	A	88	THR	5.8
1	B	171	GLY	5.6
1	C	69	LYS	5.6
1	B	201	GLN	5.5
1	C	151	PRO	5.4
1	A	87	ASP	5.1
1	C	88	THR	5.1
1	B	6	GLY	5.0
1	B	150	ALA	4.9
1	C	170	ARG	4.6
1	C	57	PHE	4.5
1	C	205[A]	ARG	4.5
1	C	287	ASN	4.5
1	A	148	SER	4.3
1	A	289	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	90	VAL	4.2
1	A	86	MET	4.2
1	A	153	SER	4.1
1	A	69	LYS	4.0
1	B	203	LYS	3.9
1	A	169	LYS	3.9
1	C	250[A]	GLN	3.8
1	C	68	LEU	3.8
1	C	91	ALA	3.8
1	B	204	SER	3.7
1	B	86	MET	3.7
1	A	170[A]	ARG	3.6
1	B	170[A]	ARG	3.5
1	A	201[A]	GLN	3.5
1	A	89	GLY	3.4
1	A	204	SER	3.4
1	C	7	GLN	3.4
1	A	205	ARG	3.4
1	A	21	ASP	3.4
1	C	171	GLY	3.3
1	A	149[A]	ARG	3.3
1	C	73	THR	3.1
1	B	151	PRO	3.1
1	B	43	TYR	3.0
1	B	287	ASN	3.0
1	B	54	SER	3.0
1	A	171	GLY	3.0
1	C	149[A]	ARG	2.9
1	A	26	ARG	2.9
1	C	62	PHE	2.8
1	C	56	SER	2.7
1	C	150	ALA	2.6
1	C	24	GLN	2.6
1	A	174[A]	MET	2.6
1	A	154	ARG	2.6
1	A	73	THR	2.5
1	B	175	MET	2.5
1	B	56	SER	2.5
1	C	87	ASP	2.5
1	B	289	PRO	2.5
1	C	260	LEU	2.5
1	C	6	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	89	GLY	2.4
1	B	153	SER	2.4
1	A	286	THR	2.4
1	C	126	ASN	2.4
1	C	172[A]	GLN	2.4
1	B	200	ARG	2.4
1	B	73	THR	2.4
1	B	149[A]	ARG	2.3
1	C	169[A]	LYS	2.3
1	C	203	LYS	2.2
1	B	87	ASP	2.2
1	B	288	ASN	2.2
1	C	270[A]	ASN	2.1
1	B	221	GLU	2.1
1	C	86	MET	2.1
1	C	123	VAL	2.1
1	A	31	LYS	2.1
1	C	12	LEU	2.1
1	B	7	GLN	2.1
1	C	189	ARG	2.0
1	B	45	PRO	2.0
1	B	169	LYS	2.0
1	C	267	ILE	2.0
1	C	202	ASN	2.0
1	A	172	GLN	2.0
1	B	251[A]	GLU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO4	B	1290	5/5	0.13	-0.40	48,49,50,50	0
2	PO4	A	1290	5/5	0.11	-0.69	37,38,40,41	0
2	PO4	C	1288	5/5	0.12	-0.96	46,47,47,49	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.