



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2018 – 10:29 am GMT

PDB ID : 4XRU  
Title : Structure of Pnkp1/Rnl/Hen1 complex  
Authors : Wang, P.  
Deposited on : 2015-01-21  
Resolution : 3.41 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

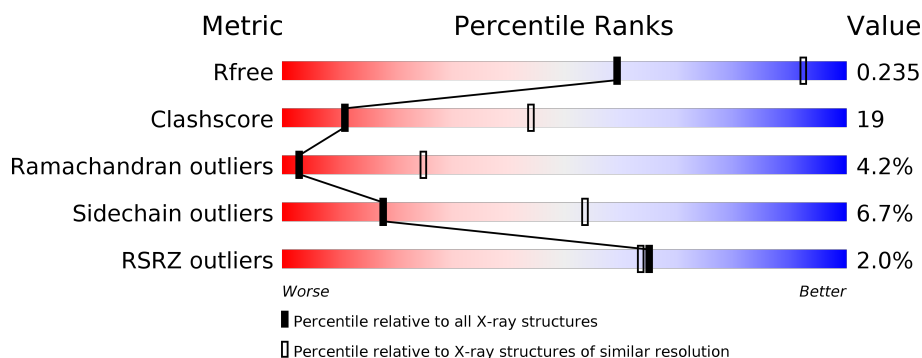
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.41 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))
$R_{free}$	111664	1244 (3.50-3.34)
Clashscore	122126	1323 (3.50-3.34)
Ramachandran outliers	120053	1291 (3.50-3.34)
Sidechain outliers	120020	1292 (3.50-3.34)
RSRZ outliers	108989	1165 (3.50-3.34)

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	312	<div> <div>3%</div> <div> <div></div> <div>54%</div> <div>36%</div> <div>•</div> <div>7%</div> </div> </div>
1	D	312	<div> <div>2%</div> <div> <div></div> <div>53%</div> <div>34%</div> <div>•</div> <div>8%</div> </div> </div>
2	B	394	<div> <div>3%</div> <div> <div></div> <div>57%</div> <div>37%</div> <div>6%</div> </div> </div>
2	E	394	<div> <div>4%</div> <div> <div></div> <div>53%</div> <div>41%</div> <div>5%</div> <div>•</div> </div> </div>
3	C	436	<div> <div></div> <div> <div></div> <div>57%</div> <div>36%</div> <div>•</div> <div>•</div> </div> </div>
3	F	436	<div> <div></div> <div> <div></div> <div>54%</div> <div>37%</div> <div>6%</div> <div>•</div> <div>•</div> </div> </div>

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
8	PO4	C	503	-	-	-	X
8	PO4	E	503	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 18713 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 Pnkp1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	Se	0	0	0
			2388	1524	405	448	3	8			
1	D	287	Total	C	N	O	S	Se	0	0	0
			2358	1506	399	443	2	8			

- Molecule 2 is a protein called Rnl.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	394	Total	C	N	O	S		0	0	0
			3290	2117	556	608	9				
2	E	393	Total	C	N	O	S		0	0	0
			3282	2112	555	607	8				

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	269	THR	ALA	conflict	UNP C2M8N4
B	329	GLU	GLN	conflict	UNP C2M8N4
E	269	THR	ALA	conflict	UNP C2M8N4
E	329	GLU	GLN	conflict	UNP C2M8N4

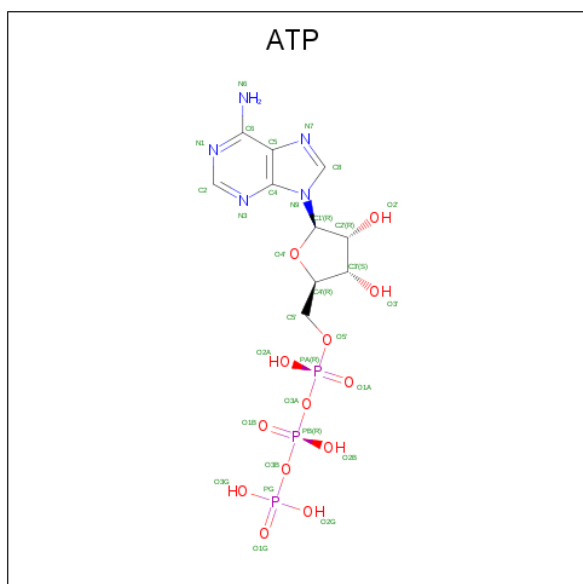
- Molecule 3 is a protein called Hen1.

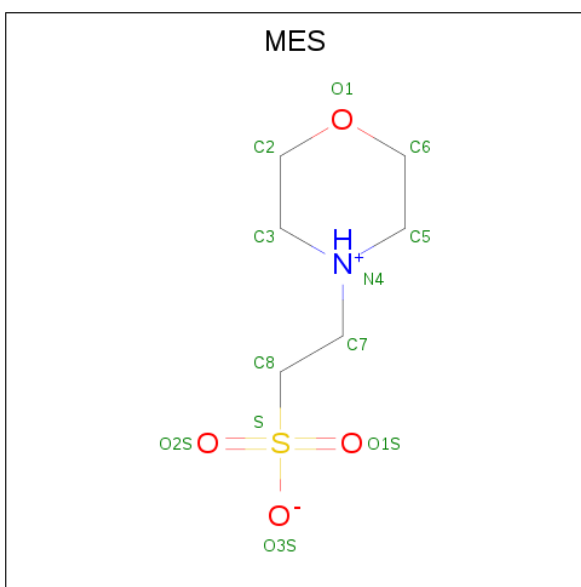
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	424	Total	C	N	O	S		0	0	0
			3536	2286	579	654	17				
3	F	424	Total	C	N	O	S		0	0	0
			3536	2286	579	654	17				

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

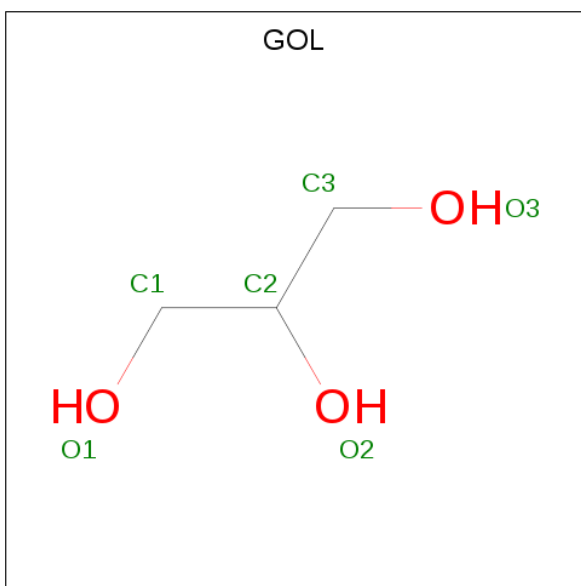
- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).





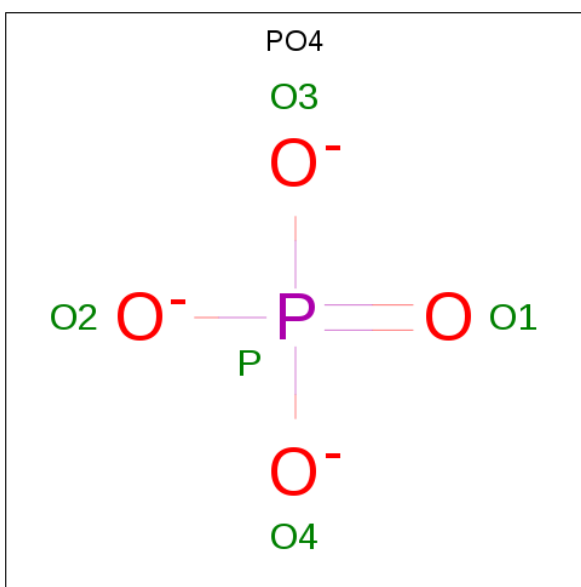
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



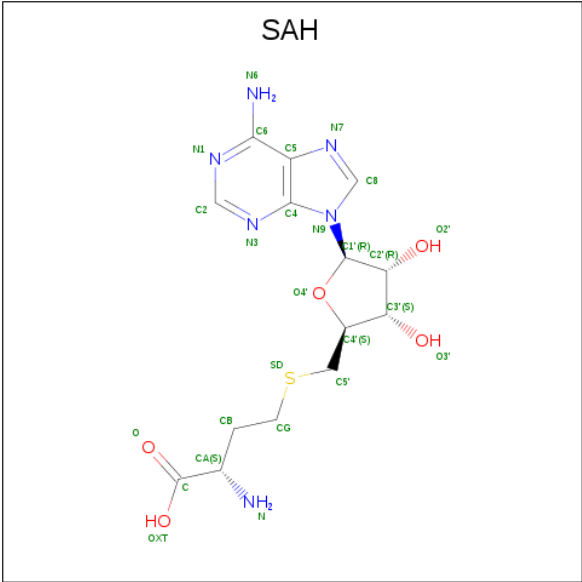
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	O	P	0	0
			5	4	1		
8	C	1	Total	O	P	0	0
			5	4	1		
8	E	1	Total	O	P	0	0
			5	4	1		
8	F	1	Total	O	P	0	0
			5	4	1		
8	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
9	F	1	Total	C	N	O	S	5	0
			26	14	6	5	1		

- Molecule 10 is water.

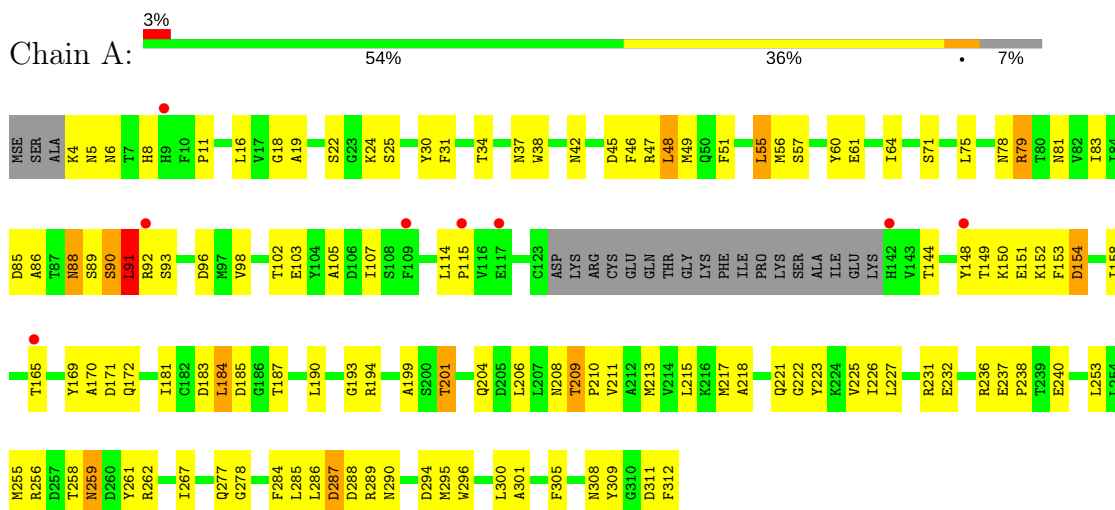
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	8	Total	O	0	0
			8	8		
10	B	28	Total	O	0	0
			28	28		
10	C	16	Total	O	0	0
			16	16		
10	D	10	Total	O	0	0
			10	10		
10	E	17	Total	O	0	0
			17	17		
10	F	13	Total	O	0	0
			13	13		



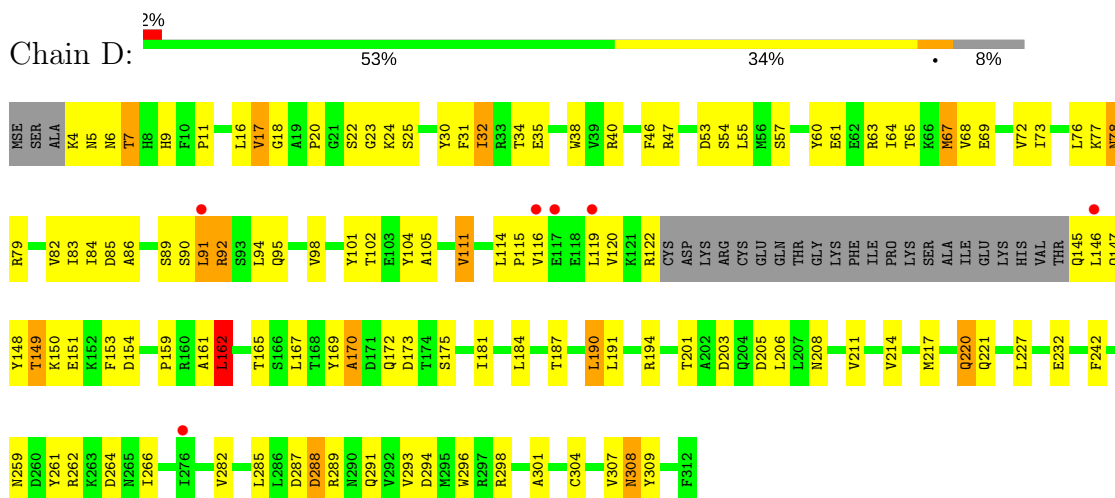
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Pnkp1



#### • Molecule 1: Pnkp1

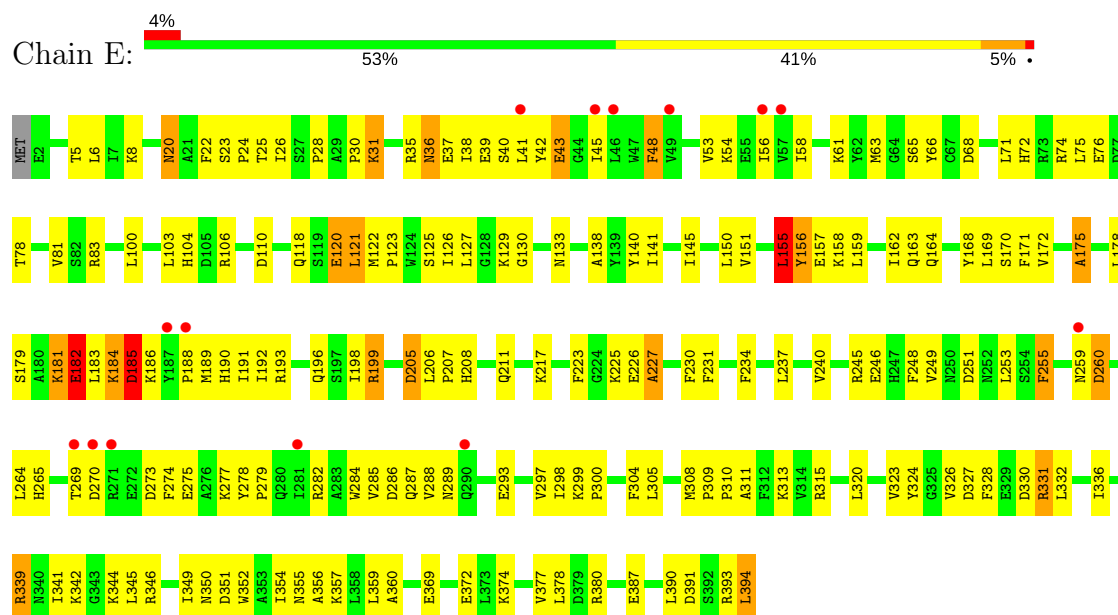


#### • Molecule 2: Rnl

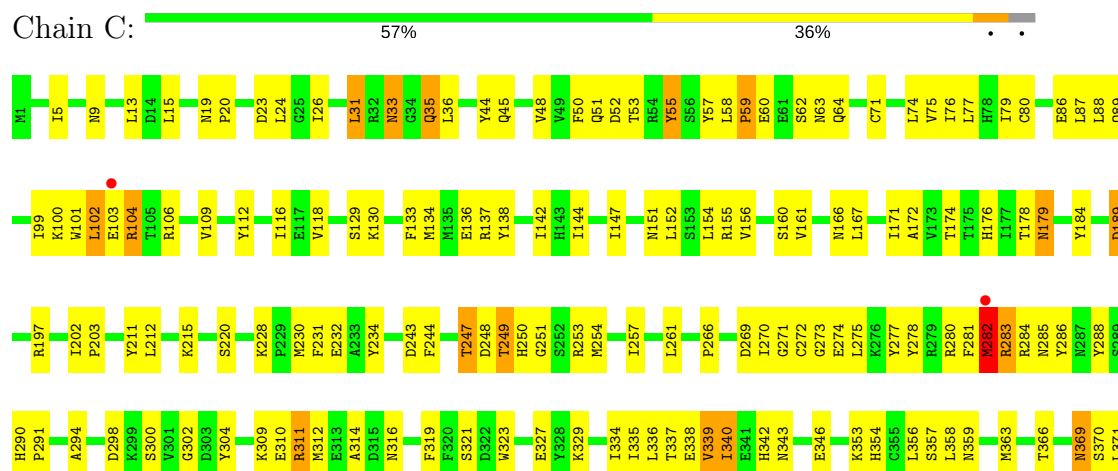




### • Molecule 2: Rnl

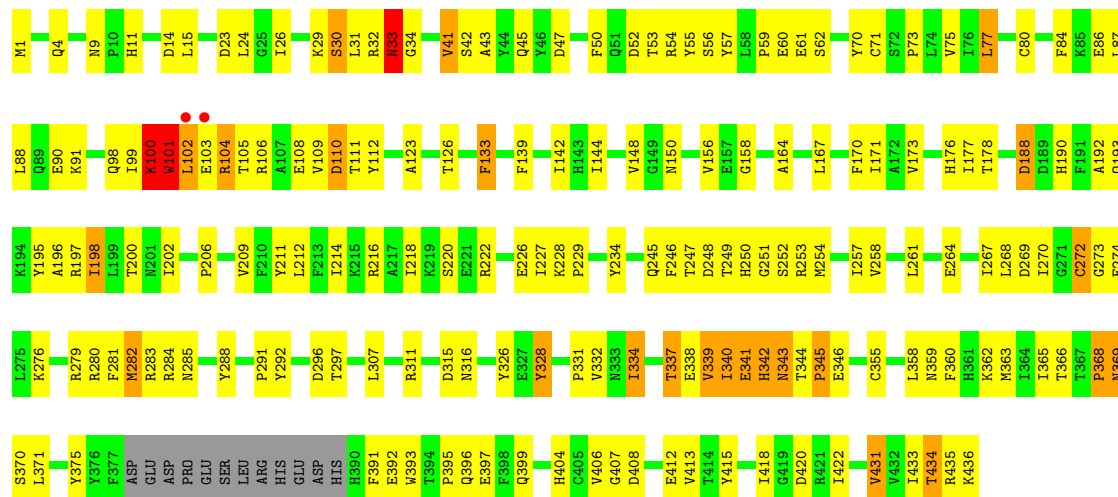


### • Molecule 3: Hen1





### ● Molecule 3: Hen1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.48Å 187.25Å 112.00Å 90.00° 106.04° 90.00°	Depositor
Resolution (Å)	42.93 – 3.41 46.13 – 3.41	Depositor EDS
% Data completeness (in resolution range)	98.2 (42.93-3.41) 94.8 (46.13-3.41)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.176 , 0.233 0.181 , 0.235	Depositor DCC
$R_{free}$ test set	2175 reflections (3.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	103.2	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 62.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for l,k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18713	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, SAH, MES, PO4, ATP

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	0.43	0/2427	0.65	0/3266
1	D	0.42	0/2396	0.67	1/3223 (0.0%)
2	B	0.56	0/3367	0.76	1/4547 (0.0%)
2	E	0.49	0/3359	0.73	0/4537
3	C	0.49	0/3634	0.73	1/4928 (0.0%)
3	F	0.54	0/3634	0.76	1/4928 (0.0%)
All	All	0.50	0/18817	0.72	4/25429 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
2	E	0	2
3	C	0	2
3	F	0	2
All	All	0	7

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	91	LEU	CA-CB-CG	6.84	131.02	115.30
3	F	273	GLY	N-CA-C	-6.09	97.89	113.10
2	B	264	LEU	CA-CB-CG	5.70	128.40	115.30
3	C	212	LEU	CA-CB-CG	-5.13	103.49	115.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	129	SER	Peptide
3	C	342	HIS	Peptide
1	D	92	ARG	Peptide
2	E	181	LYS	Peptide
2	E	185	ASP	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	2388	0	2380	84	0
1	D	2358	0	2352	85	0
2	B	3290	0	3251	130	0
2	E	3282	0	3239	163	0
3	C	3536	0	3410	128	0
3	F	3536	0	3410	158	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	31	0	12	2	0
5	B	31	0	12	5	0
5	D	31	0	12	2	0
5	E	31	0	12	5	0
6	B	12	0	12	3	0
7	B	12	0	16	2	0
8	B	5	0	0	0	0
8	C	5	0	0	0	0
8	E	5	0	0	1	0
8	F	10	0	0	0	0
9	C	26	0	19	1	0
9	F	26	0	19	1	0
10	A	8	0	0	1	0
10	B	28	0	0	1	0
10	C	16	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	10	0	0	0	0
10	E	17	0	0	1	0
10	F	13	0	0	0	0
All	All	18713	0	18156	705	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 19.

The worst 5 of 705 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)
2:B:339:ARG:HG3	2:B:339:ARG:HH11	1.01	1.09
2:E:72:HIS:H	2:E:78:THR:HG22	1.25	0.98
2:E:315:ARG:HH22	2:E:394:LEU:HA	1.29	0.95
2:B:339:ARG:HG3	2:B:339:ARG:NH1	1.76	0.92
2:B:72:HIS:H	2:B:78:THR:HG22	1.31	0.92

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	287/312 (92%)	235 (82%)	40 (14%)	12 (4%)	3	25
1	D	283/312 (91%)	220 (78%)	47 (17%)	16 (6%)	2	17
2	B	392/394 (100%)	330 (84%)	48 (12%)	14 (4%)	4	29
2	E	391/394 (99%)	323 (83%)	55 (14%)	13 (3%)	4	30
3	C	420/436 (96%)	344 (82%)	61 (14%)	15 (4%)	4	29
3	F	420/436 (96%)	342 (81%)	56 (13%)	22 (5%)	2	19
All	All	2193/2284 (96%)	1794 (82%)	307 (14%)	92 (4%)	3	25

5 of 92 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	GLU
1	A	151	GLU
1	A	154	ASP
2	B	184	LYS
2	B	186	LYS

### 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	265/274 (97%)	248 (94%)	17 (6%)	19	55
1	D	261/274 (95%)	243 (93%)	18 (7%)	17	52
2	B	359/359 (100%)	329 (92%)	30 (8%)	12	43
2	E	358/359 (100%)	336 (94%)	22 (6%)	20	56
3	C	387/399 (97%)	362 (94%)	25 (6%)	19	54
3	F	387/399 (97%)	364 (94%)	23 (6%)	21	57
All	All	2017/2064 (98%)	1882 (93%)	135 (7%)	18	53

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	275	LEU
1	D	57	SER
3	F	246	PHE
3	C	282	MET
3	C	410	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	369	ASN
3	F	343	ASN

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Mol	Chain	Res	Type
2	E	84	ASN
2	B	235	ASN
3	F	250	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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	ATP	A	402	-	27,33,33	1.08	1 (3%)	27,52,52	1.66	4 (14%)
5	ATP	B	501	4	27,33,33	1.06	1 (3%)	27,52,52	1.42	4 (14%)
6	MES	B	502	-	12,12,12	2.00	1 (8%)	14,16,16	2.70	8 (57%)
7	GOL	B	503	-	5,5,5	0.39	0	5,5,5	0.70	0
7	GOL	B	504	-	5,5,5	0.39	0	5,5,5	0.24	0
8	PO4	B	506	-	4,4,4	0.76	0	6,6,6	0.41	0
9	SAH	C	501	-	20,28,28	1.23	2 (10%)	19,40,40	2.64	2 (10%)
8	PO4	C	503	-	4,4,4	0.76	0	6,6,6	0.36	0
5	ATP	D	402	-	27,33,33	1.09	2 (7%)	27,52,52	1.78	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ATP	E	501	4	27,33,33	1.01	1 (3%)	27,52,52	1.92	5 (18%)
8	PO4	E	503	-	4,4,4	0.79	0	6,6,6	0.31	0
9	SAH	F	501	-	20,28,28	1.20	2 (10%)	19,40,40	2.75	3 (15%)
8	PO4	F	503	-	4,4,4	0.70	0	6,6,6	0.39	0
8	PO4	F	504	-	4,4,4	0.74	0	6,6,6	0.43	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	ATP	A	402	-	-	0/18/38/38	0/3/3/3
5	ATP	B	501	4	-	0/18/38/38	0/3/3/3
6	MES	B	502	-	-	0/6/14/14	0/1/1/1
7	GOL	B	503	-	-	0/4/4/4	0/0/0/0
7	GOL	B	504	-	-	0/4/4/4	0/0/0/0
8	PO4	B	506	-	-	0/0/0/0	0/0/0/0
9	SAH	C	501	-	-	0/7/31/31	0/3/3/3
8	PO4	C	503	-	-	0/0/0/0	0/0/0/0
5	ATP	D	402	-	-	0/18/38/38	0/3/3/3
5	ATP	E	501	4	-	0/18/38/38	0/3/3/3
8	PO4	E	503	-	-	0/0/0/0	0/0/0/0
9	SAH	F	501	-	-	0/7/31/31	0/3/3/3
8	PO4	F	503	-	-	0/0/0/0	0/0/0/0
8	PO4	F	504	-	-	0/0/0/0	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	502	MES	C8-S	-6.61	1.68	1.77
5	D	402	ATP	O4'-C1'	2.03	1.44	1.41
9	C	501	SAH	C2-N1	2.29	1.38	1.33
9	F	501	SAH	C2-N1	2.46	1.38	1.33
5	A	402	ATP	C5-C4	3.08	1.47	1.40

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	501	SAH	N3-C2-N1	-10.61	119.78	128.86
9	C	501	SAH	N3-C2-N1	-10.24	120.10	128.86
5	E	501	ATP	N3-C2-N1	-5.73	123.96	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	402	ATP	N3-C2-N1	-5.52	124.14	128.86
5	D	402	ATP	N3-C2-N1	-5.31	124.32	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	402	ATP	2	0
5	B	501	ATP	5	0
6	B	502	MES	3	0
7	B	503	GOL	1	0
7	B	504	GOL	1	0
9	C	501	SAH	1	0
5	D	402	ATP	2	0
5	E	501	ATP	5	0
8	E	503	PO4	1	0
9	F	501	SAH	1	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 [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	283/312 (90%)	0.03	8 (2%) 53 51	51, 87, 134, 147	0
1	D	279/312 (89%)	0.02	6 (2%) 62 60	51, 92, 136, 163	0
2	B	394/394 (100%)	-0.05	12 (3%) 50 48	42, 63, 128, 159	0
2	E	393/394 (99%)	0.07	14 (3%) 42 41	55, 93, 128, 149	0
3	C	424/436 (97%)	-0.11	2 (0%) 90 89	44, 82, 122, 147	0
3	F	424/436 (97%)	-0.20	2 (0%) 90 89	49, 74, 120, 145	0
All	All	2197/2284 (96%)	-0.05	44 (2%) 65 63	42, 82, 129, 163	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	177	VAL	6.4
1	D	117	GLU	4.9
1	D	119	LEU	4.6
2	B	195	TYR	4.3
2	B	192	ILE	4.2

### 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
8	PO4	E	503	5/5	0.64	0.55	166,168,170,171	0
8	PO4	C	503	5/5	0.69	0.45	145,146,146,148	0
4	MG	F	502	1/1	0.72	0.26	54,54,54,54	0
8	PO4	B	506	5/5	0.78	0.27	136,137,139,141	0
9	SAH	C	501	26/26	0.82	0.34	124,138,150,188	0
8	PO4	F	504	5/5	0.83	0.42	134,135,135,137	0
9	SAH	F	501	26/26	0.84	0.54	83,101,121,196	9
7	GOL	B	504	6/6	0.89	0.51	95,103,106,108	0
5	ATP	E	501	31/31	0.90	0.31	57,67,171,189	0
5	ATP	D	402	31/31	0.90	0.15	121,127,140,179	0
6	MES	B	502	12/12	0.91	0.24	64,80,120,122	0
8	PO4	F	503	5/5	0.92	0.34	115,117,120,125	0
7	GOL	B	503	6/6	0.93	0.20	58,77,81,82	0
5	ATP	A	402	31/31	0.93	0.14	98,119,150,150	0
4	MG	C	502	1/1	0.93	0.41	41,41,41,41	0
5	ATP	B	501	31/31	0.94	0.27	39,53,168,198	0
4	MG	E	502	1/1	0.95	0.56	68,68,68,68	0
4	MG	D	401	1/1	0.97	0.35	56,56,56,56	0
4	MG	A	401	1/1	0.99	0.46	54,54,54,54	0
4	MG	B	505	1/1	0.99	0.37	48,48,48,48	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.