



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 11:24 pm BST

PDB ID : 6BYS  
Title : Structures of the PKA RI alpha holoenzyme with the FLHCC driver J-PKAc alpha or native PRKAc alpha  
Authors : Cao, B.; Lu, T.W.; Martinez Fiesco, J.A.; Tomasini, M.; Fan, L.; Simon, S.M.; Taylor, S.S.; Zhang, P.  
Deposited on : 2017-12-21  
Resolution : 4.75 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

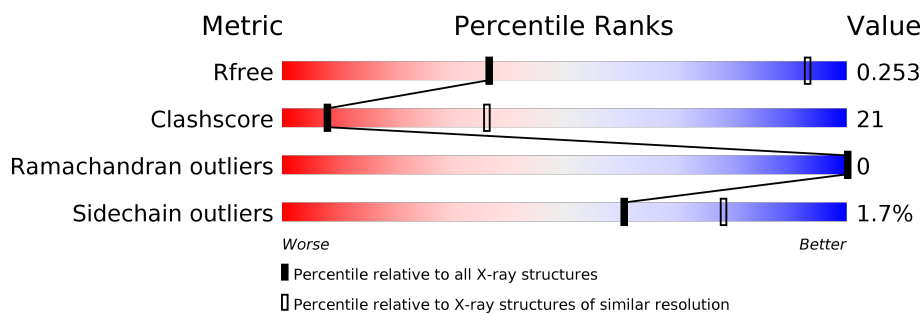
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.75 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))
$R_{free}$	130704	1089 (5.70-3.80)
Clashscore	141614	1163 (5.70-3.80)
Ramachandran outliers	138981	1098 (5.70-3.80)
Sidechain outliers	138945	1078 (5.70-3.80)

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 respectively. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	350	61% 35% . .
1	C	350	58% 36% . .
1	E	350	61% 34% . .
1	G	350	61% 33% . .
2	B	379	44% 31% . 24%
2	D	379	46% 28% . 24%
2	F	379	45% 30% . 24%

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Mol	Chain	Length	Quality of chain
2	H	379	

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	SEP	C	338	-	-	X	-
1	SEP	G	338	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20336 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 cAMP-dependent protein kinase catalytic subunit alpha.

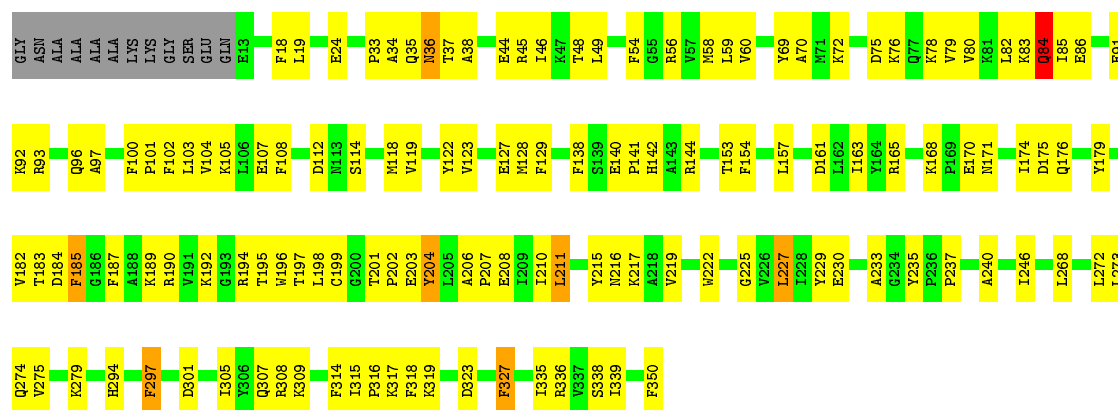
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	P	S	0	0	0
			2798	1811	468	508	3	8			
1	C	338	Total	C	N	O	P	S	0	0	0
			2798	1811	468	508	3	8			
1	E	338	Total	C	N	O	P	S	0	0	0
			2798	1811	468	508	3	8			
1	G	338	Total	C	N	O	P	S	0	0	0
			2798	1811	468	508	3	8			

- Molecule 2 is a protein called cAMP-dependent protein kinase type I-alpha regulatory subunit.

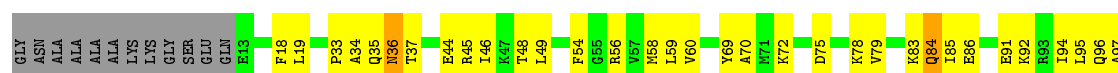
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	288	Total	C	N	O	S	0	0	0
			2286	1444	397	437	8			
2	D	288	Total	C	N	O	S	0	0	0
			2286	1444	397	437	8			
2	F	288	Total	C	N	O	S	0	0	0
			2286	1444	397	437	8			
2	H	288	Total	C	N	O	S	0	0	0
			2286	1444	397	437	8			

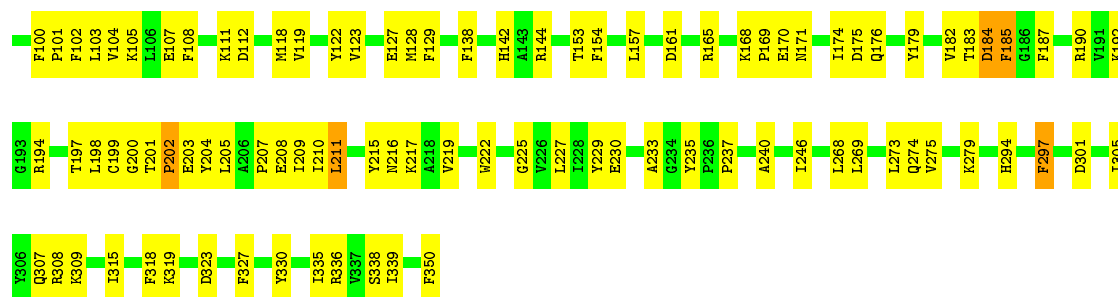
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

- Chain A:  61% 35% ..



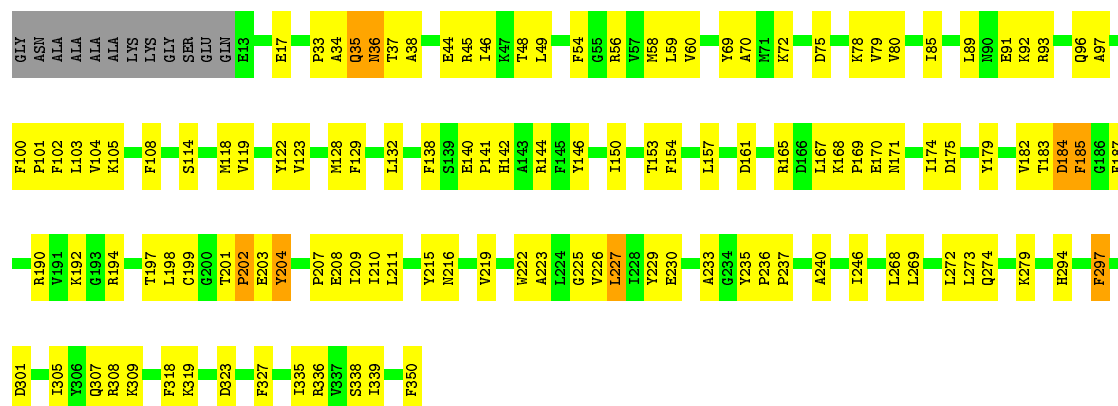
- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha





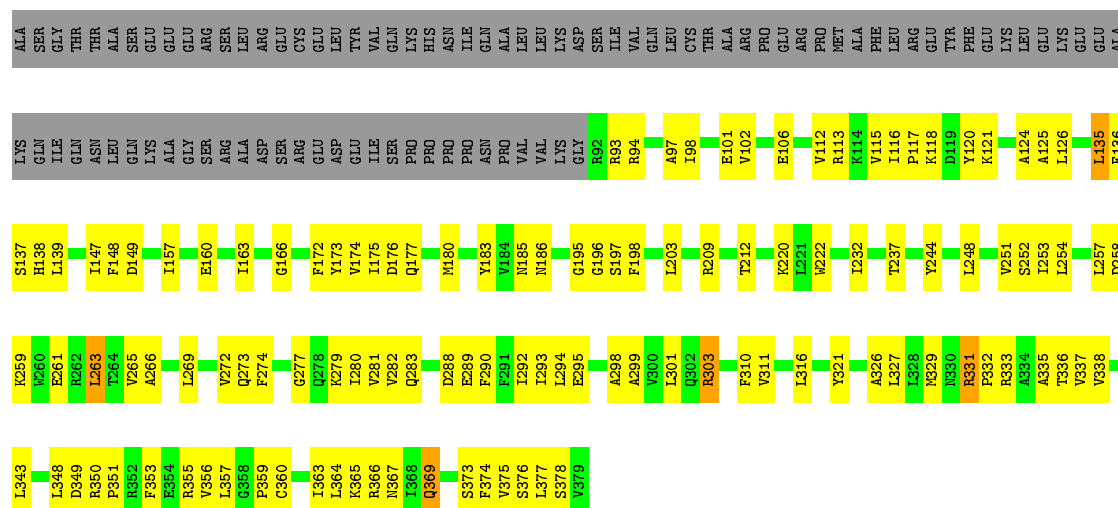
- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

Chain G: 61% 33%



- Molecule 2: cAMP-dependent protein kinase type I-alpha regulatory subunit

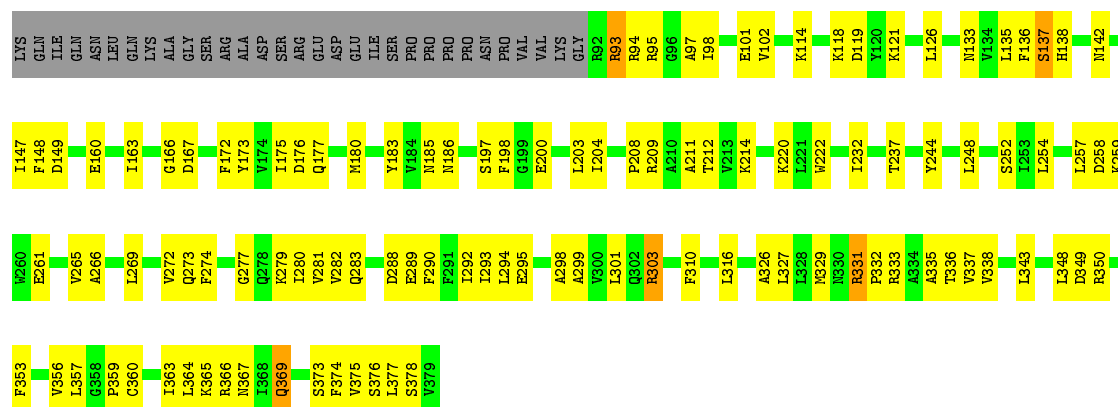
Chain B: 44% 31% 24%



- Molecule 2: cAMP-dependent protein kinase type I-alpha regulatory subunit

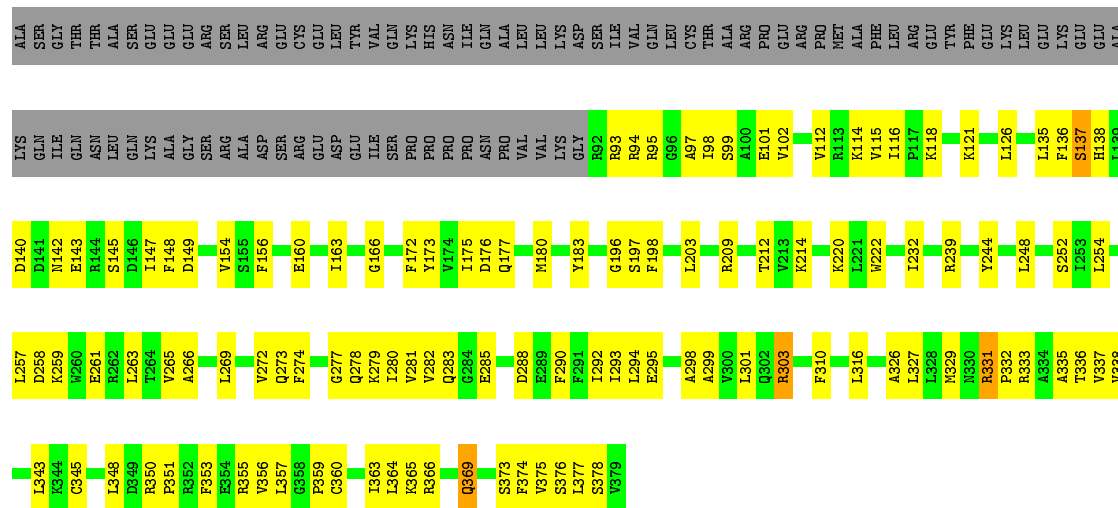
Chain D: 46% 28% 24%





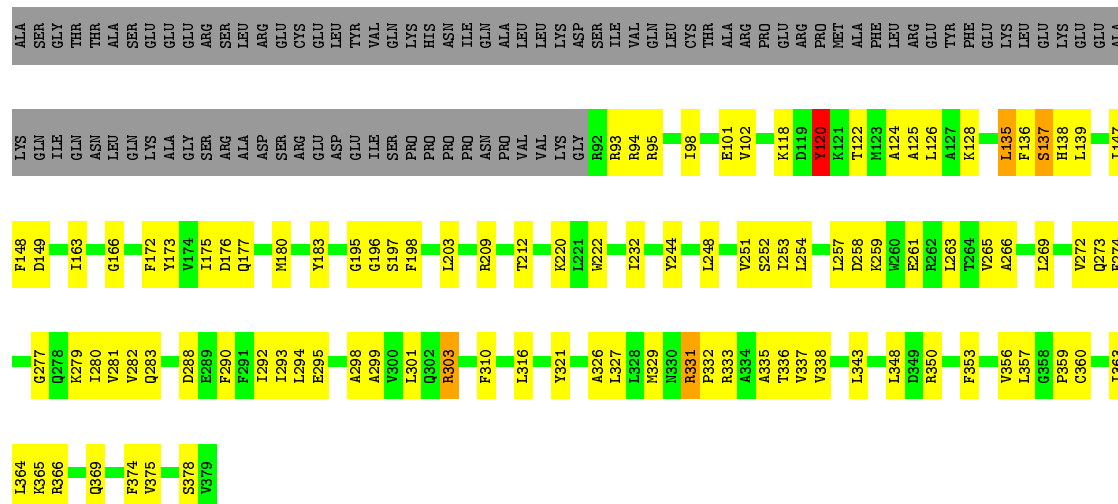
- Molecule 2: cAMP-dependent protein kinase type I-alpha regulatory subunit

Chain F: 45% 30% 24%



- Molecule 2: cAMP-dependent protein kinase type I-alpha regulatory subunit

Chain H: 49% 26% 24%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.50Å 186.16Å 186.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.16 – 4.75 48.54 – 4.75	Depositor EDS
% Data completeness (in resolution range)	95.6 (45.16-4.75) 88.4 (48.54-4.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.34 (at 4.86Å)	Xtriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, $R_{free}$	0.212 , 0.255 0.214 , 0.253	Depositor DCC
$R_{free}$ test set	1995 reflections (8.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	187.0	Xtriage
Anisotropy	0.742	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 213.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.027 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	20336	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	269.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.29% 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 ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.57	0/2837	0.86	7/3819 (0.2%)
1	C	0.56	1/2837 (0.0%)	0.85	10/3819 (0.3%)
1	E	0.56	0/2837	0.85	10/3819 (0.3%)
1	G	0.53	0/2837	0.83	7/3819 (0.2%)
2	B	0.58	0/2326	0.77	2/3136 (0.1%)
2	D	0.57	0/2326	0.78	0/3136
2	F	0.57	0/2326	0.78	0/3136
2	H	0.61	2/2326 (0.1%)	0.91	6/3136 (0.2%)
All	All	0.57	3/20652 (0.0%)	0.83	42/27820 (0.2%)

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	C	0	1
2	H	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	84	GLN	CD-OE1	-7.89	1.06	1.24
2	H	120	TYR	CG-CD1	-7.40	1.29	1.39
2	H	120	TYR	CE1-CZ	-6.15	1.30	1.38

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	120	TYR	CB-CG-CD2	-20.04	108.97	121.00
2	H	120	TYR	CD1-CG-CD2	-12.38	104.28	117.90
1	A	35	GLN	CB-CA-C	-11.08	88.25	110.40
1	C	35	GLN	CB-CA-C	-10.55	89.31	110.40
2	H	120	TYR	CB-CG-CD1	10.43	127.26	121.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	84	GLN	Sidechain
2	H	120	TYR	Sidechain

## 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	2798	0	2773	104	0
1	C	2798	0	2774	127	0
1	E	2798	0	2774	112	0
1	G	2798	0	2774	120	0
2	B	2286	0	2274	134	0
2	D	2286	0	2274	119	0
2	F	2286	0	2274	131	0
2	H	2286	0	2274	106	0
All	All	20336	0	20191	867	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 21.

The worst 5 of 867 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:G:204:TYR:OH	1:G:227:LEU:CB	1.90	1.20
2:B:195:GLY:HA3	2:H:120:TYR:CE2	1.79	1.18
1:G:204:TYR:OH	1:G:227:LEU:HB2	0.99	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:GLU:OE1	2:D:94:ARG:NH2	1.80	1.13
2:B:195:GLY:HA3	2:H:120:TYR:HE2	1.00	1.08

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	333/350 (95%)	280 (84%)	53 (16%)	0	100	100
1	C	333/350 (95%)	277 (83%)	56 (17%)	0	100	100
1	E	333/350 (95%)	277 (83%)	56 (17%)	0	100	100
1	G	333/350 (95%)	275 (83%)	58 (17%)	0	100	100
2	B	286/379 (76%)	246 (86%)	40 (14%)	0	100	100
2	D	286/379 (76%)	247 (86%)	39 (14%)	0	100	100
2	F	286/379 (76%)	247 (86%)	39 (14%)	0	100	100
2	H	286/379 (76%)	245 (86%)	41 (14%)	0	100	100
All	All	2476/2916 (85%)	2094 (85%)	382 (15%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	296/302 (98%)	292 (99%)	4 (1%)	67	81
1	C	296/302 (98%)	293 (99%)	3 (1%)	76	86
1	E	296/302 (98%)	291 (98%)	5 (2%)	60	78
1	G	296/302 (98%)	291 (98%)	5 (2%)	60	78
2	B	244/324 (75%)	240 (98%)	4 (2%)	62	79
2	D	244/324 (75%)	239 (98%)	5 (2%)	55	73
2	F	244/324 (75%)	239 (98%)	5 (2%)	55	73
2	H	244/324 (75%)	238 (98%)	6 (2%)	47	68
All	All	2160/2504 (86%)	2123 (98%)	37 (2%)	60	78

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	36	ASN
1	E	297	PHE
2	H	303	ARG
1	E	184	ASP
1	E	185	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	138	HIS
1	E	84	GLN
1	E	87	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	SEP	E	338	1	8,9,10	1.53	1 (12%)	8,12,14	1.79	2 (25%)
1	TPO	G	197	1	8,10,11	1.62	1 (12%)	10,14,16	2.35	2 (20%)
1	SEP	C	338	1	8,9,10	1.49	1 (12%)	8,12,14	1.79	3 (37%)
1	TPO	C	197	1	8,10,11	1.69	1 (12%)	10,14,16	2.35	2 (20%)
1	TPO	E	197	1	8,10,11	1.65	2 (25%)	10,14,16	2.46	2 (20%)
1	SEP	C	139	1	8,9,10	1.67	1 (12%)	8,12,14	1.84	1 (12%)
1	SEP	E	139	1	8,9,10	1.74	1 (12%)	8,12,14	2.23	1 (12%)
1	SEP	G	139	1	8,9,10	1.61	1 (12%)	8,12,14	1.94	2 (25%)
1	TPO	A	197	1	8,10,11	1.58	2 (25%)	10,14,16	2.33	2 (20%)
1	SEP	A	338	1	8,9,10	1.93	1 (12%)	8,12,14	1.69	2 (25%)
1	SEP	A	139	1	8,9,10	1.65	1 (12%)	8,12,14	1.82	1 (12%)
1	SEP	G	338	1	8,9,10	1.54	1 (12%)	8,12,14	1.87	2 (25%)

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	SEP	E	338	1	-	4/5/8/10	-
1	TPO	G	197	1	-	1/9/11/13	-
1	SEP	C	338	1	-	5/5/8/10	-
1	TPO	C	197	1	-	1/9/11/13	-
1	TPO	E	197	1	-	1/9/11/13	-
1	SEP	C	139	1	-	1/5/8/10	-
1	SEP	E	139	1	-	1/5/8/10	-
1	SEP	G	139	1	-	3/5/8/10	-
1	TPO	A	197	1	-	1/9/11/13	-
1	SEP	A	338	1	-	4/5/8/10	-
1	SEP	A	139	1	-	2/5/8/10	-
1	SEP	G	338	1	-	4/5/8/10	-

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	SEP	P-O1P	4.77	1.65	1.50
1	E	139	SEP	P-O1P	3.64	1.62	1.50
1	C	139	SEP	P-O1P	3.62	1.62	1.50
1	G	338	SEP	P-O1P	3.57	1.62	1.50
1	C	197	TPO	P-O1P	3.48	1.61	1.50

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	197	TPO	P-OG1-CB	-6.92	102.30	123.21
1	G	197	TPO	P-OG1-CB	-6.60	103.28	123.21
1	C	197	TPO	P-OG1-CB	-6.43	103.78	123.21
1	A	197	TPO	P-OG1-CB	-6.41	103.84	123.21
1	E	139	SEP	OG-CB-CA	5.64	113.63	108.14

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	338	SEP	CB-OG-P-O2P
1	E	338	SEP	CB-OG-P-O3P
1	C	338	SEP	CB-OG-P-O2P
1	C	338	SEP	CB-OG-P-O3P
1	C	139	SEP	N-CA-CB-OG

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	338	SEP	3	0
1	G	197	TPO	2	0
1	C	338	SEP	4	0
1	C	197	TPO	1	0
1	E	197	TPO	1	0
1	A	197	TPO	1	0
1	A	338	SEP	2	0
1	G	338	SEP	4	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.