



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:21 AM GMT

PDB ID : 3E8C  
Title : Crystal structures of the kinase domain of PKA in complex with ATP-competitive inhibitors  
Authors : Concha, N.O.; Elkins, P.A.; Smallwood, A.; Ward, P.  
Deposited on : 2008-08-19  
Resolution : 2.20 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

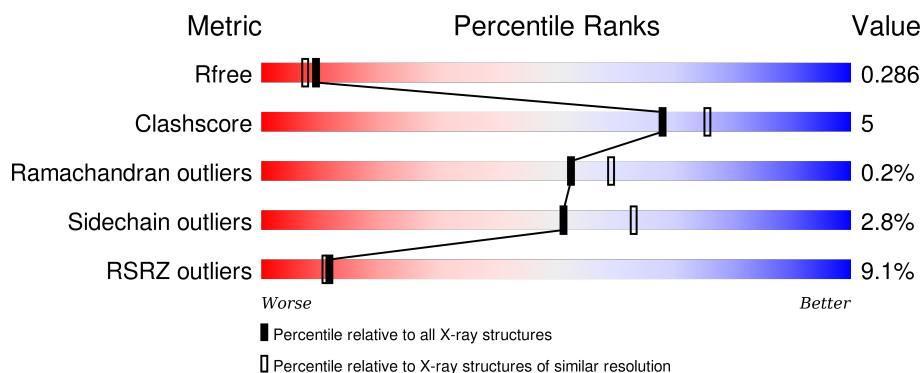
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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. 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	350	<div> <div>7%</div> <div>90%</div> <div>8%</div> </div>
1	B	350	<div> <div>5%</div> <div>89%</div> <div>10%</div> </div>
1	C	350	<div> <div>8%</div> <div>86%</div> <div>12%</div> </div>
1	D	350	<div> <div>5%</div> <div>86%</div> <div>13%</div> </div>
1	E	350	<div> <div>9%</div> <div>87%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	350	<div><div></div><div>16%</div><div>84%</div><div>14%</div><div></div></div>
2	G	20	<div><div></div><div>10%</div><div>85%</div><div>5%</div><div>10%</div><div></div></div>
2	H	20	<div><div></div><div>10%</div><div>90%</div><div>10%</div><div></div></div>
2	I	20	<div><div></div><div>20%</div><div>65%</div><div>35%</div><div></div></div>
2	J	20	<div><div></div><div>10%</div><div>55%</div><div>35%</div><div>5%</div><div>5%</div><div></div></div>
2	K	20	<div><div></div><div>15%</div><div>90%</div><div>10%</div><div></div></div>
2	L	20	<div><div></div><div>55%</div><div>60%</div><div>35%</div><div>5%</div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18893 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.

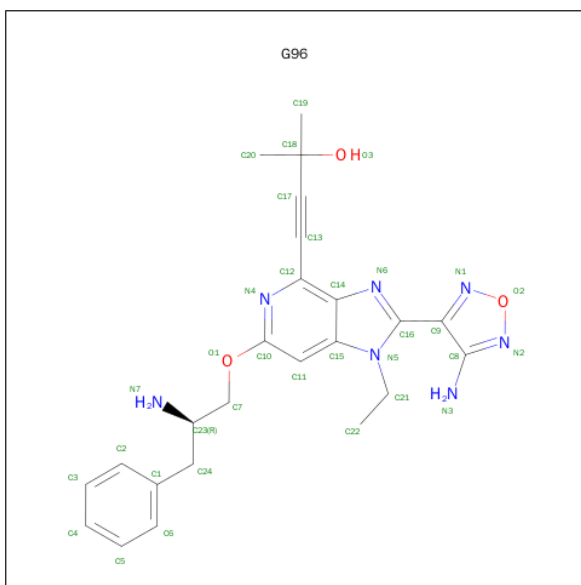
- Molecule 1 is a protein called cAMP-dependent protein kinase catalytic subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	P	S	0	0	0
			2845	1838	477	518	3	9			
1	B	347	Total	C	N	O	P	S	0	0	0
			2860	1847	480	521	3	9			
1	C	344	Total	C	N	O	P	S	0	1	0
			2844	1838	477	517	3	9			
1	D	347	Total	C	N	O	P	S	0	0	0
			2842	1838	475	517	3	9			
1	E	338	Total	C	N	O	P	S	0	0	0
			2785	1804	467	503	2	9			
1	F	344	Total	C	N	O	P	S	0	0	0
			2845	1838	477	518	3	9			

- Molecule 2 is a protein called cAMP-dependent protein kinase inhibitor peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	18	Total	C	N	O	0	0	0
			138	84	28	26			
2	H	20	Total	C	N	O	0	0	0
			157	94	32	31			
2	I	20	Total	C	N	O	0	0	0
			157	94	32	31			
2	J	19	Total	C	N	O	0	0	0
			148	90	31	27			
2	K	20	Total	C	N	O	0	0	0
			157	94	32	31			
2	L	19	Total	C	N	O	0	0	0
			149	90	30	29			

- Molecule 3 is 4-[2-(4-AMINO-1,2,5-OXADIAZOL-3-YL)-6-{{[(2R)-2-AMINO-3-PHENYLPROPYL]OXY}}-1-ETHYL-1H-IMIDAZO[4,5-C]PYRIDIN-4-YL]-2-METHYLBUT-3-YN-2-OL (three-letter code: G96) (formula: C<sub>24</sub>H<sub>27</sub>N<sub>7</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			34	24	7	3		
3	B	1	Total	C	N	O	0	0
			34	24	7	3		
3	C	1	Total	C	N	O	0	0
			34	24	7	3		
3	D	1	Total	C	N	O	0	0
			34	24	7	3		
3	E	1	Total	C	N	O	0	0
			34	24	7	3		
3	F	1	Total	C	N	O	0	0
			34	24	7	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	130	Total	O	0	0
			130	130		
4	B	160	Total	O	0	0
			160	160		
4	C	122	Total	O	0	0
			122	122		
4	D	106	Total	O	0	0
			106	106		
4	E	95	Total	O	0	0
			95	95		
4	F	103	Total	O	0	0
			103	103		

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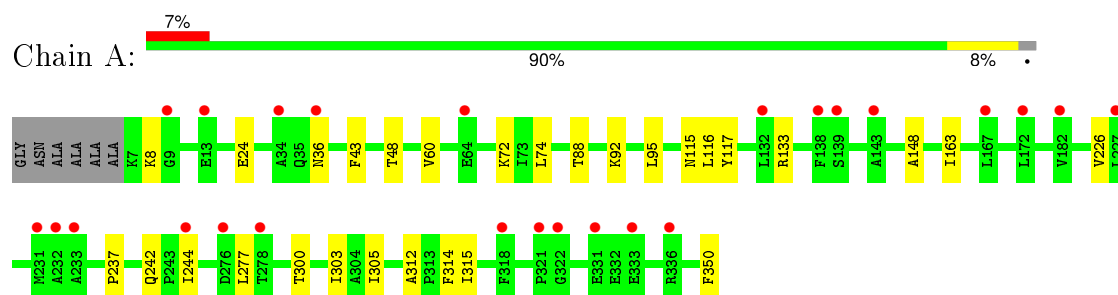
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	4	Total 4	O 4	0	0
4	H	12	Total 12	O 12	0	0
4	I	12	Total 12	O 12	0	0
4	J	6	Total 6	O 6	0	0
4	K	8	Total 8	O 8	0	0
4	L	4	Total 4	O 4	0	0

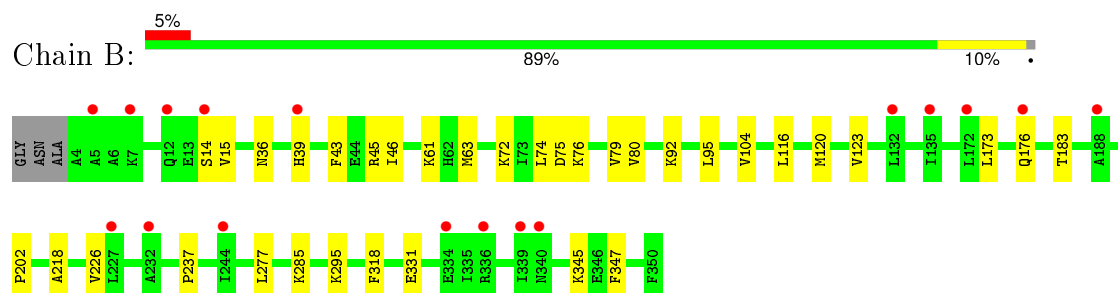
### 3 Residue-property plots [i](#)

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

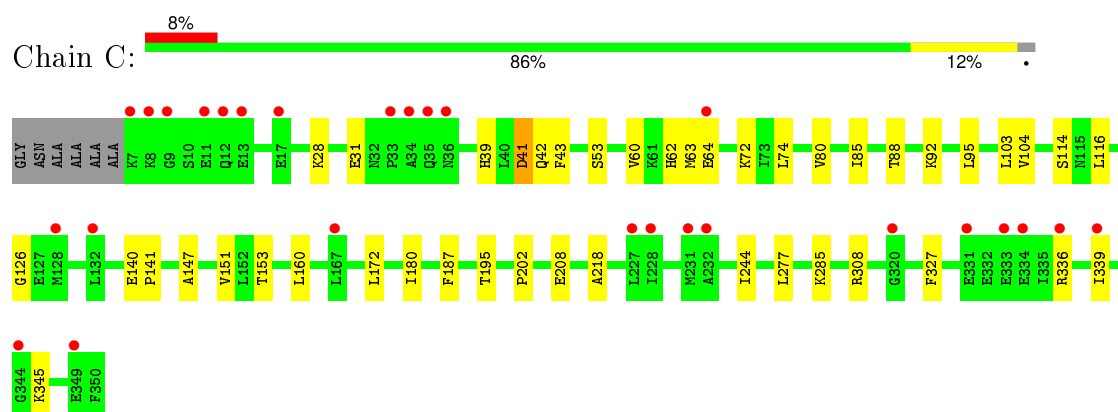
- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha



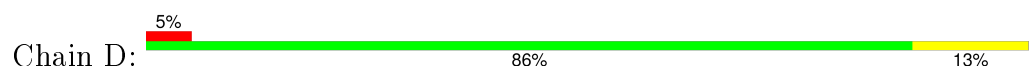
- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

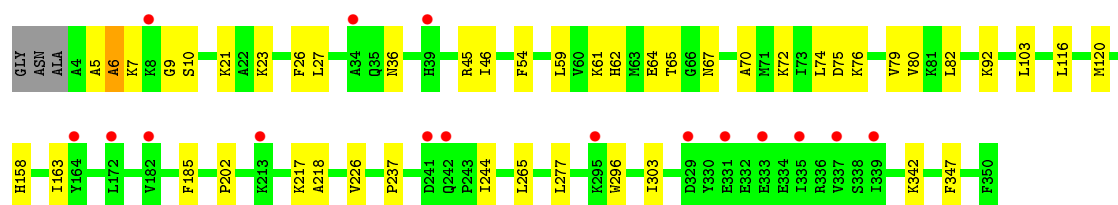


- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

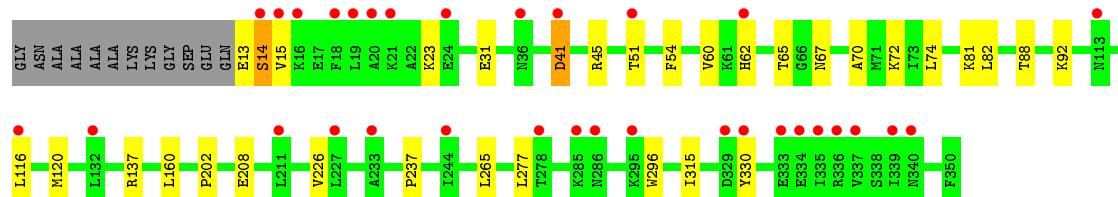
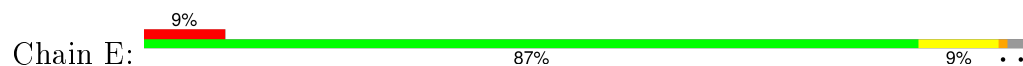


- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

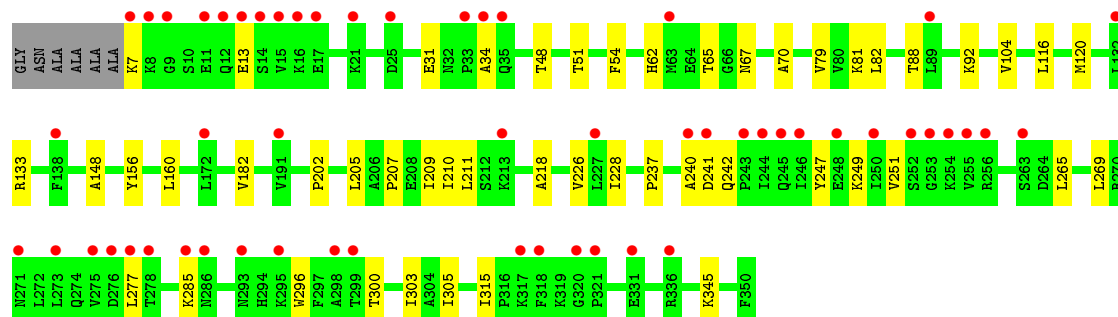
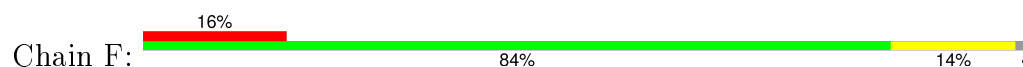




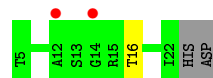
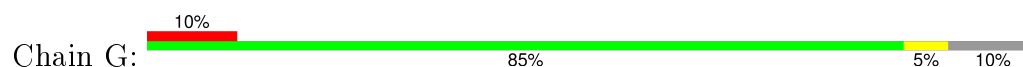
- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha



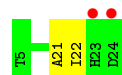
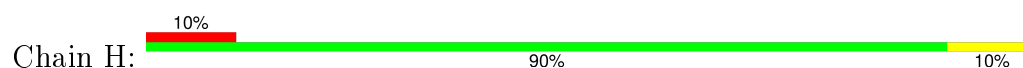
- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha



- Molecule 2: cAMP-dependent protein kinase inhibitor peptide



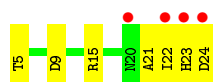
- Molecule 2: cAMP-dependent protein kinase inhibitor peptide



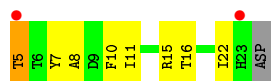
- Molecule 2: cAMP-dependent protein kinase inhibitor peptide



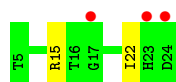
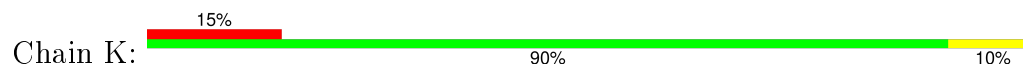




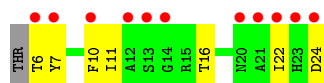
- Molecule 2: cAMP-dependent protein kinase inhibitor peptide



- Molecule 2: cAMP-dependent protein kinase inhibitor peptide



- Molecule 2: cAMP-dependent protein kinase inhibitor peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.46Å 96.39Å 180.04Å 90.00° 102.66° 90.00°	Depositor
Resolution (Å)	46.93 – 2.20 43.06 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.8 (46.93-2.20) 95.8 (43.06-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.264 , 0.290 0.263 , 0.286	Depositor DCC
$R_{free}$ test set	6759 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.3	Xtriage
Anisotropy	0.772	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.8	EDS
Estimated twinning fraction	0.001 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	5 of 134346 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	18893	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.06 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.8220e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: TPO, G96, 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	0.38	0/2884	0.57	0/3880
1	B	0.39	0/2899	0.58	0/3901
1	C	0.38	0/2886	0.57	1/3884 (0.0%)
1	D	0.37	0/2881	0.53	0/3880
1	E	0.35	0/2835	0.53	0/3820
1	F	0.36	0/2884	0.52	0/3880
2	G	0.61	0/139	0.69	0/186
2	H	0.44	0/159	0.68	0/212
2	I	0.43	0/159	0.66	0/212
2	J	0.40	0/150	0.64	0/201
2	K	0.40	0/159	0.63	0/212
2	L	0.42	0/150	0.59	0/197
All	All	0.38	0/18185	0.55	1/24465 (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	E	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	345	LYS	N-CA-CB	-5.03	101.55	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	15	VAL	Peptide

## 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	2845	0	2819	17	0
1	B	2860	0	2834	15	0
1	C	2844	0	2813	26	0
1	D	2842	0	2800	34	0
1	E	2785	0	2750	21	0
1	F	2845	0	2819	39	0
2	G	138	0	135	1	0
2	H	157	0	146	3	0
2	I	157	0	146	5	0
2	J	148	0	142	5	0
2	K	157	0	146	1	0
2	L	149	0	137	6	0
3	A	34	0	27	2	0
3	B	34	0	27	4	0
3	C	34	0	27	2	0
3	D	34	0	27	2	0
3	E	34	0	27	0	0
3	F	34	0	27	0	0
4	A	130	0	0	3	0
4	B	160	0	0	3	0
4	C	122	0	0	3	0
4	D	106	0	0	1	0
4	E	95	0	0	0	0
4	F	103	0	0	6	0
4	G	4	0	0	0	0
4	H	12	0	0	1	0
4	I	12	0	0	0	0
4	J	6	0	0	0	0
4	K	8	0	0	0	0
4	L	4	0	0	0	0
All	All	18893	0	17849	168	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 5.

The worst 5 of 168 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:E:208:GLU:HG2	1:E:277:LEU:HD21	1.58	0.84
1:A:48:THR:HG23	4:A:408:HOH:O	1.83	0.79
1:C:180:ILE:O	4:C:467:HOH:O	2.00	0.78
2:J:5:THR:HG23	2:J:8:ALA:HB3	1.68	0.75
1:F:210:ILE:CD1	1:F:251:VAL:CG1	2.67	0.72

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	339/350 (97%)	330 (97%)	9 (3%)	0	100	100
1	B	342/350 (98%)	330 (96%)	10 (3%)	2 (1%)	30	29
1	C	340/350 (97%)	331 (97%)	9 (3%)	0	100	100
1	D	342/350 (98%)	330 (96%)	11 (3%)	1 (0%)	46	50
1	E	334/350 (95%)	324 (97%)	9 (3%)	1 (0%)	46	50
1	F	339/350 (97%)	331 (98%)	8 (2%)	0	100	100
2	G	16/20 (80%)	15 (94%)	1 (6%)	0	100	100
2	H	18/20 (90%)	16 (89%)	2 (11%)	0	100	100
2	I	18/20 (90%)	15 (83%)	3 (17%)	0	100	100
2	J	17/20 (85%)	16 (94%)	1 (6%)	0	100	100
2	K	18/20 (90%)	16 (89%)	2 (11%)	0	100	100
2	L	16/20 (80%)	14 (88%)	2 (12%)	0	100	100
All	All	2139/2220 (96%)	2068 (97%)	67 (3%)	4 (0%)	52	59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	14	SER
1	B	15	VAL
1	D	6	ALA
1	B	14	SER

### 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	301/302 (100%)	296 (98%)	5 (2%)	68	81
1	B	301/302 (100%)	291 (97%)	10 (3%)	45	56
1	C	300/302 (99%)	289 (96%)	11 (4%)	41	50
1	D	296/302 (98%)	290 (98%)	6 (2%)	63	76
1	E	294/302 (97%)	287 (98%)	7 (2%)	57	69
1	F	301/302 (100%)	292 (97%)	9 (3%)	48	60
2	G	13/15 (87%)	13 (100%)	0	100	100
2	H	15/15 (100%)	15 (100%)	0	100	100
2	I	15/15 (100%)	14 (93%)	1 (7%)	20	21
2	J	14/15 (93%)	12 (86%)	2 (14%)	4	3
2	K	15/15 (100%)	14 (93%)	1 (7%)	20	21
2	L	13/15 (87%)	12 (92%)	1 (8%)	16	16
All	All	1878/1902 (99%)	1825 (97%)	53 (3%)	51	63

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	195	THR
1	D	92	LYS
2	I	15	ARG
1	C	285	LYS
1	D	21	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	286	ASN
1	E	271	ASN
1	E	32	ASN
1	B	293	ASN
1	E	62	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

17 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	A	10	1	8,9,10	1.57	1 (12%)	8,12,14	1.79	1 (12%)
1	TPO	A	197	1	8,10,11	0.73	0	7,14,16	1.25	0
1	SEP	A	338	1	8,9,10	1.44	1 (12%)	8,12,14	1.93	2 (25%)
1	SEP	B	10	1	8,9,10	1.57	1 (12%)	8,12,14	1.58	2 (25%)
1	TPO	B	197	1	8,10,11	0.58	0	7,14,16	1.34	0
1	SEP	B	338	1	8,9,10	1.55	1 (12%)	8,12,14	1.71	1 (12%)
1	SEP	C	10	1	8,9,10	1.59	1 (12%)	8,12,14	2.00	1 (12%)
1	TPO	C	197	1	8,10,11	0.68	0	7,14,16	1.23	1 (14%)
1	SEP	C	338	1	8,9,10	1.47	1 (12%)	8,12,14	1.58	2 (25%)
1	SEP	D	10	1	8,9,10	1.54	1 (12%)	8,12,14	1.71	2 (25%)
1	TPO	D	197	1	8,10,11	0.69	0	7,14,16	1.32	0
1	SEP	D	338	1	8,9,10	1.51	1 (12%)	8,12,14	1.79	1 (12%)
1	TPO	E	197	1	8,10,11	0.70	0	7,14,16	1.33	1 (14%)
1	SEP	E	338	1	8,9,10	1.51	1 (12%)	8,12,14	1.84	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	SEP	F	10	1	8,9,10	1.56	1 (12%)	8,12,14	1.51	1 (12%)
1	TPO	F	197	1	8,10,11	0.68	0	7,14,16	1.39	1 (14%)
1	SEP	F	338	1	8,9,10	1.52	1 (12%)	8,12,14	2.14	1 (12%)

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	A	10	1	-	0/6/8/10	0/0/0/0
1	TPO	A	197	1	-	0/8/11/13	0/0/0/0
1	SEP	A	338	1	-	0/6/8/10	0/0/0/0
1	SEP	B	10	1	-	0/6/8/10	0/0/0/0
1	TPO	B	197	1	-	0/8/11/13	0/0/0/0
1	SEP	B	338	1	-	0/6/8/10	0/0/0/0
1	SEP	C	10	1	-	0/6/8/10	0/0/0/0
1	TPO	C	197	1	-	0/8/11/13	0/0/0/0
1	SEP	C	338	1	-	0/6/8/10	0/0/0/0
1	SEP	D	10	1	-	0/6/8/10	0/0/0/0
1	TPO	D	197	1	-	0/8/11/13	0/0/0/0
1	SEP	D	338	1	-	0/6/8/10	0/0/0/0
1	TPO	E	197	1	-	0/8/11/13	0/0/0/0
1	SEP	E	338	1	-	0/6/8/10	0/0/0/0
1	SEP	F	10	1	-	0/6/8/10	0/0/0/0
1	TPO	F	197	1	-	0/8/11/13	0/0/0/0
1	SEP	F	338	1	-	0/6/8/10	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	SEP	P-O1P	2.90	1.60	1.51
1	C	338	SEP	P-O1P	2.97	1.60	1.51
1	E	338	SEP	P-O1P	3.10	1.61	1.51
1	D	338	SEP	P-O1P	3.13	1.61	1.51
1	D	10	SEP	P-O1P	3.13	1.61	1.51

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	10	SEP	O-C-CA	-2.43	119.15	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	10	SEP	O-C-CA	-2.00	120.28	125.49
1	C	197	TPO	O3P-P-O2P	2.06	115.23	107.38
1	E	197	TPO	O3P-P-O2P	2.15	115.56	107.38
1	C	338	SEP	OG-P-O1P	2.18	112.70	107.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	10	SEP	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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	$\# Z  > 2$
3	G96	A	351	-	30,37,37	2.08	3 (10%)	33,53,53	1.90	6 (18%)
3	G96	B	351	-	30,37,37	2.18	3 (10%)	33,53,53	1.84	5 (15%)
3	G96	C	351	-	30,37,37	2.11	3 (10%)	33,53,53	1.77	6 (18%)
3	G96	D	351	-	30,37,37	2.15	3 (10%)	33,53,53	1.87	5 (15%)
3	G96	E	351	-	30,37,37	2.23	4 (13%)	33,53,53	1.82	6 (18%)
3	G96	F	351	-	30,37,37	2.09	4 (13%)	33,53,53	1.84	5 (15%)

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
3	G96	A	351	-	-	0/12/21/21	0/3/4/4
3	G96	B	351	-	-	0/12/21/21	0/3/4/4
3	G96	C	351	-	-	0/12/21/21	0/3/4/4
3	G96	D	351	-	-	0/12/21/21	0/3/4/4
3	G96	E	351	-	-	0/12/21/21	0/3/4/4
3	G96	F	351	-	-	0/12/21/21	0/3/4/4

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	351	G96	C12-C13	-10.01	1.28	1.43
3	B	351	G96	C12-C13	-9.96	1.28	1.43
3	D	351	G96	C12-C13	-9.71	1.28	1.43
3	C	351	G96	C12-C13	-9.40	1.29	1.43
3	A	351	G96	C12-C13	-9.28	1.29	1.43

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	351	G96	C11-C10-N4	-3.25	120.13	124.06
3	F	351	G96	C11-C10-N4	-3.21	120.17	124.06
3	B	351	G96	C11-C10-N4	-3.18	120.20	124.06
3	E	351	G96	C11-C10-N4	-3.04	120.37	124.06
3	C	351	G96	C11-C10-N4	-2.94	120.50	124.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	351	G96	2	0
3	B	351	G96	4	0
3	C	351	G96	2	0
3	D	351	G96	2	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	341/350 (97%)	0.67	25 (7%)	18 17	14, 16, 25, 48	0
1	B	344/350 (98%)	0.53	17 (4%)	33 33	14, 16, 26, 35	0
1	C	341/350 (97%)	0.78	27 (7%)	15 15	14, 16, 25, 53	0
1	D	344/350 (98%)	0.66	16 (4%)	35 34	14, 16, 23, 31	0
1	E	336/350 (96%)	0.79	32 (9%)	10 9	14, 16, 22, 31	0
1	F	341/350 (97%)	1.00	55 (16%)	3 2	14, 16, 25, 39	0
2	G	18/20 (90%)	0.90	2 (11%)	7 7	20, 21, 29, 32	0
2	H	20/20 (100%)	1.06	2 (10%)	9 8	20, 22, 37, 38	0
2	I	20/20 (100%)	1.78	4 (20%)	1 1	20, 22, 37, 38	0
2	J	19/20 (95%)	1.10	2 (10%)	8 7	20, 22, 32, 35	0
2	K	20/20 (100%)	1.41	3 (15%)	3 3	20, 22, 35, 36	0
2	L	19/20 (95%)	3.43	11 (57%)	0 0	20, 22, 35, 36	0
All	All	2163/2220 (97%)	0.78	196 (9%)	11 11	14, 16, 26, 53	0

The worst 5 of 196 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	24	ASP	10.9
1	F	9	GLY	10.2
2	I	24	ASP	9.7
1	C	9	GLY	9.3
2	I	23	HIS	8.6

### 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	SEP	B	10	10/11	0.89	0.16	-	30,31,32,32	0
1	TPO	D	197	11/12	0.97	0.14	-	11,13,14,15	0
1	SEP	D	10	10/11	0.85	0.19	-	22,23,23,24	0
1	SEP	B	338	10/11	0.92	0.17	-	26,27,27,27	0
1	SEP	A	10	10/11	0.70	0.26	-	45,46,46,46	0
1	TPO	F	197	11/12	0.96	0.16	-	12,14,15,15	0
1	SEP	C	10	10/11	0.58	0.45	-	49,50,52,52	0
1	SEP	A	338	10/11	0.92	0.14	-	25,26,27,27	0
1	SEP	C	338	10/11	0.88	0.17	-	25,27,27,27	0
1	SEP	F	338	10/11	0.94	0.11	-	25,26,27,27	0
1	TPO	B	197	11/12	0.97	0.12	-	10,13,14,15	0
1	SEP	F	10	10/11	0.70	0.39	-	37,38,38,38	0
1	TPO	A	197	11/12	0.98	0.14	-	11,13,15,15	0
1	TPO	E	197	11/12	0.95	0.12	-	11,13,15,15	0
1	SEP	E	338	10/11	0.87	0.17	-	26,26,27,27	0
1	SEP	D	338	10/11	0.90	0.17	-	26,26,27,27	0
1	TPO	C	197	11/12	0.97	0.14	-	11,13,15,15	0

### 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	G96	C	351	34/34	0.92	0.14	-0.95	10,11,12,13	0
3	G96	F	351	34/34	0.92	0.13	-1.15	13,14,17,17	0
3	G96	D	351	34/34	0.94	0.12	-1.17	8,10,15,15	0
3	G96	E	351	34/34	0.92	0.13	-1.21	13,14,19,20	0
3	G96	B	351	34/34	0.94	0.11	-1.96	5,6,12,12	0
3	G96	A	351	34/34	0.94	0.10	-2.64	4,5,7,7	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.