



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 21, 2024 – 11:58 PM EDT

PDB ID : 3MVJ  
Title : Human cyclic AMP-dependent protein kinase PKA inhibitor complex  
Authors : Pandit, J.; Vajdos, F.  
Deposited on : 2010-05-04  
Resolution : 2.49 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

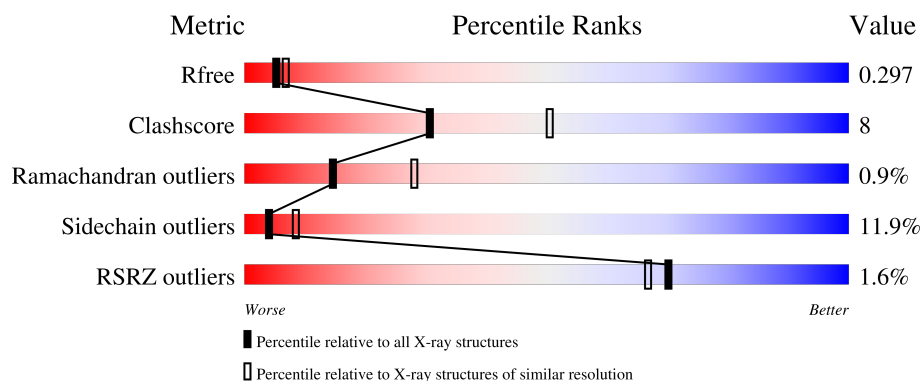
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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))
$R_{free}$	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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 of 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  $\leq 5\%$ . 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	371	 68% 20% 9%
1	B	371	 61% 22% 13%
1	E	371	 72% 15% 9%
2	I	20	 10% 80% 20%
2	J	20	 5% 75% 10% 15%

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Mol	Chain	Length	Quality of chain
2	K	20	

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
3	XFE	E	351	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8959 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	336	Total	C	N	O	P	S	0	0	0
			2779	1803	466	500	2	8			
1	B	322	Total	C	N	O	P	S	0	0	0
			2667	1733	450	474	2	8			
1	E	336	Total	C	N	O	P	S	0	0	0
			2779	1803	466	500	2	8			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP P17612
A	-19	GLY	-	expression tag	UNP P17612
A	-18	SER	-	expression tag	UNP P17612
A	-17	SER	-	expression tag	UNP P17612
A	-16	HIS	-	expression tag	UNP P17612
A	-15	HIS	-	expression tag	UNP P17612
A	-14	HIS	-	expression tag	UNP P17612
A	-13	HIS	-	expression tag	UNP P17612
A	-12	HIS	-	expression tag	UNP P17612
A	-11	HIS	-	expression tag	UNP P17612
A	-10	SER	-	expression tag	UNP P17612
A	-9	SER	-	expression tag	UNP P17612
A	-8	GLY	-	expression tag	UNP P17612
A	-7	LEU	-	expression tag	UNP P17612
A	-6	VAL	-	expression tag	UNP P17612
A	-5	PRO	-	expression tag	UNP P17612
A	-4	ARG	-	expression tag	UNP P17612
A	-3	GLY	-	expression tag	UNP P17612
A	-2	SER	-	expression tag	UNP P17612
A	-1	HIS	-	expression tag	UNP P17612
B	-20	MET	-	expression tag	UNP P17612
B	-19	GLY	-	expression tag	UNP P17612
B	-18	SER	-	expression tag	UNP P17612

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP P17612
B	-16	HIS	-	expression tag	UNP P17612
B	-15	HIS	-	expression tag	UNP P17612
B	-14	HIS	-	expression tag	UNP P17612
B	-13	HIS	-	expression tag	UNP P17612
B	-12	HIS	-	expression tag	UNP P17612
B	-11	HIS	-	expression tag	UNP P17612
B	-10	SER	-	expression tag	UNP P17612
B	-9	SER	-	expression tag	UNP P17612
B	-8	GLY	-	expression tag	UNP P17612
B	-7	LEU	-	expression tag	UNP P17612
B	-6	VAL	-	expression tag	UNP P17612
B	-5	PRO	-	expression tag	UNP P17612
B	-4	ARG	-	expression tag	UNP P17612
B	-3	GLY	-	expression tag	UNP P17612
B	-2	SER	-	expression tag	UNP P17612
B	-1	HIS	-	expression tag	UNP P17612
E	-20	MET	-	expression tag	UNP P17612
E	-19	GLY	-	expression tag	UNP P17612
E	-18	SER	-	expression tag	UNP P17612
E	-17	SER	-	expression tag	UNP P17612
E	-16	HIS	-	expression tag	UNP P17612
E	-15	HIS	-	expression tag	UNP P17612
E	-14	HIS	-	expression tag	UNP P17612
E	-13	HIS	-	expression tag	UNP P17612
E	-12	HIS	-	expression tag	UNP P17612
E	-11	HIS	-	expression tag	UNP P17612
E	-10	SER	-	expression tag	UNP P17612
E	-9	SER	-	expression tag	UNP P17612
E	-8	GLY	-	expression tag	UNP P17612
E	-7	LEU	-	expression tag	UNP P17612
E	-6	VAL	-	expression tag	UNP P17612
E	-5	PRO	-	expression tag	UNP P17612
E	-4	ARG	-	expression tag	UNP P17612
E	-3	GLY	-	expression tag	UNP P17612
E	-2	SER	-	expression tag	UNP P17612
E	-1	HIS	-	expression tag	UNP P17612

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

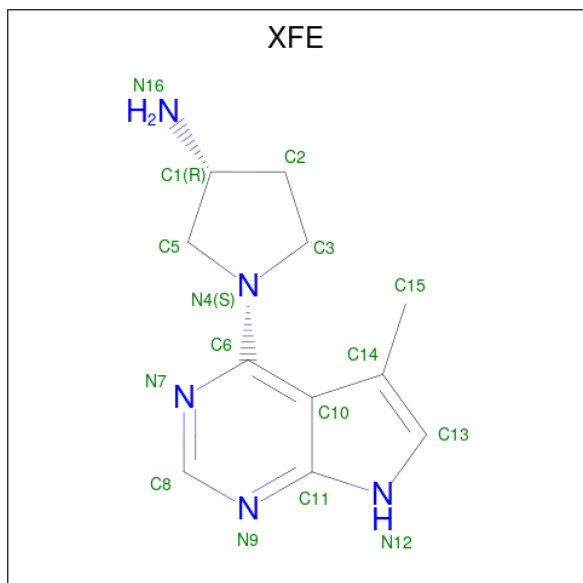
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	20	Total	C	N	O	0	0	0
			157	94	32	31			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	20	Total	C	N	O	0	0	0
			157	94	32	31			
2	K	20	Total	C	N	O	0	0	0
			157	94	32	31			

- Molecule 3 is (3R)-1-(5-methyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl)pyrrolidin-3-amine (three-letter code: XFE) (formula: C<sub>11</sub>H<sub>15</sub>N<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			16	11	5		
3	E	1	Total	C	N	0	0
			16	11	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	75	Total	O	0	0
			75	75		
4	B	73	Total	O	0	0
			73	73		
4	E	63	Total	O	0	0
			63	63		
4	I	8	Total	O	0	0
			8	8		
4	J	9	Total	O	0	0
			9	9		

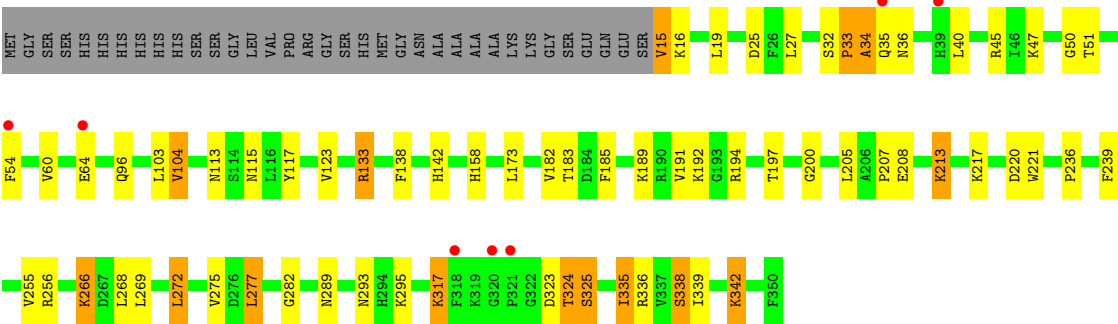
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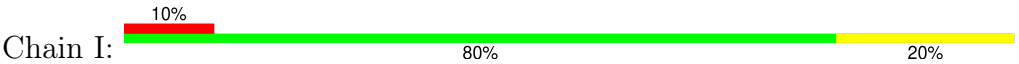
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	3	Total	O	0	0
			3	3		







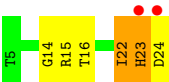
• Molecule 2: cAMP-dependent protein kinase inhibitor alpha



• Molecule 2: cAMP-dependent protein kinase inhibitor alpha



• Molecule 2: cAMP-dependent protein kinase inhibitor alpha



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.16Å 120.83Å 162.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 2.49 29.75 – 2.49	Depositor EDS
% Data completeness (in resolution range)	97.6 (29.75-2.49) 97.6 (29.75-2.49)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.49 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.212 , 0.304 0.208 , 0.297	Depositor DCC
$R_{free}$ test set	2103 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 29.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8959	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: XFE, SEP, TPO

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	0.83	1/2829 (0.0%)	0.88	5/3810 (0.1%)
1	B	0.83	0/2712	0.90	4/3650 (0.1%)
1	E	0.84	0/2829	0.86	5/3810 (0.1%)
2	I	0.82	0/159	1.01	0/212
2	J	0.80	0/159	1.08	1/212 (0.5%)
2	K	0.85	0/159	1.14	0/212
All	All	0.84	1/8847 (0.0%)	0.89	15/11906 (0.1%)

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	B	0	1
2	K	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	239	PHE	CE1-CZ	5.01	1.46	1.37

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	133	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	E	133	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	A	133	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	B	277	LEU	CA-CB-CG	6.86	131.07	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	VAL	CB-CA-C	-6.85	98.38	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	52	GLY	Peptide
2	K	14	GLY	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	2779	0	2763	40	0
1	B	2667	0	2674	53	0
1	E	2779	0	2764	33	0
2	I	157	0	146	5	0
2	J	157	0	146	5	0
2	K	157	0	146	4	0
3	A	16	0	15	4	0
3	E	16	0	15	7	0
4	A	75	0	0	7	0
4	B	73	0	0	8	0
4	E	63	0	0	6	0
4	I	8	0	0	1	0
4	J	9	0	0	0	0
4	K	3	0	0	0	0
All	All	8959	0	8669	142	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 8.

The worst 5 of 142 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:B:76:LYS:NZ	1:B:342:LYS:O	1.87	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:GLU:OE2	1:B:288:VAL:HG11	1.83	0.78
1:B:103:LEU:HD22	1:B:185:PHE:HZ	1.48	0.76
1:B:286:ASN:HB3	4:B:360:HOH:O	1.89	0.72
1:A:39:HIS:HD2	1:A:40:LEU:N	1.88	0.71

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	332/371 (90%)	312 (94%)	18 (5%)	2 (1%)	22	39
1	B	316/371 (85%)	296 (94%)	17 (5%)	3 (1%)	14	28
1	E	332/371 (90%)	314 (95%)	14 (4%)	4 (1%)	11	21
2	I	18/20 (90%)	17 (94%)	1 (6%)	0	100	100
2	J	18/20 (90%)	17 (94%)	1 (6%)	0	100	100
2	K	18/20 (90%)	17 (94%)	1 (6%)	0	100	100
All	All	1034/1173 (88%)	973 (94%)	52 (5%)	9 (1%)	14	28

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	53	SER
1	E	34	ALA
1	E	33	PRO
1	E	35	GLN
1	E	36	ASN

### 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	295/321 (92%)	258 (88%)	37 (12%)	3	7
1	B	283/321 (88%)	246 (87%)	37 (13%)	3	6
1	E	295/321 (92%)	267 (90%)	28 (10%)	7	14
2	I	15/15 (100%)	15 (100%)	0	100	100
2	J	15/15 (100%)	12 (80%)	3 (20%)	1	2
2	K	15/15 (100%)	11 (73%)	4 (27%)	0	0
All	All	918/1008 (91%)	809 (88%)	109 (12%)	4	8

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	183	THR
1	B	315	ILE
1	E	335	ILE
1	B	191	VAL
1	B	269	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	113	ASN
1	E	307	GLN
2	K	20	ASN
2	J	20	ASN
1	E	158	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	B	338	1	8,9,10	1.45	1 (12%)	7,12,14	2.44	4 (57%)
1	TPO	B	197	1	8,10,11	0.54	0	10,14,16	1.01	1 (10%)
1	TPO	A	197	1	8,10,11	0.40	0	10,14,16	1.03	0
1	SEP	A	338	1	8,9,10	1.72	1 (12%)	7,12,14	1.74	2 (28%)
1	TPO	E	197	1	8,10,11	0.95	0	10,14,16	1.29	2 (20%)
1	SEP	E	338	1	8,9,10	1.56	1 (12%)	7,12,14	2.58	3 (42%)

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	B	338	1	-	4/6/8/10	-
1	TPO	B	197	1	-	1/9/11/13	-
1	TPO	A	197	1	-	1/9/11/13	-
1	SEP	A	338	1	-	3/6/8/10	-
1	TPO	E	197	1	-	1/9/11/13	-
1	SEP	E	338	1	-	3/6/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	SEP	P-O1P	3.79	1.62	1.50
1	E	338	SEP	P-O1P	3.13	1.60	1.50
1	B	338	SEP	P-O1P	2.83	1.59	1.50

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	338	SEP	OG-CB-CA	5.50	113.49	108.14
1	B	338	SEP	O3P-P-OG	-3.71	97.01	106.67
1	B	338	SEP	OG-P-O1P	3.17	115.00	106.44
1	E	338	SEP	OG-P-O1P	2.99	114.51	106.44
1	A	338	SEP	OG-CB-CA	2.75	110.82	108.14

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	338	SEP	CA-CB-OG-P
1	A	338	SEP	CB-OG-P-O2P
1	B	197	TPO	O-C-CA-CB
1	B	338	SEP	N-CA-CB-OG
1	B	338	SEP	C-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	338	SEP	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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	XFE	A	351	-	17,18,18	0.95	1 (5%)	10,26,26	3.96	8 (80%)
3	XFE	E	351	-	17,18,18	1.02	1 (5%)	10,26,26	3.29	8 (80%)



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	XFE	A	351	-	-	0/4/13/13	0/3/3/3
3	XFE	E	351	-	-	0/4/13/13	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	351	XFE	C6-N7	2.65	1.36	1.32
3	A	351	XFE	C6-N7	2.39	1.36	1.32

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	351	XFE	C8-N7-C6	7.52	124.22	116.84
3	E	351	XFE	C8-N7-C6	5.52	122.25	116.84
3	A	351	XFE	C10-C6-N7	-5.50	114.62	123.09
3	E	351	XFE	N9-C8-N7	-5.25	121.54	128.67
3	A	351	XFE	C10-C6-N4	4.82	128.17	120.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	351	XFE	4	0
3	E	351	XFE	7	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	334/371 (90%)	-0.32	3 (0%) 81 78	11, 23, 44, 59	0
1	B	320/371 (86%)	-0.32	2 (0%) 85 83	13, 25, 41, 49	0
1	E	334/371 (90%)	-0.23	7 (2%) 63 60	11, 24, 48, 65	0
2	I	20/20 (100%)	-0.11	2 (10%) 14 13	12, 21, 56, 56	0
2	J	20/20 (100%)	-0.25	1 (5%) 35 32	13, 20, 51, 52	0
2	K	20/20 (100%)	0.06	2 (10%) 14 13	18, 26, 41, 46	0
All	All	1048/1173 (89%)	-0.28	17 (1%) 70 67	11, 24, 44, 65	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	320	GLY	3.9
1	A	15	VAL	3.7
1	E	318	PHE	3.6
1	A	335	ILE	3.1
2	K	24	ASP	3.0

### 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. 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
1	SEP	A	338	10/11	0.92	0.08	37,45,47,48	0
1	SEP	B	338	10/11	0.94	0.08	22,25,27,28	0
1	SEP	E	338	10/11	0.95	0.08	29,30,32,32	0
1	TPO	B	197	11/12	0.96	0.07	23,24,25,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	TPO	E	197	11/12	0.97	0.07	21,24,26,26	0
1	TPO	A	197	11/12	0.98	0.05	15,18,19,20	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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( $\text{\AA}^2$ )	Q<0.9
3	XFE	E	351	16/16	0.91	0.10	26,31,38,40	0
3	XFE	A	351	16/16	0.93	0.08	18,22,27,29	0

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

There are no such residues in this entry.