



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:43 AM GMT

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/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

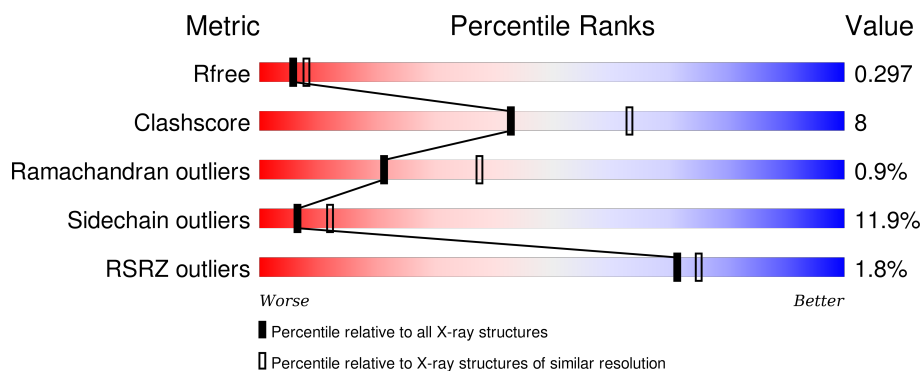
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 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	371	<div> <div>68%</div> <div>19%</div> <div>•</div> <div>9%</div> </div>
1	B	371	<div> <div>62%</div> <div>22%</div> <div>• •</div> <div>13%</div> </div>
1	E	371	<div> <div>2%</div> <div>72%</div> <div>15%</div> <div>•</div> <div>9%</div> </div>
2	I	20	<div> <div>10%</div> <div>80%</div> <div>20%</div> </div>
2	J	20	<div> <div>10%</div> <div>75%</div> <div>10%</div> <div>15%</div> </div>

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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

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.

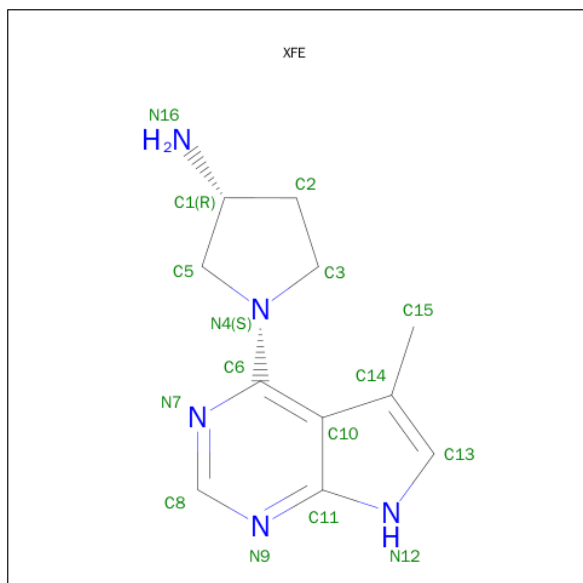
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	20	Total	C	N	O	0	0	0
			157	94	32	31			

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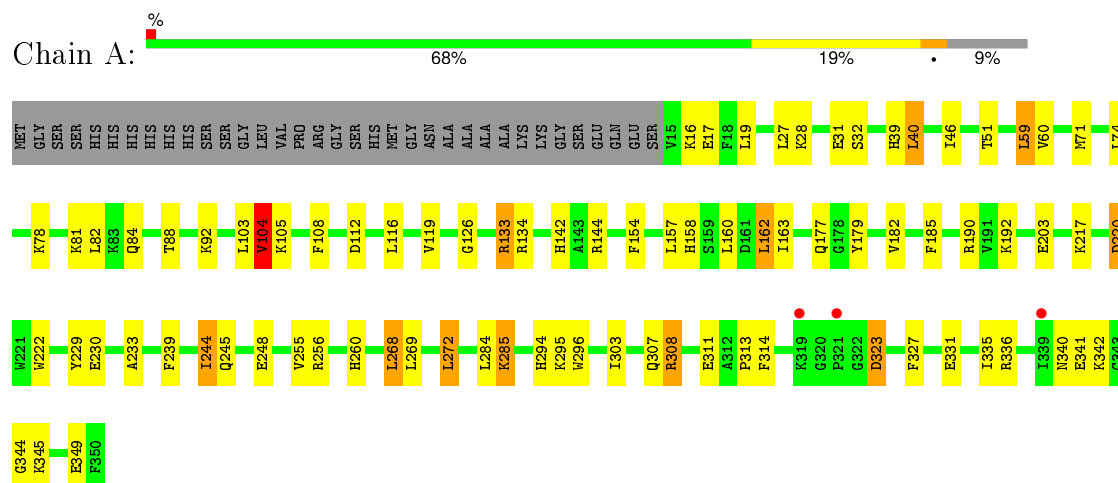
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	3	Total	O	0	0
			3	3		

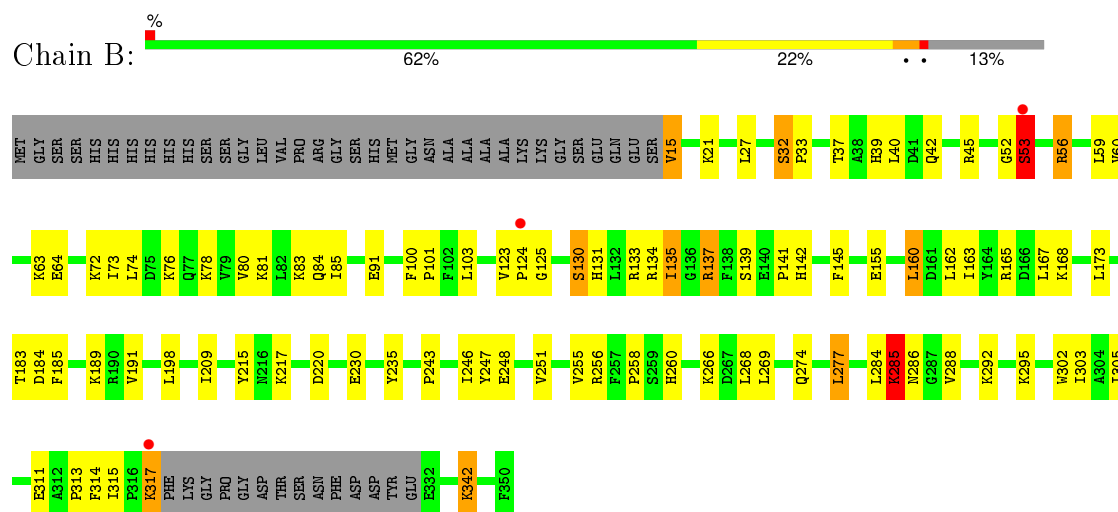
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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



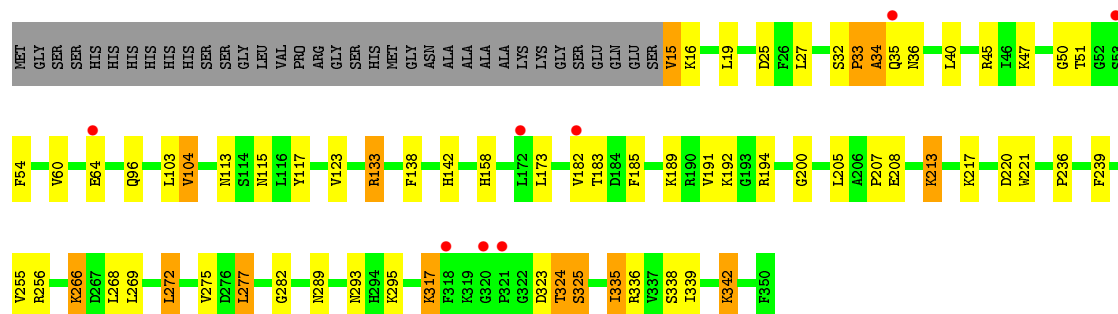
- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha



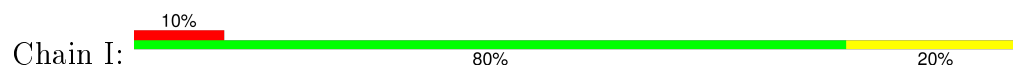
- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha







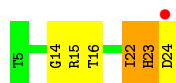
- Molecule 2: cAMP-dependent protein kinase inhibitor alpha



- 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 29.65 – 2.49	Depositor EDS
% Data completeness (in resolution range)	97.6 (29.75-2.49) 97.7 (29.65-2.49)	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 5.5.0109	Depositor
R, $R_{free}$	0.212 , 0.304 0.208 , 0.297	Depositor DCC
$R_{free}$ test set	2103 reflections (5.30%)	DCC
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> )	0.32 , 36.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 41778 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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: TPO, XFE, 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	0.83	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

All (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
1	A	220	ASP	CB-CG-OD1	6.60	124.24	118.30
1	B	137	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	B	160	LEU	CA-CB-CG	5.89	128.85	115.30
1	E	25	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	133	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	E	266	LYS	CD-CE-NZ	5.64	124.67	111.70
1	A	308	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	E	272	LEU	CA-CB-CG	5.58	128.12	115.30
2	J	15	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	B	220	ASP	CB-CG-OD2	5.17	122.95	118.30

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 ⓘ

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
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
1:A:248:GLU:HG3	2:I:7:TYR:CD2	2.27	0.70
1:E:123:VAL:HB	1:E:173:LEU:HD13	1.73	0.69
3:E:351:XFE:H3	3:E:351:XFE:H15A	1.73	0.69
1:E:104:VAL:HG21	1:E:183:THR:HG22	1.74	0.69
1:E:15:VAL:N	4:E:408:HOH:O	2.27	0.68
3:E:351:XFE:C3	3:E:351:XFE:H15A	2.23	0.68
1:E:189:LYS:HG2	1:E:191:VAL:HG23	1.75	0.68
1:E:208:GLU:HG2	1:E:277:LEU:HD22	1.76	0.67
1:B:103:LEU:HD22	1:B:185:PHE:CZ	2.29	0.66
1:A:311:GLU:OE1	1:B:83:LYS:NZ	2.29	0.65
1:A:177:GLN:HG3	4:A:416:HOH:O	1.97	0.65
1:B:142:HIS:CD2	1:B:313:PRO:HB3	2.32	0.64
1:B:53:SER:HB3	4:B:404:HOH:O	1.97	0.63
1:E:208:GLU:CG	1:E:277:LEU:HD22	2.28	0.63
1:B:130:SER:O	1:B:134:ARG:HG3	2.00	0.62
1:A:39:HIS:CD2	1:A:40:LEU:N	2.67	0.62
1:B:209:ILE:HG12	1:B:215:TYR:CD1	2.34	0.61
1:E:158:HIS:HE1	1:E:220:ASP:OD2	1.84	0.60
1:B:286:ASN:HB3	4:B:420:HOH:O	2.02	0.60
1:A:158:HIS:HE1	1:A:220:ASP:OD2	1.84	0.59
1:A:192:LYS:HB3	4:A:417:HOH:O	2.02	0.59
2:J:7:TYR:CZ	2:J:11:ILE:CD1	2.85	0.59
1:A:133:ARG:NH2	1:A:230:GLU:OE2	2.35	0.59
3:E:351:XFE:C3	3:E:351:XFE:C15	2.80	0.58
1:E:104:VAL:HG22	1:E:182:VAL:O	2.04	0.58
1:B:56:ARG:NH1	1:B:56:ARG:H	2.02	0.58
1:A:103:LEU:HD22	1:A:185:PHE:HZ	1.69	0.57
1:A:294:HIS:ND1	1:A:295:LYS:N	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LYS:HG3	1:A:192:LYS:O	2.05	0.56
1:E:15:VAL:N	4:E:410:HOH:O	2.37	0.56
1:E:64:GLU:HB3	4:E:414:HOH:O	2.03	0.56
1:A:268:LEU:HD22	1:A:272:LEU:HD22	1.88	0.56
1:B:131:HIS:HE1	1:B:314:PHE:CD2	2.24	0.55
1:B:317:LYS:C	4:B:366:HOH:O	2.45	0.55
1:B:131:HIS:CD2	1:B:135:ILE:HD13	2.42	0.55
1:A:71:MET:HG3	1:A:119:VAL:HG22	1.89	0.55
1:B:15:VAL:HG13	4:B:416:HOH:O	2.07	0.54
1:E:221:TRP:CD1	1:E:282:GLY:HA3	2.42	0.54
1:A:154:PHE:CE2	1:A:220:ASP:HB3	2.42	0.54
1:A:157:LEU:O	1:A:162:LEU:HB2	2.08	0.54
1:B:64:GLU:N	1:B:64:GLU:OE1	2.40	0.54
1:B:247:TYR:O	1:B:251:VAL:HG13	2.08	0.54
1:E:33:PRO:O	1:E:34:ALA:CB	2.55	0.54
1:E:323:ASP:OD1	1:E:325:SER:OG	2.26	0.54
1:A:133:ARG:NH1	4:A:388:HOH:O	2.41	0.53
1:B:80:VAL:HG13	1:B:85:ILE:HD11	1.90	0.53
1:B:133:ARG:HD2	2:K:16:THR:O	2.08	0.53
1:B:167:LEU:O	1:B:168:LYS:HB3	2.09	0.53
2:I:7:TYR:O	2:I:11:ILE:HG12	2.09	0.52
1:B:284:LEU:O	1:B:285:LYS:C	2.47	0.52
3:A:351:XFE:C15	3:A:351:XFE:H5A	2.40	0.52
1:E:104:VAL:CG2	1:E:183:THR:HG22	2.39	0.52
3:A:351:XFE:C5	3:A:351:XFE:H15A	2.40	0.52
1:B:131:HIS:CE1	1:B:314:PHE:CD2	2.98	0.51
1:E:96:GLN:HG2	4:E:404:HOH:O	2.10	0.51
1:A:104:VAL:HG22	1:A:182:VAL:O	2.10	0.51
1:B:100:PHE:HB3	1:B:103:LEU:HD12	1.91	0.51
1:B:100:PHE:CD2	1:B:101:PRO:HD2	2.45	0.51
1:E:138:PHE:CG	1:E:142:HIS:CD2	2.99	0.51
1:A:59:LEU:HD22	1:A:60:VAL:H	1.75	0.50
3:E:351:XFE:C15	3:E:351:XFE:H3A	2.41	0.50
1:B:303:ILE:HD12	1:B:303:ILE:H	1.75	0.50
1:A:28:LYS:HE2	1:A:28:LYS:HA	1.94	0.50
1:B:258:PRO:HB2	1:B:260:HIS:ND1	2.28	0.49
3:E:351:XFE:H15A	3:E:351:XFE:H3A	1.95	0.48
1:E:103:LEU:HD22	1:E:185:PHE:HZ	1.77	0.48
1:B:131:HIS:NE2	1:B:135:ILE:HD13	2.28	0.48
1:A:142:HIS:ND1	1:A:313:PRO:HB3	2.28	0.48
1:B:163:ILE:HG22	1:B:165:ARG:CG	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:HD2	4:A:396:HOH:O	2.14	0.48
1:B:198:LEU:HD11	2:K:22:ILE:HD12	1.96	0.48
1:B:198:LEU:HD11	2:K:22:ILE:CD1	2.45	0.47
1:A:179:TYR:CZ	1:A:308:ARG:HA	2.50	0.47
1:A:88:THR:HG21	1:A:116:LEU:CD1	2.44	0.47
3:A:351:XFE:C5	3:A:351:XFE:C15	2.93	0.47
2:I:23:HIS:CG	4:I:207:HOH:O	2.68	0.47
1:B:155:GLU:OE2	1:B:288:VAL:CG1	2.60	0.47
1:B:100:PHE:CG	1:B:101:PRO:HD2	2.49	0.47
3:A:351:XFE:H5	3:A:351:XFE:H15A	1.97	0.47
1:E:339:ILE:HD11	4:E:371:HOH:O	2.13	0.47
1:E:50:GLY:HA3	3:E:351:XFE:HN1A	1.78	0.47
1:B:163:ILE:HG22	1:B:165:ARG:HG3	1.95	0.47
1:E:338:SEP:OG	1:E:342:LYS:HE2	2.15	0.47
1:B:292:LYS:HA	1:B:302:TRP:CZ2	2.50	0.46
1:B:84:GLN:NE2	2:K:23:HIS:HD2	2.14	0.46
1:B:184:ASP:HB2	4:B:418:HOH:O	2.15	0.46
2:I:23:HIS:CD2	2:I:24:ASP:H	2.34	0.45
1:B:32:SER:N	1:B:33:PRO:HD3	2.31	0.45
1:B:100:PHE:CG	1:B:101:PRO:CD	3.00	0.45
1:E:115:ASN:HB2	1:E:117:TYR:CZ	2.51	0.45
1:B:73:ILE:C	1:B:74:LEU:HD12	2.37	0.45
1:E:207:PRO:HG2	1:E:275:VAL:HG23	1.97	0.45
1:E:317:LYS:HA	1:E:317:LYS:HE3	1.97	0.45
1:E:266:LYS:CE	4:E:397:HOH:O	2.64	0.45
1:E:289:ASN:O	1:E:293:ASN:HB2	2.16	0.45
1:A:28:LYS:HE3	4:A:413:HOH:O	2.15	0.45
1:A:284:LEU:O	1:A:285:LYS:C	2.56	0.45
1:E:47:LYS:HD2	1:E:324:THR:HG21	1.98	0.44
1:B:258:PRO:HB2	1:B:260:HIS:CE1	2.51	0.44
1:B:266:LYS:HE3	4:B:401:HOH:O	2.17	0.44
1:B:15:VAL:N	4:B:412:HOH:O	2.50	0.44
1:A:162:LEU:HD12	1:A:190:ARG:HA	2.00	0.43
1:B:258:PRO:CB	1:B:260:HIS:CE1	3.01	0.43
1:A:229:TYR:O	1:A:233:ALA:N	2.50	0.43
1:A:284:LEU:HB2	4:A:369:HOH:O	2.18	0.43
1:B:295:LYS:HE3	1:B:295:LYS:HB2	1.73	0.43
1:E:213:LYS:NZ	1:E:213:LYS:HB2	2.34	0.43
3:E:351:XFE:H3	3:E:351:XFE:C15	2.44	0.43
2:J:7:TYR:CZ	2:J:11:ILE:HD13	2.53	0.43
1:A:323:ASP:HA	4:A:404:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:GLY:HA2	1:A:327:PHE:CE1	2.54	0.42
1:E:236:PRO:HG2	1:E:239:PHE:HB3	2.00	0.42
1:A:144:ARG:NE	1:A:296:TRP:O	2.51	0.42
1:B:123:VAL:HA	1:B:124:PRO:HD2	1.89	0.42
1:B:91:GLU:OE2	1:B:184:ASP:HA	2.19	0.42
2:J:23:HIS:CD2	2:J:23:HIS:N	2.87	0.42
1:A:244:ILE:HD11	1:E:133:ARG:O	2.19	0.42
1:A:203:GLU:OE2	2:J:15:ARG:HD3	2.20	0.42
1:A:342:LYS:HD3	1:A:342:LYS:HA	1.90	0.42
1:B:230:GLU:HA	1:B:235:TYR:O	2.20	0.41
1:A:307:GLN:HB2	1:A:307:GLN:HE21	1.64	0.41
1:B:139:SER:HB2	1:B:141:PRO:HD2	2.00	0.41
1:A:82:LEU:O	1:A:84:GLN:HG2	2.21	0.41
2:I:7:TYR:CE1	2:I:11:ILE:HD11	2.55	0.41
1:E:113:ASN:O	1:E:342:LYS:HB2	2.20	0.41
1:B:39:HIS:CD2	1:B:42:GLN:HG3	2.56	0.41
1:A:112:ASP:OD1	1:A:112:ASP:C	2.59	0.41
1:E:335:ILE:H	1:E:335:ILE:HG12	1.75	0.41
1:B:145:PHE:CE2	1:B:313:PRO:HD2	2.55	0.41
2:J:7:TYR:CE2	2:J:11:ILE:HD13	2.56	0.41
1:A:303:ILE:N	1:A:303:ILE:HD12	2.36	0.41
1:B:137:ARG:NE	1:B:260:HIS:HE2	2.19	0.41
1:A:222:TRP:C	1:A:222:TRP:CD1	2.94	0.40
1:E:200:GLY:HA3	1:E:205:LEU:HD21	2.03	0.40
1:E:33:PRO:O	1:E:34:ALA:HB2	2.20	0.40
1:B:243:PRO:O	1:B:246:ILE:HB	2.22	0.40
1:A:245:GLN:HB2	1:A:245:GLN:HE21	1.69	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/371 (90%)	312 (94%)	18 (5%)	2 (1%)	30	50
1	B	316/371 (85%)	296 (94%)	17 (5%)	3 (1%)	21	37
1	E	332/371 (90%)	314 (95%)	14 (4%)	4 (1%)	16	29
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%)	21	37

All (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
1	B	285	LYS
1	B	125	GLY
1	A	344	GLY
1	A	46	ILE

### 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%)	6	10
1	B	283/321 (88%)	246 (87%)	37 (13%)	5	9
1	E	295/321 (92%)	267 (90%)	28 (10%)	11	20
2	I	15/15 (100%)	15 (100%)	0	100	100
2	J	15/15 (100%)	12 (80%)	3 (20%)	1	3
2	K	15/15 (100%)	11 (73%)	4 (27%)	0	1
All	All	918/1008 (91%)	809 (88%)	109 (12%)	6	12

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	17	GLU
1	A	19	LEU
1	A	27	LEU
1	A	31	GLU
1	A	32	SER
1	A	40	LEU
1	A	51	THR
1	A	59	LEU
1	A	74	LEU
1	A	78	LYS
1	A	81	LYS
1	A	92	LYS
1	A	104	VAL
1	A	105	LYS
1	A	108	PHE
1	A	160	LEU
1	A	162	LEU
1	A	163	ILE
1	A	217	LYS
1	A	244	ILE
1	A	255	VAL
1	A	256	ARG
1	A	260	HIS
1	A	268	LEU
1	A	269	LEU
1	A	272	LEU
1	A	285	LYS
1	A	314	PHE
1	A	323	ASP
1	A	331	GLU
1	A	335	ILE
1	A	336	ARG
1	A	340	ASN
1	A	341	GLU
1	A	345	LYS
1	A	349	GLU
1	B	15	VAL
1	B	21	LYS
1	B	27	LEU
1	B	32	SER
1	B	37	THR

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Mol	Chain	Res	Type
1	B	40	LEU
1	B	45	ARG
1	B	53	SER
1	B	56	ARG
1	B	59	LEU
1	B	60	VAL
1	B	63	LYS
1	B	72	LYS
1	B	78	LYS
1	B	81	LYS
1	B	130	SER
1	B	135	ILE
1	B	160	LEU
1	B	162	LEU
1	B	173	LEU
1	B	183	THR
1	B	189	LYS
1	B	191	VAL
1	B	217	LYS
1	B	248	GLU
1	B	255	VAL
1	B	256	ARG
1	B	268	LEU
1	B	269	LEU
1	B	274	GLN
1	B	277	LEU
1	B	285	LYS
1	B	305	ILE
1	B	311	GLU
1	B	315	ILE
1	B	317	LYS
1	B	342	LYS
1	E	15	VAL
1	E	16	LYS
1	E	19	LEU
1	E	27	LEU
1	E	32	SER
1	E	40	LEU
1	E	45	ARG
1	E	51	THR
1	E	54	PHE
1	E	60	VAL

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Mol	Chain	Res	Type
1	E	104	VAL
1	E	192	LYS
1	E	194	ARG
1	E	213	LYS
1	E	217	LYS
1	E	255	VAL
1	E	256	ARG
1	E	268	LEU
1	E	269	LEU
1	E	272	LEU
1	E	277	LEU
1	E	295	LYS
1	E	317	LYS
1	E	324	THR
1	E	325	SER
1	E	335	ILE
1	E	336	ARG
1	E	342	LYS
2	J	11	ILE
2	J	23	HIS
2	J	24	ASP
2	K	15	ARG
2	K	22	ILE
2	K	23	HIS
2	K	24	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	113	ASN
1	A	158	HIS
1	A	245	GLN
1	A	307	GLN
1	B	39	HIS
1	B	67	ASN
1	B	84	GLN
1	B	113	ASN
1	B	131	HIS
1	B	158	HIS
1	B	307	GLN
1	E	36	ASN

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Mol	Chain	Res	Type
1	E	62	HIS
1	E	113	ASN
1	E	142	HIS
1	E	158	HIS
1	E	307	GLN
2	J	20	ASN
2	J	23	HIS
2	K	20	ASN

### 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	TPO	A	197	1	8,10,11	0.36	0	7,14,16	1.53	1 (14%)
1	SEP	A	338	1	8,9,10	1.61	1 (12%)	8,12,14	1.79	2 (25%)
1	TPO	B	197	1	8,10,11	0.43	0	7,14,16	1.34	1 (14%)
1	SEP	B	338	1	8,9,10	1.37	1 (12%)	8,12,14	2.34	5 (62%)
1	TPO	E	197	1	8,10,11	0.69	0	7,14,16	1.69	2 (28%)
1	SEP	E	338	1	8,9,10	1.47	1 (12%)	8,12,14	2.66	3 (37%)

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	TPO	A	197	1	-	0/8/11/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	338	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	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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	338	SEP	P-O1P	2.46	1.59	1.51
1	E	338	SEP	P-O1P	2.75	1.60	1.51
1	A	338	SEP	P-O1P	3.37	1.62	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	338	SEP	O3P-P-OG	-3.32	97.01	106.56
1	E	338	SEP	O2P-P-O1P	-2.39	102.87	110.58
1	E	197	TPO	CG2-CB-CA	-2.28	108.54	113.17
1	B	338	SEP	O3P-P-O1P	-2.20	103.51	110.58
1	B	338	SEP	O2P-P-OG	2.17	112.81	106.56
1	E	197	TPO	O3P-P-O2P	2.31	116.16	107.38
1	A	338	SEP	O3P-P-OG	2.31	113.22	106.56
1	B	197	TPO	O3P-P-O2P	2.40	116.51	107.38
1	A	197	TPO	OG1-P-O1P	2.48	113.30	107.11
1	B	338	SEP	OG-CB-CA	2.54	110.44	108.27
1	E	338	SEP	OG-P-O1P	2.90	114.51	107.14
1	A	338	SEP	OG-CB-CA	2.98	110.82	108.27
1	B	338	SEP	OG-P-O1P	3.09	115.00	107.14
1	E	338	SEP	OG-CB-CA	6.12	113.49	108.27

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	E	338	SEP	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	0.94	0	13,26,26	3.29	9 (69%)
3	XFE	E	351	-	17,18,18	0.89	0	13,26,26	3.50	5 (38%)

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

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	351	XFE	N9-C8-N7	-9.60	121.54	128.89
3	A	351	XFE	N9-C8-N7	-7.84	122.89	128.89
3	E	351	XFE	C5-N4-C6	-3.24	114.47	123.52
3	A	351	XFE	C3-N4-C6	-2.57	116.09	123.48
3	A	351	XFE	C14-C10-C11	-2.48	102.11	106.54
3	A	351	XFE	C15-C14-C13	-2.30	122.49	127.94
3	A	351	XFE	C2-C1-C5	2.08	105.10	102.03
3	A	351	XFE	C13-C14-C10	2.10	110.24	107.51
3	A	351	XFE	C3-C2-C1	2.18	108.04	103.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	351	XFE	C2-C3-N4	2.32	106.36	103.35
3	A	351	XFE	C10-C6-N4	2.72	128.17	121.44
3	E	351	XFE	C2-C1-C5	3.19	106.74	102.03
3	E	351	XFE	C8-N7-C6	5.09	122.25	111.43
3	A	351	XFE	C8-N7-C6	6.01	124.22	111.43

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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	334/371 (90%)	-0.11	3 (0%) 85 88	11, 23, 44, 59	0
1	B	320/371 (86%)	-0.16	3 (0%) 85 88	13, 25, 41, 49	0
1	E	334/371 (90%)	-0.01	8 (2%) 62 66	11, 24, 48, 65	0
2	I	20/20 (100%)	0.05	2 (10%) 9 10	12, 21, 56, 56	0
2	J	20/20 (100%)	0.16	2 (10%) 9 10	13, 20, 51, 52	0
2	K	20/20 (100%)	0.08	1 (5%) 32 37	18, 26, 41, 46	0
All	All	1048/1173 (89%)	-0.08	19 (1%) 71 75	11, 24, 44, 65	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	321	PRO	4.9
2	J	24	ASP	4.5
1	E	35	GLN	4.1
2	I	24	ASP	4.0
1	E	320	GLY	4.0
1	E	318	PHE	3.9
2	I	23	HIS	3.8
1	A	321	PRO	3.5
2	K	24	ASP	3.2
1	E	64	GLU	3.2
1	B	317	LYS	3.1
1	E	182	VAL	2.7
1	A	319	LYS	2.7
2	J	23	HIS	2.7
1	B	53	SER	2.7
1	A	339	ILE	2.4
1	E	53	SER	2.3
1	B	124	PRO	2.3
1	E	172	LEU	2.1

## 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	TPO	B	197	11/12	0.97	0.09	-	23,24,25,26	0
1	TPO	E	197	11/12	0.97	0.09	-	21,24,26,26	0
1	SEP	B	338	10/11	0.95	0.15	-	22,25,27,28	0
1	SEP	A	338	10/11	0.94	0.12	-	37,45,47,48	0
1	TPO	A	197	11/12	0.98	0.10	-	15,18,19,20	0
1	SEP	E	338	10/11	0.96	0.09	-	29,30,32,32	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	XFE	E	351	16/16	0.94	0.17	0.37	26,31,38,40	0
3	XFE	A	351	16/16	0.94	0.14	-0.15	18,22,27,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.