



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:13 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

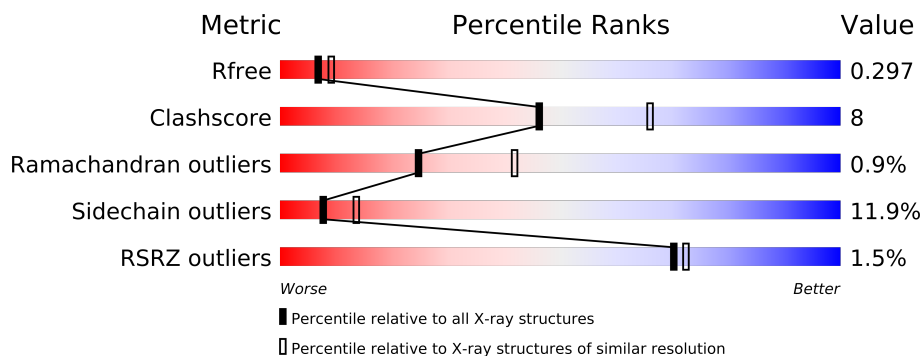
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	371	
1	B	371	
1	E	371	
2	I	20	
2	J	20	
2	K	20	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8959 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

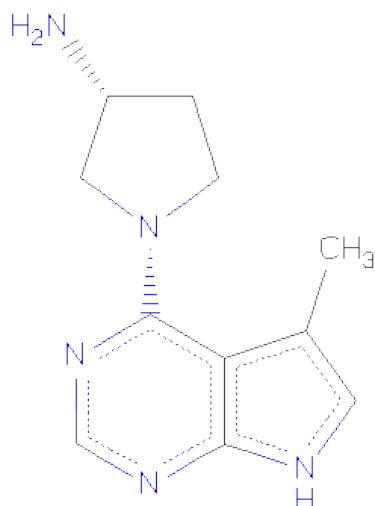
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	20	Total	C	N	O	0	0	0
			157	94	32	31			

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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: C₁₁H₁₅N₅).



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		

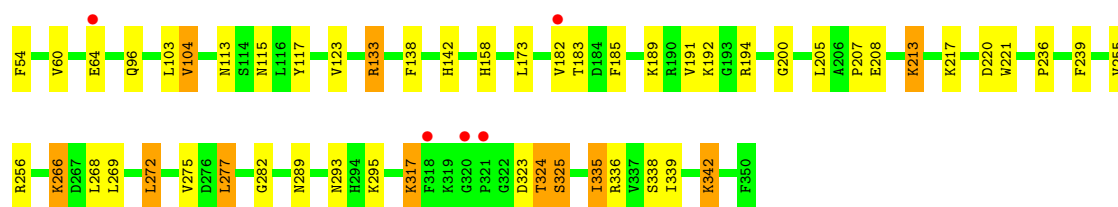
- Molecule 4 is water.

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

Chain I:



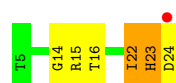
- Molecule 2: cAMP-dependent protein kinase inhibitor alpha

Chain J:



- Molecule 2: cAMP-dependent protein kinase inhibitor alpha

Chain K:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.212 , 0.304 0.209 , 0.297	Depositor DCC
R_{free} test set	2103 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 10.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	9	0	0	0	0
4	K	3	0	0	0	0
All	All	8959	0	8669	142	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (142) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
1:A:134:ARG:HD2	4:A:396:HOH:O	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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%)	33	55
1	B	316/371 (85%)	296 (94%)	17 (5%)	3 (1%)	25	42
1	E	332/371 (90%)	314 (95%)	14 (4%)	4 (1%)	19	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	25	42

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%)	7	12
1	B	283/321 (88%)	246 (87%)	37 (13%)	6	10
1	E	295/321 (92%)	267 (90%)	28 (10%)	12	22
2	I	15/15 (100%)	15 (100%)	0	100	100
2	J	15/15 (100%)	12 (80%)	3 (20%)	2	3
2	K	15/15 (100%)	11 (73%)	4 (27%)	1	1
All	All	918/1008 (91%)	809 (88%)	109 (12%)	8	13

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

Mol	Chain	Res	Type
1	A	16	LYS

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Mol	Chain	Res	Type
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
1	B	40	LEU

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Mol	Chain	Res	Type
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
1	E	104	VAL

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Mol	Chain	Res	Type
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
1	E	62	HIS

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Mol	Chain	Res	Type
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 chains 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	10,10,11	5.25	2 (20%)	12,14,16	1.32	1 (8%)
1	SEP	A	338	1	9,9,10	6.45	3 (33%)	10,12,14	2.04	2 (20%)
1	TPO	B	197	1	10,10,11	5.73	2 (20%)	12,14,16	1.19	2 (16%)
1	SEP	B	338	1	9,9,10	6.24	2 (22%)	10,12,14	2.27	5 (50%)
1	TPO	E	197	1	10,10,11	6.31	1 (10%)	12,14,16	1.53	3 (25%)
1	SEP	E	338	1	9,9,10	5.74	3 (33%)	10,12,14	1.79	4 (40%)

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	-	0/9/11/13	0/0/0/0
1	SEP	A	338	1	-	0/6/8/10	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	B	197	1	-	0/9/11/13	0/0/0/0
1	SEP	B	338	1	-	0/6/8/10	0/0/0/0
1	TPO	E	197	1	-	0/9/11/13	0/0/0/0
1	SEP	E	338	1	-	0/6/8/10	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	197	TPO	O-C	19.80	1.25	1.11
1	A	338	SEP	O-C	18.69	1.24	1.11
1	B	338	SEP	O-C	18.27	1.24	1.11
1	B	197	TPO	O-C	17.87	1.23	1.11
1	E	338	SEP	O-C	16.58	1.22	1.11
1	A	197	TPO	O-C	16.41	1.22	1.11
1	A	338	SEP	P-O1P	3.30	1.62	1.51
1	E	338	SEP	P-O1P	2.68	1.60	1.51
1	E	338	SEP	CA-C	2.43	1.52	1.48
1	B	338	SEP	P-O1P	2.40	1.59	1.51
1	A	338	SEP	CA-C	2.40	1.52	1.48
1	B	197	TPO	OG1-CB	-2.33	1.40	1.45
1	A	197	TPO	CA-C	2.28	1.52	1.48

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	SEP	C-CA-N	-5.05	108.79	113.83
1	B	338	SEP	C-CA-N	3.82	117.65	113.83
1	B	338	SEP	O3P-P-OG	-3.49	97.01	106.65
1	E	338	SEP	OG-CB-CA	3.39	113.49	108.69
1	B	338	SEP	OG-P-O1P	2.83	115.00	106.71
1	E	338	SEP	OG-P-O1P	2.66	114.51	106.71
1	B	197	TPO	CB-CA-N	2.54	113.14	109.60
1	E	197	TPO	CB-CA-N	2.38	112.93	109.60
1	A	338	SEP	O3P-P-OG	2.38	113.22	106.65
1	A	197	TPO	OG1-P-O1P	2.33	113.30	106.79
1	E	338	SEP	O2P-P-O1P	-2.32	102.87	110.44
1	B	197	TPO	O3P-P-O2P	2.29	116.51	107.61
1	E	197	TPO	CG2-CB-CA	-2.27	108.54	113.20
1	B	338	SEP	O2P-P-OG	2.23	112.81	106.65
1	E	197	TPO	O3P-P-O2P	2.20	116.16	107.61
1	E	338	SEP	C-CA-N	-2.15	111.68	113.83
1	B	338	SEP	O3P-P-O1P	-2.12	103.51	110.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	-	18,18,18	1.11	2 (11%)	24,26,26	2.60	11 (45%)
3	XFE	E	351	-	18,18,18	1.17	1 (5%)	24,26,26	2.78	11 (45%)

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	0/1/3/3
3	XFE	E	351	-	-	0/4/13/13	0/1/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	351	XFE	C14-C10	3.32	1.49	1.42
3	A	351	XFE	C14-C10	2.19	1.46	1.42
3	A	351	XFE	C6-N4	2.01	1.43	1.36

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	351	XFE	N9-C8-N7	-8.57	121.54	128.71
3	A	351	XFE	N9-C8-N7	-6.96	122.89	128.71
3	A	351	XFE	C8-N7-C6	5.85	124.22	111.53
3	E	351	XFE	C8-N7-C6	4.95	122.25	111.53
3	E	351	XFE	N12-C11-N9	3.72	131.94	125.34
3	A	351	XFE	C14-C10-C11	-3.57	102.11	106.08
3	E	351	XFE	C5-N4-C6	-3.18	114.47	123.58
3	A	351	XFE	C10-C6-N7	-2.96	114.62	123.04
3	E	351	XFE	C10-C11-N9	-2.88	119.08	125.14
3	A	351	XFE	C10-C11-N12	2.84	109.43	106.54
3	E	351	XFE	C8-N9-C11	2.80	120.30	114.82
3	E	351	XFE	C14-C10-C11	-2.80	102.97	106.08
3	A	351	XFE	C3-N4-C6	-2.61	116.09	123.58
3	A	351	XFE	C3-C2-C1	2.52	108.04	103.31
3	A	351	XFE	C15-C14-C13	-2.48	122.49	127.91
3	E	351	XFE	C10-C11-N12	2.39	108.98	106.54
3	A	351	XFE	C10-C6-N4	2.38	128.17	121.94
3	A	351	XFE	N12-C11-N9	2.34	129.50	125.34
3	E	351	XFE	C2-C3-N4	2.31	106.36	103.29
3	A	351	XFE	C13-C14-C10	2.23	110.24	107.54
3	E	351	XFE	C2-C1-N16	-2.07	107.87	113.49
3	E	351	XFE	C10-C6-N7	-2.01	117.33	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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 ²)	Q<0.9
1	A	336/371 (90%)	-0.23	2 (0%) 86 88	11, 23, 44, 59	0
1	B	322/371 (86%)	-0.26	2 (0%) 86 88	13, 25, 40, 49	0
1	E	336/371 (90%)	-0.13	7 (2%) 60 63	11, 24, 48, 65	0
2	I	20/20 (100%)	-0.05	2 (10%) 8 7	12, 21, 56, 56	0
2	J	20/20 (100%)	0.05	2 (10%) 8 7	13, 20, 51, 52	0
2	K	20/20 (100%)	-0.05	1 (5%) 28 28	18, 26, 41, 46	0
All	All	1054/1173 (89%)	-0.20	16 (1%) 70 72	11, 24, 44, 65	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	321	PRO	4.5
1	E	320	GLY	4.5
1	E	318	PHE	4.2
2	J	24	ASP	4.0
1	E	35	GLN	3.5
2	I	23	HIS	3.5
2	I	24	ASP	3.3
1	A	321	PRO	2.9
2	K	24	ASP	2.9
1	B	317	LYS	2.7
1	E	64	GLU	2.7
1	A	319	LYS	2.6
2	J	23	HIS	2.4
1	E	182	VAL	2.4
1	B	53	SER	2.3
1	E	53	SER	2.2

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

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	SEP	B	338	10/11	0.13	-0.45	22,25,27,28	0
1	TPO	B	197	11/12	0.08	-0.72	23,24,25,26	0
1	SEP	A	338	10/11	0.12	-1.21	37,45,47,48	0
1	SEP	E	338	10/11	0.09	-1.31	29,30,32,32	0
1	TPO	A	197	11/12	0.08	-1.58	15,18,19,20	0
1	TPO	E	197	11/12	0.08	-1.62	21,24,26,26	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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	XFE	E	351	16/16	0.17	0.48	26,31,38,40	0
3	XFE	A	351	16/16	0.13	-0.28	18,22,27,29	0

6.5 Other polymers ⓘ

There are no such residues in this entry.