



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:43 PM UTC

PDB ID : 3MVJ / pdb_00003mvj
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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

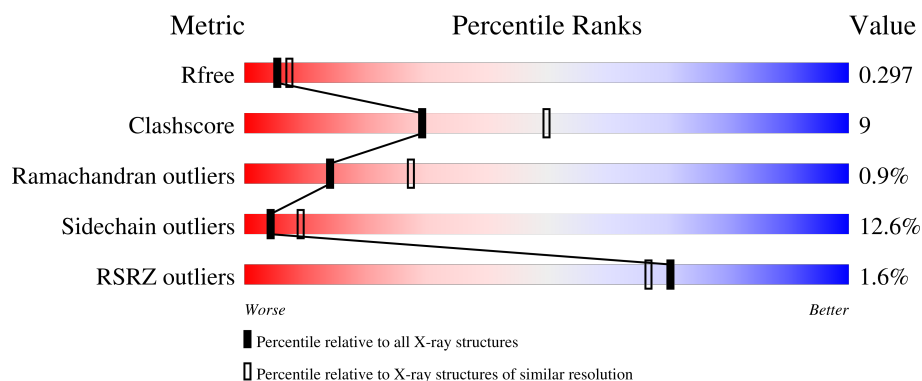
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 ≥ 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	
1	B	371	
1	E	371	
2	I	20	
2	J	20	

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Mol	Chain	Length	Quality of chain
2	K	20	10% 75% 10% 15%

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.

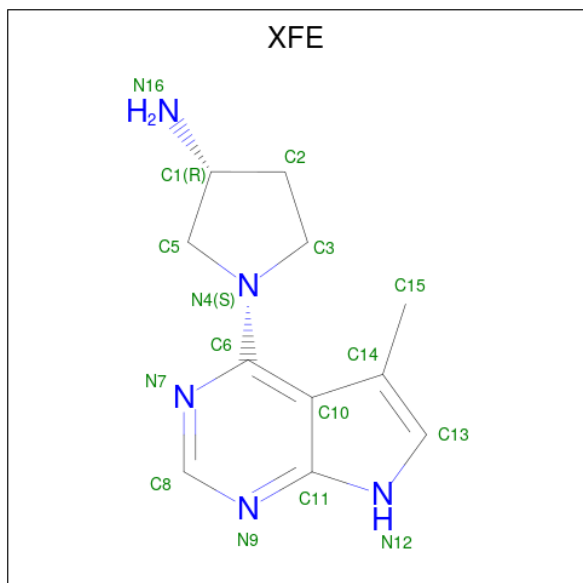
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	20	Total	C	N	O	0	0	0
			157	94	32	31			

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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 (CCD ID: 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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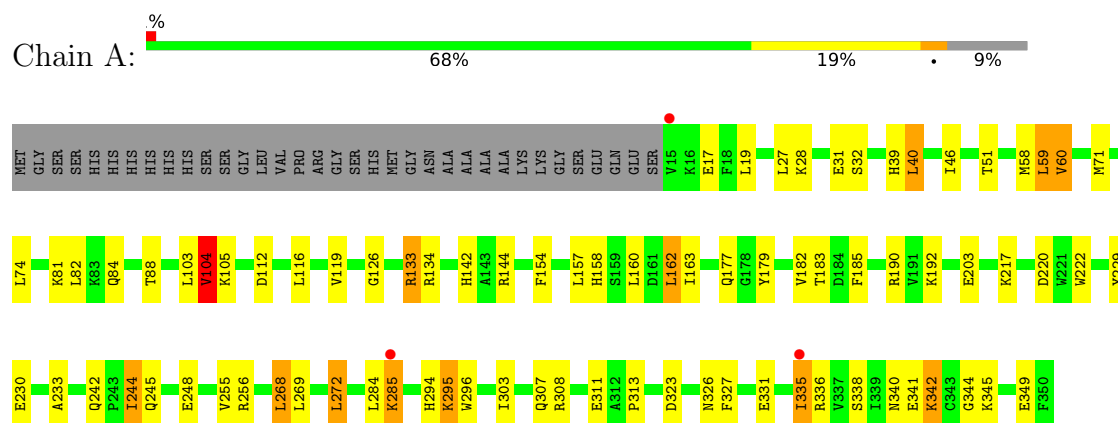
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	3	Total	O	0	0
			3	3		

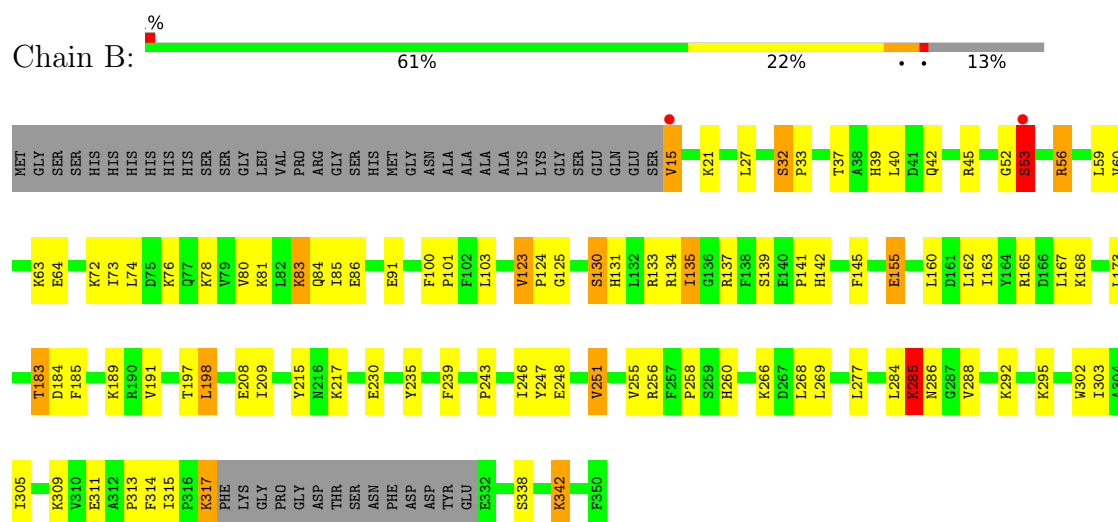
3 Residue-property plots [i](#)

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

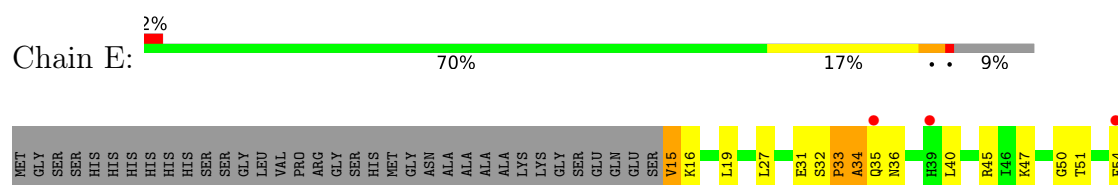
- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

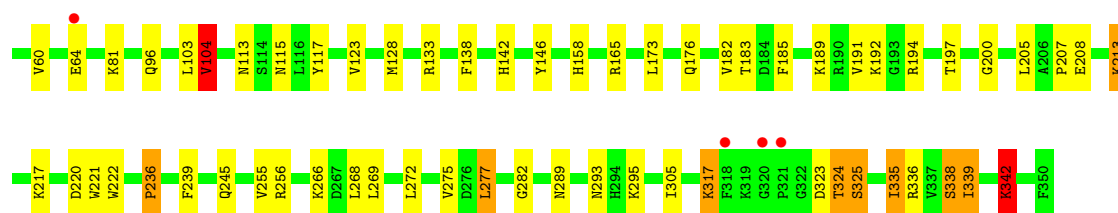


- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha



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





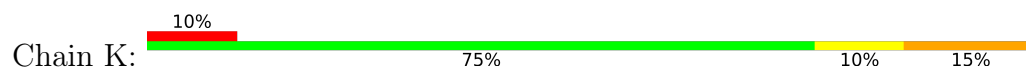
- Molecule 2: cAMP-dependent protein kinase inhibitor alpha



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 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.

²Theoretical 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	0.97	1/2829 (0.0%)	1.09	6/3810 (0.2%)
1	B	0.99	0/2712	1.11	5/3650 (0.1%)
1	E	0.96	0/2829	1.04	6/3810 (0.2%)
2	I	0.99	0/159	1.32	1/212 (0.5%)
2	J	1.03	0/159	1.18	0/212
2	K	1.05	0/159	1.43	1/212 (0.5%)
All	All	0.97	1/8847 (0.0%)	1.10	19/11906 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	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	335	ILE	CA-CB	5.21	1.58	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	VAL	CB-CA-C	-7.94	98.38	111.32
2	K	14	GLY	N-CA-C	7.91	122.22	112.73
1	A	335	ILE	CB-CA-C	-7.46	103.89	111.80
1	B	123	VAL	CA-C-N	7.28	128.94	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	VAL	C-N-CA	7.28	128.94	119.84
1	E	342	LYS	N-CA-C	6.13	120.84	112.68
1	E	165	ARG	N-CA-C	6.04	120.59	113.23
1	A	326	ASN	N-CA-C	5.85	119.89	112.87
1	B	183	THR	CB-CA-C	-5.72	100.55	111.48
1	B	155	GLU	N-CA-C	-5.46	105.41	111.36
1	E	31	GLU	N-CA-C	5.35	116.97	111.03
1	B	53	SER	N-CA-C	5.16	121.80	110.80
1	A	342	LYS	N-CA-C	5.13	120.19	113.88
2	I	22	ILE	N-CA-CB	5.13	117.28	110.26
1	A	242	GLN	CA-C-N	5.10	124.54	119.24
1	A	242	GLN	C-N-CA	5.10	124.54	119.24
1	E	104	VAL	CB-CA-C	-5.02	103.23	111.51
1	E	236	PRO	CA-C-N	5.00	124.66	119.56
1	E	236	PRO	C-N-CA	5.00	124.66	119.56

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	2764	43	0
1	B	2667	0	2674	56	0
1	E	2779	0	2764	36	0
2	I	157	0	146	5	0
2	J	157	0	146	6	0
2	K	157	0	146	4	0
3	A	16	0	15	4	0
3	E	16	0	15	5	0
4	A	75	0	0	8	0
4	B	73	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	63	0	0	7	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	8670	149	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 9.

All (149) 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
3:A:351:XFE:H5A	3:A:351:XFE:H15B	1.62	0.80
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
3:E:351:XFE:H15B	3:E:351:XFE:H3A	1.69	0.75
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
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
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
3:E:351:XFE:H15B	3:E:351:XFE:C3	2.28	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:B:317:LYS:C	4:B:366:HOH:O	2.45	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:B:56:ARG:NH1	2.02	0.58
1:E:128:MET:HE2	1:E:146:TYR:CD2	2.39	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
1:B:284:LEU:O	1:B:285:LYS:C	2.47	0.57
1:A:183:THR:HB	3:A:351:XFE:H15A	1.87	0.56
1:A:192:LYS:O	1:A:192:LYS:HG3	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: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:A:133:ARG:NH1	4:A:388:HOH:O	2.41	0.53
3:A:351:XFE:H15B	3:A:351:XFE:C5	2.34	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:E:104:VAL:CG2	1:E:183:THR:HG22	2.39	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:CD2	1:B:101:PRO:HD2	2.45	0.51
1:B:100:PHE:HB3	1:B:103:LEU:HD12	1.91	0.51
1:E:323:ASP:OD1	1:E:325:SER:OG	2.26	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
1:B:303:ILE:HD12	1:B:303:ILE:H	1.75	0.50
1:B:73:ILE:C	1:B:74:LEU:HD12	2.37	0.50
1:A:28:LYS:HA	1:A:28:LYS:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LEU:O	1:A:285:LYS:C	2.56	0.49
1:B:258:PRO:HB2	1:B:260:HIS:ND1	2.28	0.49
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
1:B:198:LEU:HD11	2:K:22:ILE:HD12	1.96	0.48
1:A:179:TYR:CZ	1:A:308:ARG:HA	2.50	0.47
1:B:198:LEU:HD11	2:K:22:ILE:CD1	2.45	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:100:PHE:CG	1:B:101:PRO:HD2	2.49	0.47
1:B:155:GLU:OE2	1:B:288:VAL:CG1	2.60	0.47
1:E:339:ILE:HD11	4:E:371:HOH:O	2.13	0.47
1:B:163:ILE:HG22	1:B:165:ARG:HG3	1.95	0.47
1:E:50:GLY:HA3	3:E:351:XFE:HN1A	1.78	0.47
1:E:338:SEP:OG	1:E:342:LYS:HE2	2.15	0.47
3:E:351:XFE:C15	3:E:351:XFE:H3	2.44	0.47
1:A:229:TYR:OH	1:A:256:ARG:O	2.31	0.46
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:A:58:MET:HE2	4:A:359:HOH:O	2.14	0.46
1:A:112:ASP:OD1	1:A:112:ASP:C	2.59	0.46
1:B:184:ASP:HB2	4:B:418:HOH:O	2.15	0.46
1:B:32:SER:N	1:B:33:PRO:HD3	2.31	0.45
2:I:23:HIS:CD2	2:I:24:ASP:H	2.34	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:A:222:TRP:CD1	1:A:222:TRP:C	2.94	0.45
1:E:207:PRO:HG2	1:E:275:VAL:HG23	1.97	0.45
1:E:317:LYS:HE3	1:E:317:LYS:HA	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:B:239:PHE:C	1:B:239:PHE:CD1	2.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LEU:HD12	1:A:190:ARG:HA	2.00	0.43
1:A:229:TYR:O	1:A:233:ALA:N	2.50	0.43
1:B:258:PRO:CB	1:B:260:HIS:CE1	3.01	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:HB2	1:E:213:LYS:NZ	2.34	0.43
2:J:7:TYR:CZ	2:J:11:ILE:HD13	2.53	0.43
1:A:126:GLY:HA2	1:A:327:PHE:CE1	2.54	0.42
1:A:323:ASP:HA	4:A:404:HOH:O	2.18	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:155:GLU:CD	1:B:288:VAL:HG11	2.45	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:203:GLU:OE2	2:J:15:ARG:HD3	2.20	0.42
1:A:244:ILE:HD11	1:E:133:ARG:O	2.19	0.42
1:A:342:LYS:HA	1:A:342:LYS:HD3	1.90	0.42
1:A:307:GLN:HE21	1:A:307:GLN:HB2	1.64	0.41
1:B:230:GLU:HA	1:B:235:TYR:O	2.20	0.41
1:B:139:SER:HB2	1:B:141:PRO:HD2	2.00	0.41
1:E:266:LYS:NZ	4:E:397:HOH:O	2.42	0.41
2:J:17:GLY:O	2:J:18:ARG:C	2.62	0.41
1:A:82:LEU:O	1:A:84:GLN:HG2	2.21	0.41
1:E:222:TRP:CD1	1:E:222:TRP:C	2.99	0.41
1:B:39:HIS:CD2	1:B:42:GLN:HG3	2.56	0.41
1:E:113:ASN:O	1:E:342:LYS:HB2	2.20	0.41
2:I:7:TYR:CE1	2:I:11:ILE:HD11	2.55	0.41
1:E:335:ILE:H	1:E:335:ILE:HG12	1.75	0.41
1:A:303:ILE:HD12	1:A:303:ILE:N	2.36	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:B:137:ARG:NE	1:B:260:HIS:HE2	2.19	0.41
1:B:155:GLU:CD	4:B:416:HOH:O	2.64	0.41
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:A:245:GLN:HE21	1:A:245:GLN:HB2	1.69	0.40
1:B:243:PRO:O	1:B:246:ILE:HB	2.22	0.40

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%)	21	38
1	B	316/371 (85%)	296 (94%)	17 (5%)	3 (1%)	14	27
1	E	332/371 (90%)	314 (95%)	14 (4%)	4 (1%)	10	20
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	27

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	295/321 (92%)	263 (89%)	32 (11%)	6	13
1	B	283/321 (88%)	241 (85%)	42 (15%)	3	6
1	E	295/321 (92%)	262 (89%)	33 (11%)	6	12
2	I	15/15 (100%)	12 (80%)	3 (20%)	1	2
2	J	15/15 (100%)	12 (80%)	3 (20%)	1	2
2	K	15/15 (100%)	12 (80%)	3 (20%)	1	2
All	All	918/1008 (91%)	802 (87%)	116 (13%)	4	9

All (116) residues with a non-rotameric sidechain are listed below:

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	60	VAL
1	A	74	LEU
1	A	81	LYS
1	A	104	VAL
1	A	105	LYS
1	A	133	ARG
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	268	LEU
1	A	269	LEU
1	A	272	LEU
1	A	285	LYS
1	A	295	LYS
1	A	331	GLU
1	A	335	ILE
1	A	336	ARG
1	A	340	ASN
1	A	341	GLU

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Mol	Chain	Res	Type
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
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	83	LYS
1	B	86	GLU
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	198	LEU
1	B	208	GLU
1	B	217	LYS
1	B	248	GLU
1	B	251	VAL
1	B	255	VAL
1	B	256	ARG
1	B	268	LEU
1	B	269	LEU
1	B	277	LEU
1	B	285	LYS
1	B	305	ILE
1	B	309	LYS
1	B	311	GLU
1	B	315	ILE

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Mol	Chain	Res	Type
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	81	LYS
1	E	104	VAL
1	E	176	GLN
1	E	192	LYS
1	E	194	ARG
1	E	213	LYS
1	E	217	LYS
1	E	245	GLN
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	305	ILE
1	E	317	LYS
1	E	324	THR
1	E	325	SER
1	E	335	ILE
1	E	336	ARG
1	E	339	ILE
1	E	342	LYS
2	I	15	ARG
2	I	22	ILE
2	I	23	HIS
2	J	11	ILE
2	J	22	ILE
2	J	23	HIS
2	K	15	ARG

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Mol	Chain	Res	Type
2	K	22	ILE
2	K	23	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	42	GLN
1	A	62	HIS
1	A	113	ASN
1	A	158	HIS
1	A	177	GLN
1	A	242	GLN
1	A	245	GLN
1	A	307	GLN
1	B	39	HIS
1	B	113	ASN
1	B	131	HIS
1	B	158	HIS
1	B	177	GLN
1	B	245	GLN
1	B	271	ASN
1	B	307	GLN
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	SEP	A	338	1	8,9,10	1.72	1 (12%)	7,12,14	1.74	2 (28%)
1	SEP	E	338	1	8,9,10	1.56	1 (12%)	7,12,14	2.58	3 (42%)
1	TPO	A	197	1	8,10,11	0.40	0	10,14,16	1.03	0
1	TPO	E	197	1	8,10,11	0.95	0	10,14,16	1.29	2 (20%)
1	TPO	B	197	1	8,10,11	0.54	0	10,14,16	1.01	1 (10%)
1	SEP	B	338	1	8,9,10	1.45	1 (12%)	7,12,14	2.44	4 (57%)

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

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

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	A	338	SEP	O3P-P-OG	2.51	113.22	106.67
1	E	197	TPO	CG2-CB-CA	-2.43	108.54	113.26
1	B	338	SEP	OG-CB-CA	2.36	110.44	108.14
1	B	338	SEP	O2P-P-OG	2.35	112.81	106.67
1	B	197	TPO	O3P-P-O2P	2.32	116.51	107.80
1	E	197	TPO	O3P-P-O2P	2.23	116.16	107.80
1	E	338	SEP	O2P-P-O1P	-2.04	102.87	110.83

There are no chirality outliers.

All (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
1	E	197	TPO	O-C-CA-CB
1	E	338	SEP	C-CA-CB-OG
1	B	338	SEP	CA-CB-OG-P
1	E	338	SEP	CA-CB-OG-P
1	B	338	SEP	CB-OG-P-O1P
1	A	338	SEP	N-CA-CB-OG
1	E	338	SEP	N-CA-CB-OG
1	A	197	TPO	CB-OG1-P-O3P

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

There are no oligosaccharides 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	1.00	1 (5%)	17,26,26	3.56	11 (64%)
3	XFE	E	351	-	18,18,18	0.87	0	17,26,26	4.00	10 (58%)

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	-	-	1/4/13/13	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	351	XFE	C6-N4	2.24	1.43	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	351	XFE	C11-N12-C13	8.40	112.44	108.48
3	E	351	XFE	C10-C11-N9	-7.09	119.08	126.64
3	A	351	XFE	C11-C10-C14	-7.08	102.11	106.83
3	E	351	XFE	C11-C10-C14	-5.79	102.97	106.83
3	A	351	XFE	C6-C10-C11	5.62	120.20	115.61
3	A	351	XFE	C10-C11-N9	-5.22	121.08	126.64
3	A	351	XFE	C8-N7-C6	5.07	124.22	111.83
3	A	351	XFE	C11-N12-C13	4.96	110.82	108.48
3	E	351	XFE	C6-C10-C11	4.72	119.47	115.61
3	E	351	XFE	N9-C8-N7	-4.65	121.54	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	351	XFE	C8-N7-C6	4.27	122.25	111.83
3	A	351	XFE	N9-C8-N7	-3.76	122.89	128.58
3	E	351	XFE	C14-C13-N12	-3.52	105.81	109.50
3	A	351	XFE	C10-C6-N4	3.42	128.17	122.08
3	E	351	XFE	N12-C11-N9	3.24	131.94	126.69
3	E	351	XFE	C5-N4-C6	-3.14	114.47	123.60
3	E	351	XFE	C2-C1-C5	2.85	106.74	102.20
3	A	351	XFE	C15-C14-C13	-2.75	122.49	126.14
3	A	351	XFE	C3-N4-C6	-2.60	116.09	123.53
3	A	351	XFE	C6-C10-C14	2.05	137.68	134.28
3	A	351	XFE	C14-C13-N12	-2.01	107.40	109.50

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	351	XFE	N7-C6-N4-C3

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	351	XFE	4	0
3	E	351	XFE	5	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, 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	334/371 (90%)	-0.22	3 (0%) 81 78	11, 23, 44, 59	0
1	B	320/371 (86%)	-0.21	2 (0%) 85 83	13, 25, 41, 49	0
1	E	334/371 (90%)	-0.12	7 (2%) 63 59	11, 24, 48, 65	0
2	I	20/20 (100%)	-0.01	2 (10%) 12 10	12, 21, 56, 56	0
2	J	20/20 (100%)	-0.15	1 (5%) 34 30	13, 20, 51, 52	0
2	K	20/20 (100%)	0.16	2 (10%) 12 10	18, 26, 41, 46	0
All	All	1048/1173 (89%)	-0.17	17 (1%) 70 67	11, 24, 44, 65	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	320	GLY	4.0
1	A	15	VAL	3.7
1	E	318	PHE	3.7
1	A	335	ILE	3.2
2	K	24	ASP	3.0
1	B	15	VAL	3.0
1	E	321	PRO	3.0
1	E	54	PHE	2.6
2	I	23	HIS	2.6
1	E	64	GLU	2.5
1	A	285	LYS	2.4
2	J	23	HIS	2.3
2	K	23	HIS	2.3
1	B	53	SER	2.2
1	E	39	HIS	2.2
1	E	35	GLN	2.1
2	I	22	ILE	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. 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	RSCC	RSR	B-factors(Å ²)	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
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 oligosaccharides 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, 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	RSCC	RSR	B-factors(Å 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.