



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:56 PM GMT

PDB ID : 4GKH
Title : Crystal structure of the aminoglycoside phosphotransferase APH(3')-Ia, with substrate kanamycin and small molecule inhibitor 1-NA-PP1
Authors : Stogios, P.J.; Evdokimova, E.; Wawrzak, Z.; Minasov, G.; Egorova, O.; Di Leo, R.; Shakya, T.; Spanogiannopoulos, P.; Todorovic, N.; Capretta, A.; Wright, G.D.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2012-08-11
Resolution : 1.86 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

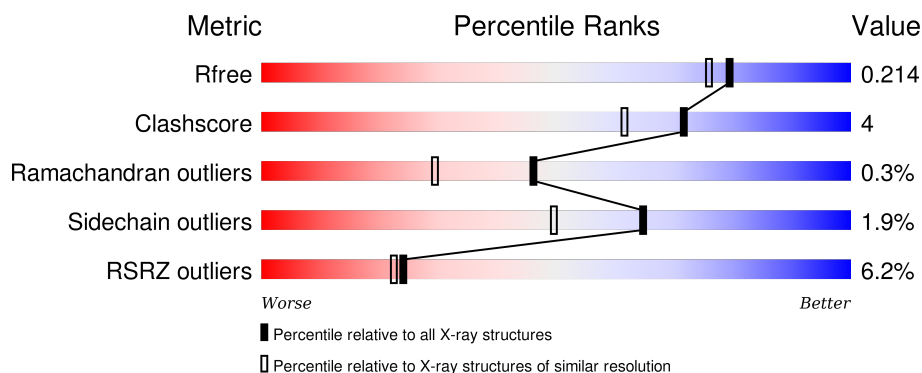
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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. 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	272	<div> <div>88%</div> <div>6% 7%</div> </div>
1	B	272	<div> <div>4%</div> <div>93%</div> <div>6%</div> </div>
1	C	272	<div> <div>6%</div> <div>90%</div> <div>6%</div> </div>
1	D	272	<div> <div>11%</div> <div>87%</div> <div>10%</div> </div>
1	E	272	<div> <div>4%</div> <div>90%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	272	
1	G	272	
1	H	272	
1	I	272	
1	J	272	
1	K	272	
1	L	272	

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	0J9	B	302	-	-	-	X
3	0J9	G	302	-	-	-	X
4	NA	F	304	-	-	-	X
4	NA	G	304	-	-	-	X
4	NA	K	304	-	-	-	X
4	NA	L	303	-	-	-	X
5	ACT	A	304	-	-	-	X
5	ACT	C	306	-	-	-	X
5	ACT	D	305	-	-	-	X
5	ACT	E	304	-	-	-	X
5	ACT	H	304	-	-	-	X
5	ACT	I	306	-	-	-	X
5	ACT	K	306	-	-	-	X
5	ACT	K	307	-	-	-	X
5	ACT	L	304	-	-	X	-
5	ACT	L	306	-	-	-	X
7	PEG	D	306	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 29502 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 Aminoglycoside 3'-phosphotransferase AphA1-IAB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	Se	0	5	0
			2065	1325	350	380	4	6			
1	B	268	Total	C	N	O	S	Se	0	7	0
			2209	1404	385	408	5	7			
1	C	267	Total	C	N	O	S	Se	0	3	0
			2164	1377	374	402	5	6			
1	D	265	Total	C	N	O	S	Se	0	2	0
			2152	1371	374	396	5	6			
1	E	261	Total	C	N	O	S	Se	0	4	0
			2119	1354	364	391	4	6			
1	F	271	Total	C	N	O	S	Se	0	7	0
			2220	1412	385	411	5	7			
1	G	267	Total	C	N	O	S	Se	0	4	0
			2169	1382	374	401	5	7			
1	H	255	Total	C	N	O	S	Se	0	4	0
			2065	1322	350	383	4	6			
1	I	266	Total	C	N	O	S	Se	0	2	0
			2152	1369	374	398	5	6			
1	J	267	Total	C	N	O	S	Se	0	2	0
			2164	1379	374	399	5	7			
1	K	269	Total	C	N	O	S	Se	0	5	0
			2194	1398	379	405	5	7			
1	L	254	Total	C	N	O	S	Se	0	2	0
			2052	1314	349	379	4	6			

There are 12 discrepancies between the modelled and reference sequences:

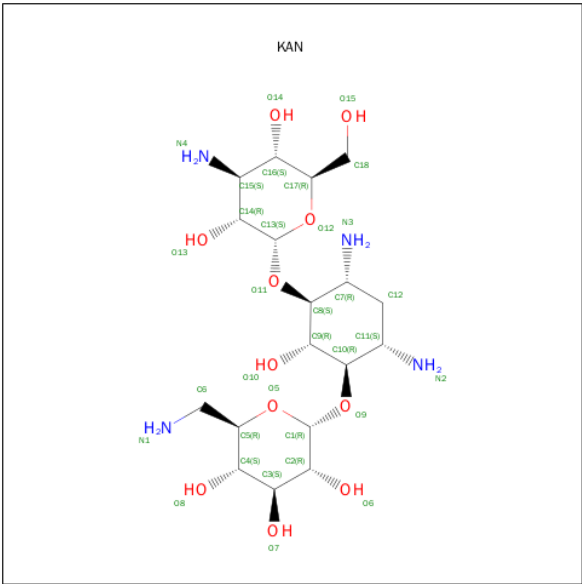
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP B0VD92
B	0	GLY	-	EXPRESSION TAG	UNP B0VD92
C	0	GLY	-	EXPRESSION TAG	UNP B0VD92
D	0	GLY	-	EXPRESSION TAG	UNP B0VD92
E	0	GLY	-	EXPRESSION TAG	UNP B0VD92

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	GLY	-	EXPRESSION TAG	UNP B0VD92
G	0	GLY	-	EXPRESSION TAG	UNP B0VD92
H	0	GLY	-	EXPRESSION TAG	UNP B0VD92
I	0	GLY	-	EXPRESSION TAG	UNP B0VD92
J	0	GLY	-	EXPRESSION TAG	UNP B0VD92
K	0	GLY	-	EXPRESSION TAG	UNP B0VD92
L	0	GLY	-	EXPRESSION TAG	UNP B0VD92

- Molecule 2 is KANAMYCIN A (three-letter code: KAN) (formula: C₁₈H₃₆N₄O₁₁).



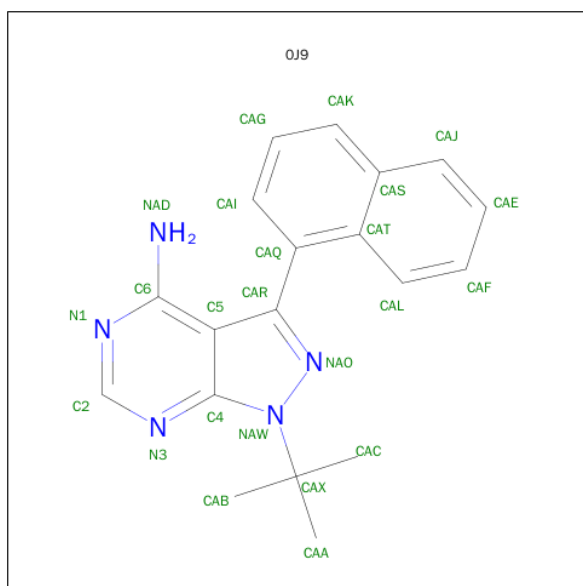
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	18	4	11		
2	B	1	Total	C	N	O	0	0
			33	18	4	11		
2	C	1	Total	C	N	O	0	0
			33	18	4	11		
2	D	1	Total	C	N	O	0	0
			33	18	4	11		
2	E	1	Total	C	N	O	0	0
			33	18	4	11		
2	F	1	Total	C	N	O	0	0
			33	18	4	11		
2	G	1	Total	C	N	O	0	0
			33	18	4	11		
2	H	1	Total	C	N	O	0	0
			33	18	4	11		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	I	1	Total	C	N	O	0	0
			33	18	4	11		
2	J	1	Total	C	N	O	0	0
			33	18	4	11		
2	K	1	Total	C	N	O	0	0
			33	18	4	11		
2	L	1	Total	C	N	O	0	0
			33	18	4	11		

- Molecule 3 is 1-TERT-BUTYL-3-(NAPHTHALEN-1-YL)-1H-PYRAZOLO[3,4-D]PYRIMIDIN-4-AMINE (three-letter code: OJ9) (formula: C₁₉H₁₉N₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N		0	0
			24	19	5			
3	B	1	Total	C	N		0	0
			24	19	5			
3	C	1	Total	C	N		0	0
			24	19	5			
3	C	1	Total	C	N		0	0
			24	19	5			
3	E	1	Total	C	N		0	0
			24	19	5			
3	F	1	Total	C	N		0	0
			24	19	5			
3	G	1	Total	C	N		0	0
			24	19	5			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	N	0	0
			24	19	5		
3	I	1	Total	C	N	0	0
			24	19	5		
3	J	1	Total	C	N	0	0
			24	19	5		
3	K	1	Total	C	N	0	0
			24	19	5		
3	L	1	Total	C	N	0	0
			24	19	5		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	2	Total	Na	0	0
			2	2		
4	K	2	Total	Na	0	0
			2	2		
4	E	1	Total	Na	0	0
			1	1		
4	H	1	Total	Na	0	0
			1	1		
4	B	2	Total	Na	0	0
			2	2		
4	I	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		
4	A	1	Total	Na	0	0
			1	1		
4	L	1	Total	Na	0	0
			1	1		
4	F	2	Total	Na	0	0
			2	2		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	G	1	Total 4	C 2	O 2	0	0
5	G	1	Total 4	C 2	O 2	0	0
5	G	1	Total 4	C 2	O 2	0	0
5	H	1	Total 4	C 2	O 2	0	0
5	H	1	Total 4	C 2	O 2	0	0
5	I	1	Total 4	C 2	O 2	0	0
5	I	1	Total 4	C 2	O 2	0	0
5	I	1	Total 4	C 2	O 2	0	0
5	J	1	Total 4	C 2	O 2	0	0
5	K	1	Total 4	C 2	O 2	0	0
5	K	1	Total 4	C 2	O 2	0	0
5	K	1	Total 4	C 2	O 2	0	0
5	L	1	Total 4	C 2	O 2	0	0
5	L	1	Total 4	C 2	O 2	0	0
5	L	1	Total 4	C 2	O 2	0	0
5	L	1	Total 4	C 2	O 2	0	0

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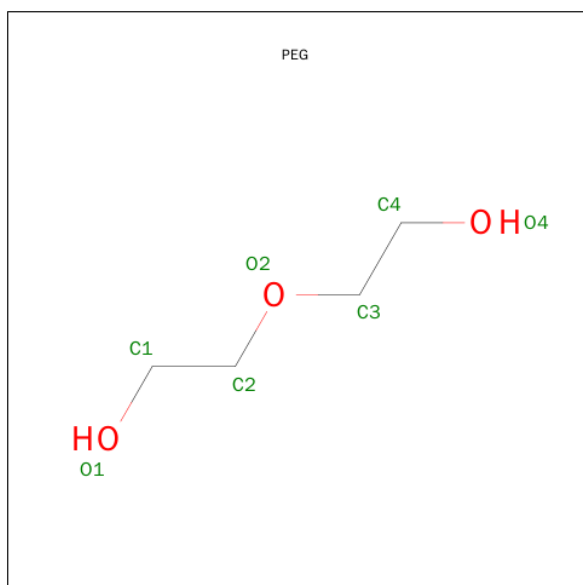
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	I	1	Total	Cl		0	0
			1	1			
6	C	1	Total	Cl		0	0
			1	1			

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			7	4	3		
7	D	1	Total	C	O	0	0
			7	4	3		
7	H	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	261	Total	O		0	2
			263	263			

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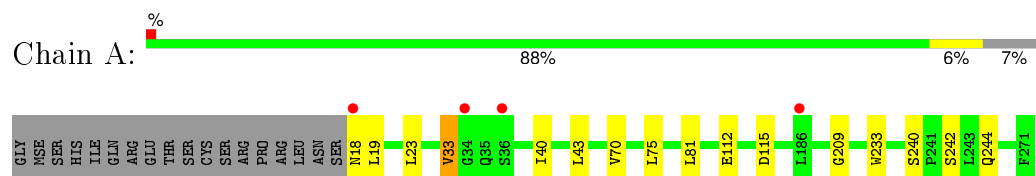
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	252	Total 255	O 255	0	4
8	D	183	Total 185	O 185	0	3
8	G	254	Total 258	O 258	0	4
8	C	245	Total 247	O 247	0	2
8	K	259	Total 263	O 263	0	4
8	E	256	Total 265	O 265	0	9
8	F	245	Total 247	O 247	0	4
8	H	226	Total 230	O 230	0	4
8	I	274	Total 276	O 276	0	2
8	J	153	Total 156	O 156	0	3
8	L	262	Total 267	O 267	0	5

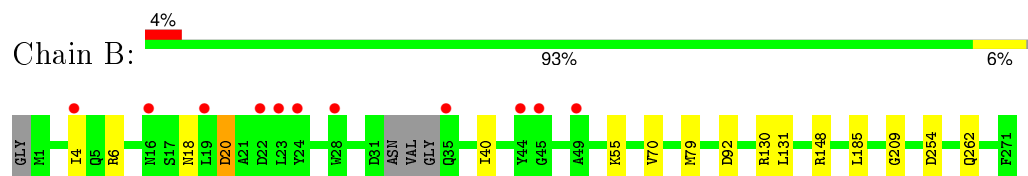
3 Residue-property plots [i](#)

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

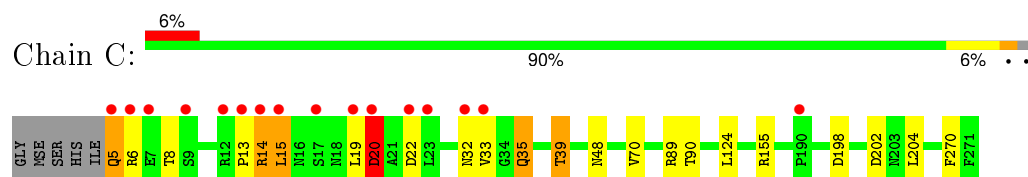
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



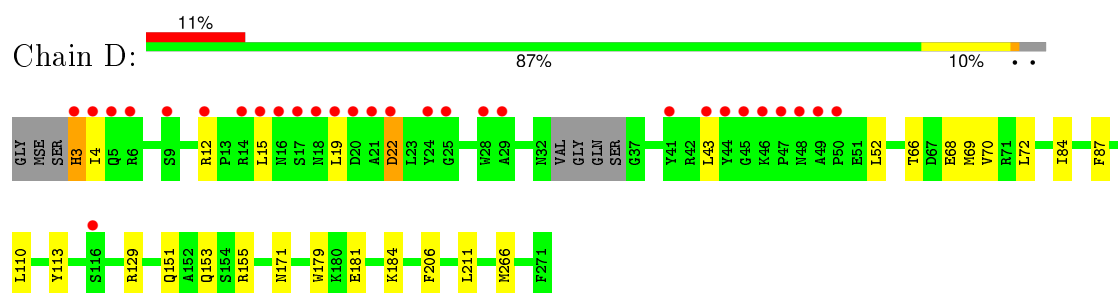
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



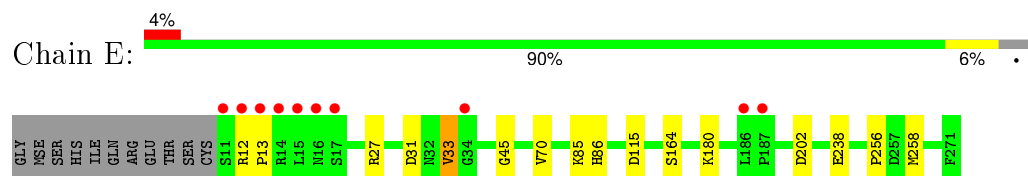
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



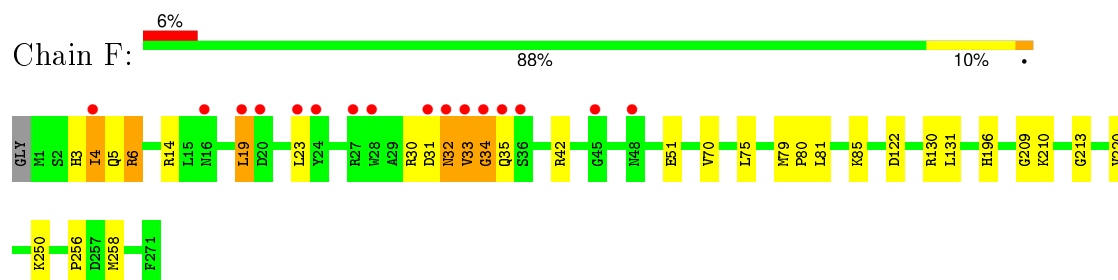
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



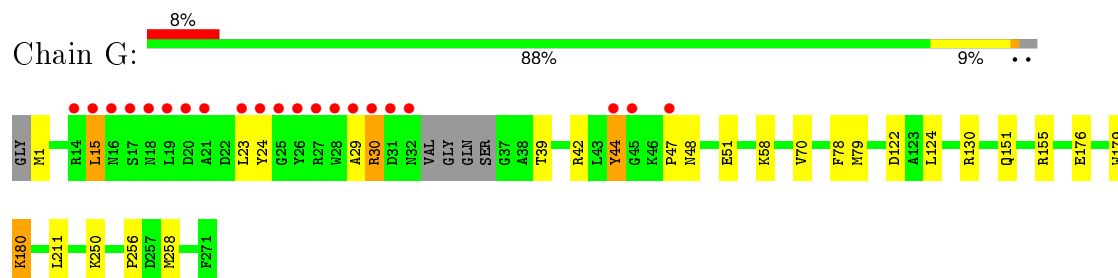
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



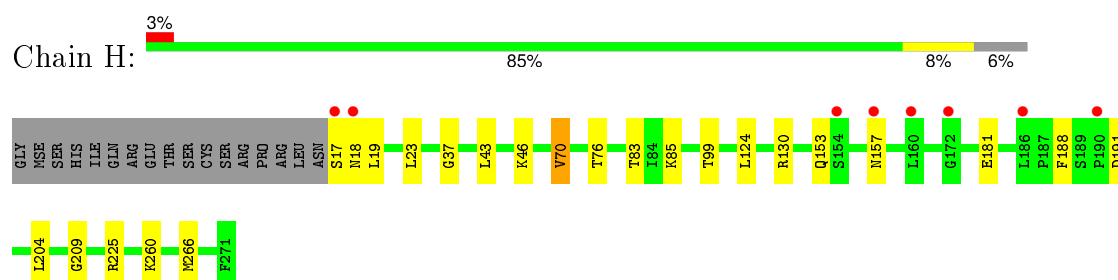
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



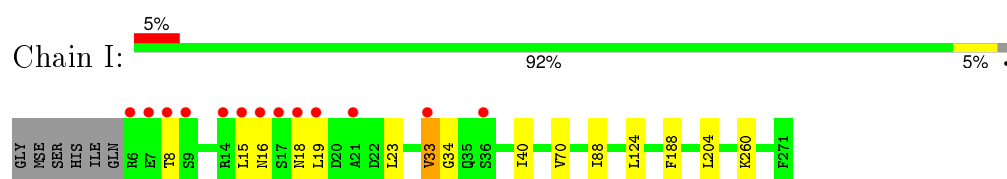
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



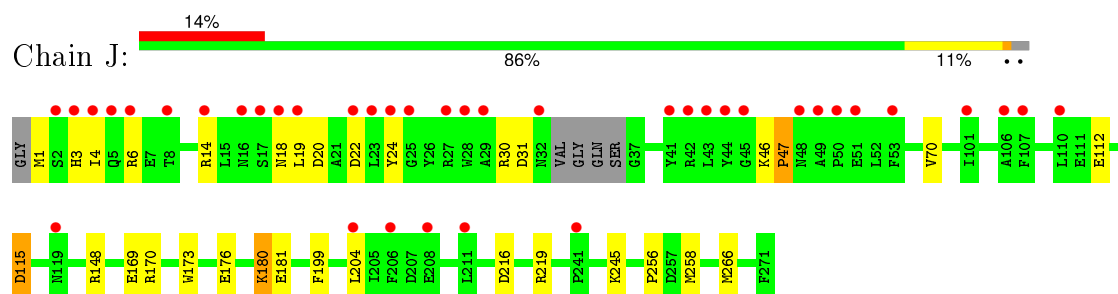
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



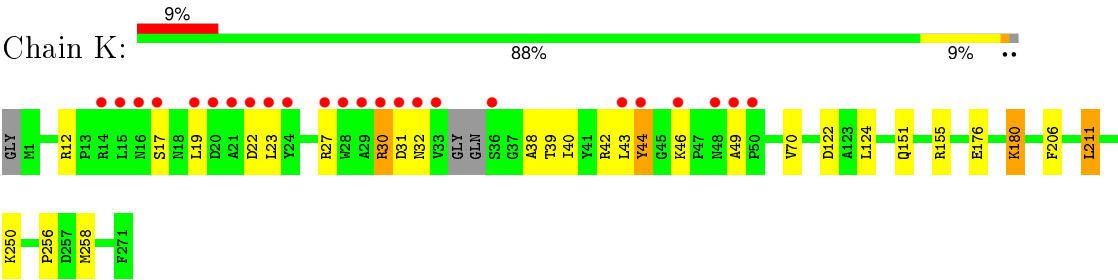
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



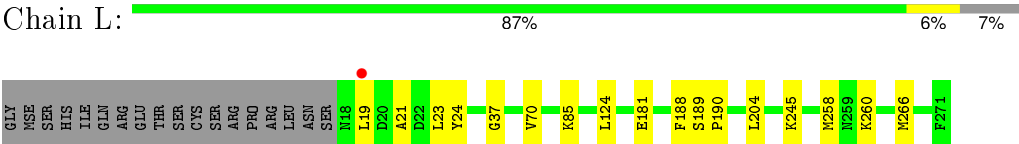
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



● Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	97.19Å 97.30Å 112.74Å 102.97° 106.21° 112.66°	Depositor
Resolution (Å)	54.78 – 1.86 80.87 – 1.86	Depositor EDS
% Data completeness (in resolution range)	94.6 (54.78-1.86) 76.6 (80.87-1.86)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 1.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.164 , 0.216 0.163 , 0.214	Depositor DCC
R_{free} test set	13946 reflections (5.60%)	DCC
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.2	EDS
Estimated twinning fraction	0.000 for k,h,-h-k-l 0.009 for -k,-h,-l 0.000 for -h,-k,h+k+l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 268419 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	29502	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 82.06 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.0598e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: CL, NA, KAN, 0J9, ACT, PEG

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	0.39	0/2125	0.54	0/2876
1	B	0.36	0/2270	0.51	0/3066
1	C	0.38	0/2219	0.56	0/3001
1	D	0.33	0/2204	0.50	0/2981
1	E	0.39	0/2177	0.54	0/2946
1	F	0.38	0/2287	0.52	0/3091
1	G	0.36	0/2230	0.52	0/3014
1	H	0.37	0/2125	0.53	0/2876
1	I	0.39	0/2207	0.54	0/2984
1	J	0.30	0/2219	0.48	0/2999
1	K	0.38	0/2255	0.51	0/3047
1	L	0.39	0/2106	0.53	0/2850
All	All	0.37	0/26424	0.52	0/35731

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2065	0	2016	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2209	0	2150	10	0
1	C	2164	0	2100	20	0
1	D	2152	0	2089	22	0
1	E	2119	0	2064	12	0
1	F	2220	0	2166	23	0
1	G	2169	0	2113	16	0
1	H	2065	0	2007	15	0
1	I	2152	0	2090	15	0
1	J	2164	0	2106	19	0
1	K	2194	0	2142	19	0
1	L	2052	0	1990	12	0
2	A	33	0	36	0	0
2	B	33	0	36	0	0
2	C	33	0	36	0	0
2	D	33	0	36	0	0
2	E	33	0	36	0	0
2	F	33	0	36	0	0
2	G	33	0	36	0	0
2	H	33	0	36	0	0
2	I	33	0	36	0	0
2	J	33	0	36	0	0
2	K	33	0	36	1	0
2	L	33	0	36	0	0
3	A	24	0	19	5	0
3	B	24	0	19	4	0
3	C	48	0	38	8	0
3	E	24	0	19	5	0
3	F	24	0	19	5	0
3	G	24	0	19	4	0
3	H	24	0	19	4	0
3	I	24	0	19	5	0
3	J	24	0	19	5	0
3	K	24	0	19	4	0
3	L	24	0	19	4	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	2	0	0	0	0
4	L	1	0	0	0	0
5	A	12	0	9	1	0
5	B	8	0	6	1	0
5	C	12	0	9	0	0
5	D	16	0	12	0	0
5	E	12	0	9	1	0
5	F	16	0	12	1	0
5	G	12	0	9	0	0
5	H	8	0	6	1	0
5	I	12	0	9	0	0
5	J	4	0	3	0	0
5	K	12	0	9	1	0
5	L	20	0	15	3	0
6	C	1	0	0	0	0
6	I	1	0	0	0	0
7	D	14	0	16	2	0
7	H	7	0	8	1	0
8	A	263	0	0	2	0
8	B	255	0	0	1	0
8	C	247	0	0	2	0
8	D	185	0	0	2	0
8	E	265	0	0	2	0
8	F	247	0	0	1	0
8	G	258	0	0	0	0
8	H	230	0	0	2	0
8	I	276	0	0	1	0
8	J	156	0	0	1	0
8	K	263	0	0	2	0
8	L	267	0	0	1	0
All	All	29502	0	25825	225	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 4.

All (225) 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)
3:G:302:0J9:H12	3:G:302:0J9:H15	1.06	1.07
3:K:302:0J9:H15	3:K:302:0J9:H12	1.16	1.06
3:F:302:0J9:H12	3:F:302:0J9:H15	1.25	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:VAL:HG11	1:D:70[B]:VAL:HG21	1.42	1.01
3:B:302:0J9:H12	3:B:302:0J9:H15	1.26	1.00
3:J:302:0J9:H12	3:J:302:0J9:H15	1.29	0.95
1:I:70:VAL:HG11	1:J:70[B]:VAL:HG21	1.46	0.95
1:A:209:GLY:HA2	5:A:304:ACT:H2	1.52	0.91
1:G:79:MSE:HE1	1:G:130:ARG:HG2	1.54	0.90
3:G:302:0J9:H15	3:G:302:0J9:NAD	1.86	0.88
3:K:302:0J9:NAD	3:K:302:0J9:H15	1.91	0.86
3:I:302:0J9:H15	3:I:302:0J9:H12	1.39	0.86
3:C:302:0J9:H12	3:C:302:0J9:H15	1.40	0.85
3:C:303:0J9:H15	3:C:303:0J9:H12	1.42	0.83
3:F:302:0J9:CAI	3:F:302:0J9:H12	1.94	0.81
3:K:302:0J9:CAI	3:K:302:0J9:H12	1.93	0.81
3:B:302:0J9:H12	3:B:302:0J9:CAI	1.94	0.81
3:C:303:0J9:CAI	3:C:303:0J9:H12	1.95	0.80
3:F:302:0J9:NAD	3:F:302:0J9:H15	1.97	0.80
3:J:302:0J9:H12	3:J:302:0J9:CAI	1.95	0.80
3:B:302:0J9:H15	3:B:302:0J9:NAD	1.97	0.80
3:C:302:0J9:CAI	3:C:302:0J9:H12	1.95	0.79
3:J:302:0J9:NAD	3:J:302:0J9:H15	2.00	0.76
3:I:302:0J9:H12	3:I:302:0J9:CAI	1.98	0.75
3:G:302:0J9:H12	3:G:302:0J9:CAI	1.96	0.73
3:A:302:0J9:CAI	3:A:302:0J9:H12	2.03	0.71
3:C:302:0J9:NAD	3:C:302:0J9:H15	2.06	0.71
3:A:302:0J9:H15	3:A:302:0J9:H12	1.54	0.71
3:G:302:0J9:NAO	3:G:302:0J9:H18	2.07	0.70
1:K:70:VAL:HG11	1:L:70[A]:VAL:HG11	1.73	0.70
3:E:302:0J9:CAI	3:E:302:0J9:H12	2.05	0.70
3:I:302:0J9:H15	3:I:302:0J9:NAD	2.07	0.69
3:H:302:0J9:CAI	3:H:302:0J9:H12	2.07	0.68
3:E:302:0J9:H12	3:E:302:0J9:H15	1.58	0.67
3:C:303:0J9:NAD	3:C:303:0J9:H15	2.09	0.67
1:I:33:VAL:HB	1:I:40:ILE:HD12	1.77	0.66
3:K:302:0J9:H18	3:K:302:0J9:NAO	2.09	0.66
3:J:302:0J9:H18	3:J:302:0J9:NAO	2.11	0.66
3:B:302:0J9:H18	3:B:302:0J9:NAO	2.11	0.65
3:F:302:0J9:NAO	3:F:302:0J9:H18	2.12	0.65
3:I:302:0J9:NAO	3:I:302:0J9:H18	2.12	0.65
3:C:303:0J9:H18	3:C:303:0J9:NAO	2.11	0.65
1:I:70:VAL:HG11	1:J:70[A]:VAL:HG11	1.77	0.64
3:L:302:0J9:CAI	3:L:302:0J9:H12	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:176:GLU:O	1:K:180:LYS:HD2	1.99	0.63
1:C:19:LEU:HD12	1:D:15:LEU:HD21	1.81	0.62
1:H:85:LYS:NZ	8:H:622:HOH:O	2.32	0.62
1:D:22:ASP:OD1	1:D:22:ASP:N	2.32	0.62
1:G:179:TRP:HD1	1:G:180:LYS:HE3	1.64	0.62
3:C:302:0J9:H18	3:C:302:0J9:NAO	2.12	0.62
1:J:4:ILE:HG23	1:J:6:ARG:HG3	1.82	0.61
1:L:124:LEU:HD22	1:L:204:LEU:HD13	1.83	0.61
1:F:4:ILE:HG23	1:F:6:ARG:HD3	1.83	0.61
1:D:129:ARG:HG2	7:D:306:PEG:H41	1.83	0.61
1:L:258:MSE:HE3	5:L:307:ACT:H1	1.82	0.61
1:I:33:VAL:HG12	1:I:34:GLY:HA2	1.82	0.60
3:H:302:0J9:H15	3:H:302:0J9:H12	1.66	0.60
1:H:83:THR:H	1:H:99[B]:THR:HG22	1.67	0.59
3:L:302:0J9:H15	3:L:302:0J9:H12	1.68	0.59
1:C:70:VAL:HG11	1:D:70[A]:VAL:HG11	1.83	0.59
1:K:256:PRO:HB2	1:K:258:MSE:HE2	1.84	0.59
1:F:209:GLY:HA2	5:F:305:ACT:H3	1.85	0.59
3:A:302:0J9:H18	3:A:302:0J9:NAO	2.17	0.58
1:G:124:LEU:HD23	1:G:211:LEU:HD11	1.85	0.58
1:I:124:LEU:HD22	1:I:204:LEU:HD13	1.84	0.58
3:A:302:0J9:H15	3:A:302:0J9:NAD	2.18	0.57
1:G:70:VAL:HG11	1:H:70[A]:VAL:HG11	1.86	0.56
1:E:70:VAL:HG11	1:F:70[A]:VAL:HG11	1.86	0.56
1:G:256:PRO:HB2	1:G:258:MSE:CE	2.35	0.56
1:E:256:PRO:HB2	1:E:258:MSE:CE	2.36	0.56
1:C:124:LEU:HD22	1:C:204:LEU:HD13	1.88	0.56
1:C:202:ASP:OD1	1:D:3:HIS:HB3	2.06	0.56
1:B:79:MSE:SE	1:B:130[A]:ARG:HG2	2.56	0.55
1:G:176:GLU:O	1:G:180:LYS:HD2	2.06	0.55
1:L:181:GLU:HB2	1:L:266:MSE:HE1	1.89	0.55
1:F:256:PRO:HB2	1:F:258:MSE:CE	2.37	0.54
3:E:302:0J9:NAD	3:E:302:0J9:H15	2.22	0.54
1:E:202:ASP:OD1	1:F:3:HIS:HD2	1.91	0.54
1:K:155:ARG:NH2	8:K:657:HOH:O	2.33	0.53
3:E:302:0J9:NAO	3:E:302:0J9:H18	2.22	0.53
1:J:176:GLU:O	1:J:180:LYS:HD2	2.09	0.53
1:I:19:LEU:HG	1:I:23:LEU:HD11	1.91	0.53
3:L:302:0J9:H18	3:L:302:0J9:NAO	2.23	0.53
1:K:31:ASP:HB3	1:K:40:ILE:HB	1.91	0.53
1:J:115:ASP:OD1	1:J:115:ASP:N	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:VAL:HG11	1:B:70[A]:VAL:HG11	1.91	0.53
1:C:14:ARG:HA	1:C:15:LEU:CB	2.39	0.52
1:C:48:ASN:ND2	8:C:561:HOH:O	2.43	0.52
1:B:20:ASP:N	1:B:20:ASP:OD1	2.42	0.52
1:G:42:ARG:HD2	1:G:44:TYR:CE2	2.44	0.52
1:G:78:PHE:O	1:G:79:MSE:HE2	2.10	0.52
1:I:15:LEU:HD13	1:J:19:LEU:HD23	1.90	0.52
1:H:124:LEU:HD22	1:H:204:LEU:HD13	1.91	0.51
1:B:40:ILE:HG12	1:B:55:LYS:HG2	1.92	0.51
1:A:18:ASN:HD21	1:B:18:ASN:HD21	1.58	0.51
1:K:124:LEU:HD23	1:K:211:LEU:HD21	1.93	0.51
1:K:27:ARG:HB3	1:K:44:TYR:CD1	2.45	0.51
1:I:33:VAL:CB	1:I:34:GLY:HA2	2.40	0.51
1:J:169[A]:GLU:CD	1:J:169[A]:GLU:H	2.14	0.51
1:K:46:LYS:HB3	1:K:49:ALA:HB3	1.93	0.51
1:D:171:ASN:ND2	8:D:493[B]:HOH:O	2.43	0.50
3:H:302:OJ9:H18	3:H:302:OJ9:NAO	2.27	0.50
1:C:39:THR:HG21	8:C:614:HOH:O	2.11	0.50
1:A:75:LEU:HB3	1:A:81:LEU:HD11	1.94	0.50
1:C:19:LEU:O	1:C:22:ASP:N	2.45	0.49
1:A:19:LEU:HG	1:A:23:LEU:HD11	1.95	0.49
1:D:113:TYR:CD2	7:D:307:PEG:H11	2.47	0.49
1:C:20:ASP:HA	1:D:12:ARG:HH22	1.77	0.49
3:H:302:OJ9:NAD	3:H:302:OJ9:H15	2.27	0.49
1:G:30:ARG:CZ	1:G:39:THR:HG23	2.42	0.49
1:H:191:ASP:OD2	1:H:225:ARG:NE	2.29	0.49
1:L:188:PHE:CD1	1:L:260:LYS:HE2	2.49	0.48
1:K:27:ARG:N	1:K:44:TYR:O	2.38	0.48
1:I:70:VAL:HG11	1:J:70[B]:VAL:CG2	2.32	0.48
1:A:115:ASP:HB2	8:A:440:HOH:O	2.14	0.48
1:F:42:ARG:NH1	1:F:51:GLU:OE1	2.38	0.48
1:K:42:ARG:NH2	1:K:44:TYR:OH	2.46	0.48
1:H:23:LEU:HD22	1:H:43:LEU:HD22	1.96	0.48
1:H:188:PHE:HB3	1:L:24:TYR:CE1	2.48	0.47
1:I:33:VAL:CG1	1:I:34:GLY:HA2	2.44	0.47
1:C:14:ARG:HA	1:C:15:LEU:HB2	1.95	0.47
1:H:19:LEU:O	1:H:23:LEU:HG	2.14	0.47
1:K:38:ALA:HA	5:K:307:ACT:O	2.14	0.47
1:A:240:SER:HG	1:A:242[A]:SER:HG	1.61	0.47
1:L:85:LYS:HE3	1:L:85:LYS:HB3	1.70	0.46
1:I:18:ASN:ND2	1:J:18:ASN:OD1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:21:ALA:HA	5:L:304:ACT:H2	1.97	0.46
1:H:153:GLN:NE2	1:H:157:ASN:HD22	2.13	0.46
1:G:29:ALA:HB3	1:G:42:ARG:HB3	1.98	0.46
1:C:89:ARG:NH1	1:C:90:THR:O	2.48	0.46
1:G:122:ASP:OD1	1:G:250:LYS:HG3	2.15	0.46
1:C:155:ARG:HD3	1:C:270:PHE:O	2.15	0.46
1:D:181:GLU:HB2	1:D:266:MSE:HE1	1.98	0.46
1:I:188:PHE:CD1	1:I:260:LYS:HE2	2.51	0.46
1:B:4:ILE:HG23	1:B:6:ARG:HG3	1.97	0.45
1:J:46:LYS:HA	1:J:47:PRO:HD2	1.68	0.45
3:L:302:OJ9:H15	3:L:302:OJ9:NAD	2.30	0.45
1:J:256:PRO:HB2	1:J:258:MSE:HE3	1.98	0.45
1:E:12:ARG:HA	1:E:13:PRO:HD3	1.79	0.45
1:C:5:GLN:HB2	1:C:6:ARG:H	1.66	0.45
3:I:302:OJ9:NAO	3:I:302:OJ9:CAL	2.80	0.45
1:G:256:PRO:HB2	1:G:258:MSE:HE3	1.99	0.45
1:E:164:SER:O	8:E:577:HOH:O	2.21	0.45
1:D:184:LYS:NZ	8:D:580:HOH:O	2.47	0.45
1:L:24:TYR:CB	5:L:304:ACT:H1	2.47	0.44
1:F:34:GLY:O	1:F:35:GLN:HG2	2.17	0.44
1:J:14:ARG:NH2	8:J:509:HOH:O	2.46	0.44
1:K:256:PRO:HB2	1:K:258:MSE:CE	2.46	0.44
1:C:15:LEU:HD13	1:C:15:LEU:HA	1.80	0.44
1:D:66:THR:O	1:D:70[B]:VAL:HG23	2.18	0.44
1:F:32:ASN:N	1:F:32:ASN:OD1	2.50	0.44
1:A:40:ILE:HD13	3:A:302:OJ9:H7	2.00	0.43
1:G:44:TYR:HB3	1:G:51:GLU:HG3	2.00	0.43
1:J:181:GLU:HB2	1:J:266:MSE:HE1	1.99	0.43
1:K:12:ARG:NH2	8:K:588:HOH:O	2.48	0.43
1:A:233:TRP:NE1	1:A:244:GLN:HB3	2.33	0.43
1:K:122:ASP:OD1	1:K:250:LYS:HG3	2.18	0.43
1:I:8:THR:O	1:J:30:ARG:N	2.52	0.43
1:E:86:HIS:HD2	8:E:650:HOH:O	2.02	0.43
1:C:14:ARG:HG3	1:C:14:ARG:H	1.57	0.43
1:C:35:GLN:NE2	1:C:198:ASP:OD2	2.51	0.43
1:L:19:LEU:O	1:L:23:LEU:HG	2.19	0.43
3:E:302:OJ9:CAT	5:E:306:ACT:H3	2.48	0.43
1:E:27:ARG:HD3	1:E:45:GLY:HA3	2.00	0.43
1:F:256:PRO:HB2	1:F:258:MSE:HE2	2.01	0.42
1:F:122:ASP:OD1	1:F:250:LYS:HG3	2.19	0.42
1:C:13:PRO:O	1:C:15:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:189:SER:HA	1:L:190:PRO:HD3	1.94	0.42
1:A:19:LEU:O	1:A:23:LEU:HG	2.18	0.42
1:F:85:LYS:HE3	1:F:85:LYS:HB3	1.70	0.42
1:K:30:ARG:NH1	1:K:39:THR:HG23	2.34	0.42
1:D:206:PHE:CE1	1:D:211:LEU:HD13	2.54	0.42
1:C:89:ARG:HB3	1:D:87:PHE:HB3	2.01	0.42
1:H:46:LYS:O	8:H:540:HOH:O	2.22	0.42
8:I:505:HOH:O	1:J:3:HIS:HE1	2.02	0.42
1:E:256:PRO:HB2	1:E:258:MSE:HE3	1.99	0.42
1:J:18:ASN:HB3	1:J:20:ASP:H	1.84	0.42
1:K:23:LEU:HD22	1:K:43:LEU:HD22	2.00	0.42
1:F:30:ARG:HD3	1:F:33:VAL:HG22	2.02	0.42
1:F:209:GLY:C	1:F:210:LYS:HD2	2.39	0.42
1:G:58:LYS:HB3	1:G:58:LYS:HE2	1.82	0.42
1:H:209:GLY:HA2	7:H:306:PEG:H42	2.02	0.42
1:H:181:GLU:HB2	1:H:266:MSE:HE1	2.02	0.42
1:E:70:VAL:CG1	1:F:70[A]:VAL:HG11	2.49	0.42
1:F:79:MSE:HE2	1:F:131:LEU:HB2	2.01	0.42
1:D:110:LEU:HA	1:D:110:LEU:HD23	1.92	0.42
1:E:238:GLU:OE2	1:F:3:HIS:HE1	2.03	0.42
1:D:69:MSE:HE2	1:D:87:PHE:CE2	2.55	0.42
1:D:43:LEU:HB2	1:D:52:LEU:HB2	2.01	0.42
1:F:75:LEU:HB3	1:F:81:LEU:HD11	2.02	0.42
1:A:23:LEU:HD22	1:A:43:LEU:HD21	2.02	0.41
1:B:209:GLY:HA2	5:B:305:ACT:H1	2.02	0.41
1:D:151:GLN:O	1:D:155:ARG:HG3	2.20	0.41
1:F:196:HIS:HA	1:F:220:VAL:HG22	2.03	0.41
2:K:301:KAN:O10	2:K:301:KAN:H1	2.20	0.41
1:H:76:THR:O	5:H:305:ACT:H2	2.21	0.41
1:F:19:LEU:O	1:F:23:LEU:HG	2.21	0.41
1:J:199:PHE:CZ	1:J:204:LEU:HD21	2.55	0.41
3:J:302:OJ9:NAO	3:J:302:OJ9:CAL	2.79	0.41
1:D:153:GLN:HB2	1:D:179:TRP:CH2	2.56	0.41
1:B:148:ARG:HD2	8:B:601:HOH:O	2.21	0.41
1:G:15:LEU:H	1:G:15:LEU:HD12	1.85	0.41
1:G:151:GLN:O	1:G:155:ARG:HG3	2.21	0.41
1:J:148:ARG:HD2	1:J:219:ARG:HH12	1.86	0.41
3:F:302:OJ9:NAO	3:F:302:OJ9:CAL	2.80	0.41
1:K:206:PHE:CE1	1:K:211:LEU:HD13	2.55	0.41
1:L:245:LYS:HG3	8:L:491:HOH:O	2.20	0.41
1:H:17:SER:HB3	1:H:18:ASN:H	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:ASP:HB3	1:E:33:VAL:HG23	2.02	0.41
1:B:79:MSE:HE2	1:B:131:LEU:HB2	2.03	0.41
1:I:19:LEU:HB2	1:I:88:ILE:HD11	2.02	0.41
1:J:170:ARG:HG2	1:J:173:TRP:CE3	2.56	0.41
1:F:80:PRO:HD3	1:F:130:ARG:NH1	2.35	0.41
1:K:151:GLN:O	1:K:155:ARG:HG3	2.20	0.41
1:E:33:VAL:HG13	1:F:4:ILE:O	2.20	0.40
1:K:22:ASP:O	1:K:23:LEU:HD23	2.21	0.40
1:F:14:ARG:O	8:F:634:HOH:O	2.22	0.40
1:I:19:LEU:O	1:I:23:LEU:HG	2.21	0.40
1:A:112:GLU:HG3	8:A:606[B]:HOH:O	2.22	0.40
1:D:68:GLU:O	1:D:72:LEU:HB2	2.21	0.40
1:B:185:LEU:HD11	1:B:262[B]:GLN:HG2	2.02	0.40
1:C:70:VAL:CG1	1:D:70[B]:VAL:HG21	2.32	0.40
1:H:188:PHE:CD1	1:H:260:LYS:HE2	2.56	0.40
1:F:80:PRO:HG2	1:F:213:GLY:HA2	2.03	0.40
1:D:72:LEU:HB3	1:D:84:ILE:HD11	2.03	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	257/272 (94%)	252 (98%)	4 (2%)	1 (0%)	39	22
1	B	271/272 (100%)	262 (97%)	9 (3%)	0	100	100
1	C	268/272 (98%)	258 (96%)	8 (3%)	2 (1%)	26	11
1	D	263/272 (97%)	252 (96%)	11 (4%)	0	100	100
1	E	263/272 (97%)	257 (98%)	6 (2%)	0	100	100
1	F	276/272 (102%)	269 (98%)	5 (2%)	2 (1%)	26	11
1	G	267/272 (98%)	260 (97%)	6 (2%)	1 (0%)	39	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	257/272 (94%)	252 (98%)	4 (2%)	1 (0%)	39	22
1	I	266/272 (98%)	260 (98%)	6 (2%)	0	100	100
1	J	265/272 (97%)	255 (96%)	9 (3%)	1 (0%)	39	22
1	K	270/272 (99%)	264 (98%)	6 (2%)	0	100	100
1	L	254/272 (93%)	249 (98%)	4 (2%)	1 (0%)	39	22
All	All	3177/3264 (97%)	3090 (97%)	78 (2%)	9 (0%)	46	29

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	33	VAL
1	G	47	PRO
1	C	20	ASP
1	J	47	PRO
1	F	33	VAL
1	F	34	GLY
1	H	37	GLY
1	L	37	GLY
1	A	33	VAL

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	226/231 (98%)	225 (100%)	1 (0%)	93	92
1	B	243/231 (105%)	239 (98%)	4 (2%)	70	57
1	C	237/231 (103%)	229 (97%)	8 (3%)	44	24
1	D	235/231 (102%)	231 (98%)	4 (2%)	68	54
1	E	232/231 (100%)	228 (98%)	4 (2%)	68	54
1	F	245/231 (106%)	239 (98%)	6 (2%)	57	39
1	G	239/231 (104%)	231 (97%)	8 (3%)	45	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	226/231 (98%)	223 (99%)	3 (1%)	76	65
1	I	235/231 (102%)	233 (99%)	2 (1%)	84	79
1	J	237/231 (103%)	228 (96%)	9 (4%)	40	19
1	K	242/231 (105%)	235 (97%)	7 (3%)	50	31
1	L	223/231 (96%)	223 (100%)	0	100	100
All	All	2820/2772 (102%)	2764 (98%)	56 (2%)	65	47

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	B	20	ASP
1	B	92[A]	ASP
1	B	92[B]	ASP
1	B	254	ASP
1	C	5	GLN
1	C	8	THR
1	C	14	ARG
1	C	15	LEU
1	C	20	ASP
1	C	32	ASN
1	C	35	GLN
1	C	39	THR
1	D	3	HIS
1	D	4	ILE
1	D	19	LEU
1	D	22	ASP
1	E	33	VAL
1	E	85	LYS
1	E	115	ASP
1	E	180	LYS
1	F	4	ILE
1	F	5	GLN
1	F	6	ARG
1	F	19	LEU
1	F	31	ASP
1	F	32	ASN
1	G	1	MSE
1	G	15	LEU
1	G	23	LEU

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Mol	Chain	Res	Type
1	G	24	TYR
1	G	30	ARG
1	G	44	TYR
1	G	48	ASN
1	G	180	LYS
1	H	70[A]	VAL
1	H	70[B]	VAL
1	H	130	ARG
1	I	16	ASN
1	I	33	VAL
1	J	1	MSE
1	J	22	ASP
1	J	24	TYR
1	J	31	ASP
1	J	112	GLU
1	J	115	ASP
1	J	180	LYS
1	J	216	ASP
1	J	245	LYS
1	K	17	SER
1	K	19	LEU
1	K	30	ARG
1	K	32	ASN
1	K	44	TYR
1	K	180	LYS
1	K	211	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	249	GLN
1	C	18	ASN
1	D	16	ASN
1	E	73	ASN
1	F	3	HIS
1	H	157	ASN
1	I	16	ASN
1	I	18	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 79 ligands modelled in this entry, 16 are monoatomic - leaving 63 for Mogul analysis.

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$
2	KAN	A	301	-	35,35,35	0.78	1 (2%)	44,52,52	1.42	6 (13%)
3	OJ9	A	302	-	24,27,27	3.13	6 (25%)	29,41,41	3.14	2 (6%)
5	ACT	A	304	-	1,3,3	0.70	0	0,3,3	0.00	-
5	ACT	A	305	-	1,3,3	0.67	0	0,3,3	0.00	-
5	ACT	A	306	-	1,3,3	1.72	0	0,3,3	0.00	-
2	KAN	B	301	-	35,35,35	0.86	1 (2%)	44,52,52	1.52	7 (15%)
3	OJ9	B	302	-	24,27,27	4.88	5 (20%)	29,41,41	3.22	5 (17%)
5	ACT	B	305	-	1,3,3	1.29	0	0,3,3	0.00	-
5	ACT	B	306	-	1,3,3	1.51	0	0,3,3	0.00	-
2	KAN	C	301	-	35,35,35	0.73	0	44,52,52	1.39	5 (11%)
3	OJ9	C	302	-	24,27,27	2.80	5 (20%)	29,41,41	3.15	4 (13%)
3	OJ9	C	303	-	24,27,27	5.06	5 (20%)	29,41,41	3.05	4 (13%)
5	ACT	C	306	-	1,3,3	1.26	0	0,3,3	0.00	-
5	ACT	C	307	4	1,3,3	1.10	0	0,3,3	0.00	-
5	ACT	C	308	-	1,3,3	1.16	0	0,3,3	0.00	-
2	KAN	D	301	-	35,35,35	0.71	0	44,52,52	1.37	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACT	D	302	-	1,3,3	1.18	0	0,3,3	0.00	-
5	ACT	D	303	-	1,3,3	1.50	0	0,3,3	0.00	-
5	ACT	D	304	-	1,3,3	1.06	0	0,3,3	0.00	-
5	ACT	D	305	-	1,3,3	1.30	0	0,3,3	0.00	-
7	PEG	D	306	-	6,6,6	1.00	0	5,5,5	2.15	3 (60%)
7	PEG	D	307	-	6,6,6	1.08	0	5,5,5	1.46	0
2	KAN	E	301	-	35,35,35	0.65	0	44,52,52	1.34	6 (13%)
3	0J9	E	302	-	24,27,27	2.95	5 (20%)	29,41,41	3.10	5 (17%)
5	ACT	E	304	-	1,3,3	1.64	0	0,3,3	0.00	-
5	ACT	E	305	-	1,3,3	1.44	0	0,3,3	0.00	-
5	ACT	E	306	-	1,3,3	0.67	0	0,3,3	0.00	-
2	KAN	F	301	-	35,35,35	0.89	2 (5%)	44,52,52	1.45	4 (9%)
3	0J9	F	302	-	24,27,27	4.19	5 (20%)	29,41,41	3.12	4 (13%)
5	ACT	F	305	-	1,3,3	1.12	0	0,3,3	0.00	-
5	ACT	F	306	-	1,3,3	1.22	0	0,3,3	0.00	-
5	ACT	F	307	-	1,3,3	1.36	0	0,3,3	0.00	-
5	ACT	F	308	-	1,3,3	1.26	0	0,3,3	0.00	-
2	KAN	G	301	-	35,35,35	0.83	1 (2%)	44,52,52	1.39	5 (11%)
3	0J9	G	302	-	24,27,27	5.60	5 (20%)	29,41,41	3.18	3 (10%)
5	ACT	G	305	-	1,3,3	1.13	0	0,3,3	0.00	-
5	ACT	G	306	4	1,3,3	1.28	0	0,3,3	0.00	-
5	ACT	G	307	-	1,3,3	1.22	0	0,3,3	0.00	-
2	KAN	H	301	-	35,35,35	0.76	0	44,52,52	1.35	7 (15%)
3	0J9	H	302	-	24,27,27	2.71	6 (25%)	29,41,41	3.20	2 (6%)
5	ACT	H	304	-	1,3,3	0.89	0	0,3,3	0.00	-
5	ACT	H	305	4	1,3,3	1.16	0	0,3,3	0.00	-
7	PEG	H	306	-	6,6,6	0.92	0	5,5,5	2.95	3 (60%)
2	KAN	I	301	-	35,35,35	0.84	1 (2%)	44,52,52	1.18	3 (6%)
3	0J9	I	302	-	24,27,27	4.09	6 (25%)	29,41,41	3.23	4 (13%)
5	ACT	I	305	4	1,3,3	1.21	0	0,3,3	0.00	-
5	ACT	I	306	-	1,3,3	1.01	0	0,3,3	0.00	-
5	ACT	I	307	-	1,3,3	1.01	0	0,3,3	0.00	-
2	KAN	J	301	-	35,35,35	0.72	1 (2%)	44,52,52	1.29	4 (9%)
3	0J9	J	302	-	24,27,27	4.93	5 (20%)	29,41,41	3.08	4 (13%)
5	ACT	J	303	-	1,3,3	1.42	0	0,3,3	0.00	-
2	KAN	K	301	-	35,35,35	0.82	1 (2%)	44,52,52	1.41	7 (15%)
3	0J9	K	302	-	24,27,27	4.96	5 (20%)	29,41,41	3.18	2 (6%)
5	ACT	K	305	-	1,3,3	1.54	0	0,3,3	0.00	-
5	ACT	K	306	-	1,3,3	0.68	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACT	K	307	-	1,3,3	1.52	0	0,3,3	0.00	-
2	KAN	L	301	-	35,35,35	0.78	2 (5%)	44,52,52	1.47	4 (9%)
3	0J9	L	302	-	24,27,27	3.80	6 (25%)	29,41,41	3.17	4 (13%)
5	ACT	L	304	-	1,3,3	1.46	0	0,3,3	0.00	-
5	ACT	L	305	4	1,3,3	1.34	0	0,3,3	0.00	-
5	ACT	L	306	-	1,3,3	1.26	0	0,3,3	0.00	-
5	ACT	L	307	-	1,3,3	1.06	0	0,3,3	0.00	-
5	ACT	L	308	-	1,3,3	1.17	0	0,3,3	0.00	-

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
2	KAN	A	301	-	-	0/12/72/72	0/3/3/3
3	0J9	A	302	-	-	0/10/10/10	0/4/4/4
5	ACT	A	304	-	-	0/0/0/0	0/0/0/0
5	ACT	A	305	-	-	0/0/0/0	0/0/0/0
5	ACT	A	306	-	-	0/0/0/0	0/0/0/0
2	KAN	B	301	-	-	0/12/72/72	0/3/3/3
3	0J9	B	302	-	-	0/10/10/10	0/4/4/4
5	ACT	B	305	-	-	0/0/0/0	0/0/0/0
5	ACT	B	306	-	-	0/0/0/0	0/0/0/0
2	KAN	C	301	-	-	0/12/72/72	0/3/3/3
3	0J9	C	302	-	-	0/10/10/10	0/4/4/4
3	0J9	C	303	-	-	0/10/10/10	0/4/4/4
5	ACT	C	306	-	-	0/0/0/0	0/0/0/0
5	ACT	C	307	4	-	0/0/0/0	0/0/0/0
5	ACT	C	308	-	-	0/0/0/0	0/0/0/0
2	KAN	D	301	-	-	0/12/72/72	0/3/3/3
5	ACT	D	302	-	-	0/0/0/0	0/0/0/0
5	ACT	D	303	-	-	0/0/0/0	0/0/0/0
5	ACT	D	304	-	-	0/0/0/0	0/0/0/0
5	ACT	D	305	-	-	0/0/0/0	0/0/0/0
7	PEG	D	306	-	-	0/4/4/4	0/0/0/0
7	PEG	D	307	-	-	0/4/4/4	0/0/0/0
2	KAN	E	301	-	-	0/12/72/72	0/3/3/3
3	0J9	E	302	-	-	0/10/10/10	0/4/4/4
5	ACT	E	304	-	-	0/0/0/0	0/0/0/0
5	ACT	E	305	-	-	0/0/0/0	0/0/0/0
5	ACT	E	306	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KAN	F	301	-	-	0/12/72/72	0/3/3/3
3	0J9	F	302	-	-	0/10/10/10	0/4/4/4
5	ACT	F	305	-	-	0/0/0/0	0/0/0/0
5	ACT	F	306	-	-	0/0/0/0	0/0/0/0
5	ACT	F	307	-	-	0/0/0/0	0/0/0/0
5	ACT	F	308	-	-	0/0/0/0	0/0/0/0
2	KAN	G	301	-	-	0/12/72/72	0/3/3/3
3	0J9	G	302	-	-	0/10/10/10	0/4/4/4
5	ACT	G	305	-	-	0/0/0/0	0/0/0/0
5	ACT	G	306	4	-	0/0/0/0	0/0/0/0
5	ACT	G	307	-	-	0/0/0/0	0/0/0/0
2	KAN	H	301	-	-	0/12/72/72	0/3/3/3
3	0J9	H	302	-	-	0/10/10/10	0/4/4/4
5	ACT	H	304	-	-	0/0/0/0	0/0/0/0
5	ACT	H	305	4	-	0/0/0/0	0/0/0/0
7	PEG	H	306	-	-	0/4/4/4	0/0/0/0
2	KAN	I	301	-	-	0/12/72/72	0/3/3/3
3	0J9	I	302	-	-	0/10/10/10	0/4/4/4
5	ACT	I	305	4	-	0/0/0/0	0/0/0/0
5	ACT	I	306	-	-	0/0/0/0	0/0/0/0
5	ACT	I	307	-	-	0/0/0/0	0/0/0/0
2	KAN	J	301	-	-	0/12/72/72	0/3/3/3
3	0J9	J	302	-	-	0/10/10/10	0/4/4/4
5	ACT	J	303	-	-	0/0/0/0	0/0/0/0
2	KAN	K	301	-	-	0/12/72/72	0/3/3/3
3	0J9	K	302	-	-	0/10/10/10	0/4/4/4
5	ACT	K	305	-	-	0/0/0/0	0/0/0/0
5	ACT	K	306	-	-	0/0/0/0	0/0/0/0
5	ACT	K	307	-	-	0/0/0/0	0/0/0/0
2	KAN	L	301	-	-	0/12/72/72	0/3/3/3
3	0J9	L	302	-	-	0/10/10/10	0/4/4/4
5	ACT	L	304	-	-	0/0/0/0	0/0/0/0
5	ACT	L	305	4	-	0/0/0/0	0/0/0/0
5	ACT	L	306	-	-	0/0/0/0	0/0/0/0
5	ACT	L	307	-	-	0/0/0/0	0/0/0/0
5	ACT	L	308	-	-	0/0/0/0	0/0/0/0

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	302	0J9	NAO-NAW	-26.41	1.10	1.37
3	C	303	0J9	NAO-NAW	-23.53	1.13	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	302	0J9	NAO-NAW	-23.07	1.13	1.37
3	J	302	0J9	NAO-NAW	-22.92	1.13	1.37
3	B	302	0J9	NAO-NAW	-22.69	1.14	1.37
3	F	302	0J9	NAO-NAW	-19.09	1.17	1.37
3	I	302	0J9	NAO-NAW	-18.39	1.18	1.37
3	L	302	0J9	NAO-NAW	-16.92	1.20	1.37
3	A	302	0J9	NAO-NAW	-13.26	1.23	1.37
3	E	302	0J9	NAO-NAW	-12.20	1.25	1.37
3	C	302	0J9	NAO-NAW	-11.62	1.25	1.37
3	H	302	0J9	NAO-NAW	-10.56	1.26	1.37
3	J	302	0J9	CAQ-CAR	-3.45	1.36	1.48
3	C	303	0J9	CAQ-CAR	-3.41	1.36	1.48
3	I	302	0J9	CAQ-CAR	-3.34	1.36	1.48
3	C	302	0J9	CAQ-CAR	-3.32	1.37	1.48
3	B	302	0J9	CAQ-CAR	-3.27	1.37	1.48
3	H	302	0J9	CAQ-CAR	-3.24	1.37	1.48
3	K	302	0J9	CAQ-CAR	-3.23	1.37	1.48
3	A	302	0J9	CAQ-CAR	-3.22	1.37	1.48
3	C	303	0J9	C5-C4	-3.21	1.34	1.43
3	E	302	0J9	CAQ-CAR	-3.18	1.37	1.48
3	G	302	0J9	C5-C4	-3.18	1.34	1.43
3	F	302	0J9	CAQ-CAR	-3.17	1.37	1.48
3	G	302	0J9	CAQ-CAR	-3.14	1.37	1.48
3	I	302	0J9	C5-C4	-3.11	1.34	1.43
3	K	302	0J9	C5-C4	-3.11	1.34	1.43
3	B	302	0J9	C5-C4	-3.09	1.34	1.43
3	H	302	0J9	CAR-NAO	-3.08	1.32	1.35
3	J	302	0J9	C5-C4	-3.06	1.34	1.43
3	L	302	0J9	CAQ-CAR	-3.04	1.38	1.48
3	L	302	0J9	C5-C4	-2.86	1.35	1.43
3	A	302	0J9	C5-C4	-2.85	1.35	1.43
2	F	301	KAN	C16-C15	-2.83	1.50	1.53
3	C	302	0J9	C5-C4	-2.74	1.35	1.43
3	F	302	0J9	C5-C4	-2.71	1.35	1.43
3	E	302	0J9	C5-C4	-2.71	1.35	1.43
3	I	302	0J9	CAR-NAO	-2.64	1.32	1.35
3	H	302	0J9	C5-C4	-2.64	1.36	1.43
2	K	301	KAN	C16-C15	-2.39	1.50	1.53
2	B	301	KAN	C14-C15	-2.32	1.50	1.53
2	F	301	KAN	C14-C15	-2.28	1.50	1.53
3	L	302	0J9	CAR-NAO	-2.23	1.33	1.35
2	G	301	KAN	C14-C15	-2.16	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	0J9	CAR-NAO	-2.11	1.33	1.35
2	L	301	KAN	C14-C15	-2.10	1.50	1.53
2	L	301	KAN	O5-C1	2.02	1.47	1.41
2	J	301	KAN	O5-C1	2.12	1.47	1.41
2	A	301	KAN	O5-C1	2.30	1.47	1.41
3	C	302	0J9	C2-N1	2.43	1.38	1.33
2	I	301	KAN	O5-C1	2.45	1.48	1.41
3	A	302	0J9	C2-N1	2.45	1.38	1.33
3	B	302	0J9	C2-N1	2.47	1.38	1.33
3	J	302	0J9	C2-N1	2.57	1.38	1.33
3	G	302	0J9	C2-N1	2.65	1.38	1.33
3	E	302	0J9	C2-N1	2.73	1.39	1.33
3	H	302	0J9	C2-N1	2.75	1.39	1.33
3	K	302	0J9	C2-N1	2.80	1.39	1.33
3	I	302	0J9	C2-N1	2.97	1.39	1.33
3	C	303	0J9	C2-N1	3.06	1.39	1.33
3	F	302	0J9	C2-N1	3.08	1.39	1.33
3	L	302	0J9	C2-N1	3.12	1.39	1.33
3	I	302	0J9	C2-N3	3.65	1.38	1.32
3	L	302	0J9	C2-N3	3.84	1.39	1.32
3	K	302	0J9	C2-N3	3.86	1.39	1.32
3	J	302	0J9	C2-N3	3.87	1.39	1.32
3	B	302	0J9	C2-N3	3.92	1.39	1.32
3	G	302	0J9	C2-N3	3.96	1.39	1.32
3	C	302	0J9	C2-N3	3.99	1.39	1.32
3	A	302	0J9	C2-N3	4.01	1.39	1.32
3	C	303	0J9	C2-N3	4.03	1.39	1.32
3	F	302	0J9	C2-N3	4.09	1.39	1.32
3	H	302	0J9	C2-N3	4.11	1.39	1.32
3	E	302	0J9	C2-N3	4.64	1.40	1.32

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	302	0J9	N3-C2-N1	-16.12	116.56	128.89
3	I	302	0J9	N3-C2-N1	-16.11	116.56	128.89
3	B	302	0J9	N3-C2-N1	-16.01	116.64	128.89
3	A	302	0J9	N3-C2-N1	-15.90	116.72	128.89
3	L	302	0J9	N3-C2-N1	-15.89	116.73	128.89
3	C	302	0J9	N3-C2-N1	-15.82	116.78	128.89
3	G	302	0J9	N3-C2-N1	-15.82	116.78	128.89
3	K	302	0J9	N3-C2-N1	-15.81	116.79	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	302	0J9	N3-C2-N1	-15.47	117.05	128.89
3	E	302	0J9	N3-C2-N1	-15.22	117.24	128.89
3	J	302	0J9	N3-C2-N1	-15.20	117.26	128.89
3	C	303	0J9	N3-C2-N1	-15.06	117.36	128.89
2	B	301	KAN	C6-C5-C4	-5.26	103.22	113.17
2	K	301	KAN	C6-C5-C4	-4.56	104.56	113.17
2	A	301	KAN	C6-C5-C4	-4.41	104.84	113.17
2	F	301	KAN	C6-C5-C4	-4.19	105.25	113.17
2	E	301	KAN	C6-C5-C4	-4.18	105.28	113.17
2	G	301	KAN	C6-C5-C4	-4.02	105.58	113.17
2	L	301	KAN	C6-C5-C4	-3.90	105.80	113.17
2	C	301	KAN	C6-C5-C4	-3.89	105.82	113.17
2	D	301	KAN	C6-C5-C4	-3.57	106.42	113.17
2	I	301	KAN	C6-C5-C4	-3.13	107.26	113.17
2	J	301	KAN	C6-C5-C4	-2.92	107.65	113.17
2	E	301	KAN	C18-C17-C16	-2.91	105.84	113.02
3	F	302	0J9	CAJ-CAS-CAK	-2.61	117.06	123.22
3	E	302	0J9	CAJ-CAS-CAK	-2.60	117.07	123.22
3	K	302	0J9	CAJ-CAS-CAK	-2.59	117.09	123.22
3	J	302	0J9	CAJ-CAS-CAK	-2.58	117.12	123.22
3	B	302	0J9	CAJ-CAS-CAK	-2.57	117.14	123.22
3	G	302	0J9	CAJ-CAS-CAK	-2.57	117.15	123.22
3	E	302	0J9	CAI-CAQ-CAT	-2.50	114.12	118.56
2	E	301	KAN	O11-C13-C14	-2.50	102.03	108.10
3	C	303	0J9	CAJ-CAS-CAK	-2.49	117.33	123.22
3	C	302	0J9	CAJ-CAS-CAK	-2.45	117.43	123.22
3	L	302	0J9	CAJ-CAS-CAK	-2.44	117.44	123.22
3	A	302	0J9	CAJ-CAS-CAK	-2.44	117.45	123.22
2	H	301	KAN	C6-C5-C4	-2.42	108.59	113.17
7	D	306	PEG	C3-O2-C2	-2.42	102.92	113.31
2	F	301	KAN	C16-C15-N4	-2.41	106.40	110.86
2	B	301	KAN	C1-O9-C10	-2.40	111.75	118.01
3	I	302	0J9	CAJ-CAS-CAK	-2.37	117.62	123.22
2	K	301	KAN	C1-O9-C10	-2.33	111.91	118.01
3	H	302	0J9	CAJ-CAS-CAK	-2.29	117.81	123.22
3	G	302	0J9	CAR-C5-C4	-2.28	102.26	106.55
2	B	301	KAN	C14-C15-N4	-2.26	106.66	110.86
2	K	301	KAN	O14-C16-C15	-2.23	106.54	110.31
3	L	302	0J9	CAI-CAQ-CAT	-2.21	114.64	118.56
2	H	301	KAN	O12-C13-C14	-2.18	105.81	110.28
2	G	301	KAN	C14-C15-N4	-2.15	106.87	110.86
2	K	301	KAN	C4-C3-C2	-2.11	106.86	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	0J9	CAI-CAQ-CAT	-2.10	114.83	118.56
2	A	301	KAN	O11-C13-C14	-2.09	103.02	108.10
3	I	302	0J9	CAI-CAQ-CAT	-2.08	114.87	118.56
3	F	302	0J9	CAI-CAQ-CAT	-2.07	114.88	118.56
3	C	303	0J9	CAI-CAQ-CAT	-2.07	114.89	118.56
3	B	302	0J9	CAI-CAQ-CAT	-2.06	114.90	118.56
3	J	302	0J9	CAR-C5-C4	-2.02	102.75	106.55
2	D	301	KAN	O9-C1-O5	-2.02	105.57	110.68
3	J	302	0J9	CAI-CAQ-CAT	-2.01	114.98	118.56
2	E	301	KAN	O13-C14-C13	-2.01	105.61	110.02
3	B	302	0J9	CAG-CAI-CAQ	2.02	125.13	121.17
2	C	301	KAN	O12-C17-C18	2.02	111.46	106.36
3	C	302	0J9	CAG-CAI-CAQ	2.04	125.18	121.17
3	B	302	0J9	CAQ-CAR-NAO	2.04	123.35	120.71
3	F	302	0J9	CAG-CAI-CAQ	2.05	125.18	121.17
2	H	301	KAN	O5-C5-C6	2.05	110.11	106.10
3	L	302	0J9	CAK-CAS-CAT	2.06	121.91	119.10
3	I	302	0J9	CAQ-CAR-NAO	2.07	123.38	120.71
2	K	301	KAN	C10-C9-C8	2.08	113.25	109.06
2	E	301	KAN	O13-C14-C15	2.14	113.92	110.31
3	E	302	0J9	CAK-CAS-CAT	2.15	122.03	119.10
2	B	301	KAN	C10-C9-C8	2.17	113.44	109.06
2	I	301	KAN	C13-C14-C15	2.20	113.36	110.40
2	B	301	KAN	O5-C5-C6	2.24	110.48	106.10
2	K	301	KAN	O5-C5-C6	2.25	110.50	106.10
2	H	301	KAN	C13-O12-C17	2.30	118.21	113.75
2	H	301	KAN	O12-C17-C18	2.33	112.24	106.36
3	E	302	0J9	CAG-CAI-CAQ	2.35	125.77	121.17
2	G	301	KAN	C13-C14-C15	2.36	113.56	110.40
2	E	301	KAN	O11-C8-C9	2.39	113.35	107.17
2	J	301	KAN	C13-C14-C15	2.48	113.73	110.40
2	D	301	KAN	C13-C14-C15	2.53	113.80	110.40
2	A	301	KAN	O12-C17-C18	2.56	112.82	106.36
2	A	301	KAN	O5-C5-C6	2.57	111.13	106.10
2	A	301	KAN	O11-C8-C9	2.62	113.94	107.17
2	C	301	KAN	C13-C14-C15	2.70	114.03	110.40
7	D	306	PEG	O2-C3-C4	2.71	122.92	110.43
3	C	303	0J9	CAQ-CAR-NAO	2.78	124.30	120.71
7	D	306	PEG	O2-C2-C1	2.80	123.32	110.43
2	B	301	KAN	C13-C14-C15	2.82	114.19	110.40
2	J	301	KAN	O5-C5-C6	2.83	111.63	106.10
2	L	301	KAN	O5-C5-C6	2.93	111.82	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	KAN	O11-C8-C9	2.98	114.85	107.17
2	A	301	KAN	C13-C14-C15	3.02	114.46	110.40
2	C	301	KAN	O5-C5-C6	3.07	112.11	106.10
2	C	301	KAN	O11-C8-C9	3.12	115.23	107.17
2	F	301	KAN	C13-C14-C15	3.17	114.66	110.40
2	J	301	KAN	O11-C8-C9	3.19	115.39	107.17
2	D	301	KAN	O11-C8-C9	3.19	115.41	107.17
7	H	306	PEG	C3-O2-C2	3.22	127.16	113.31
2	L	301	KAN	C13-C14-C15	3.23	114.74	110.40
2	K	301	KAN	O11-C8-C9	3.23	115.52	107.17
2	H	301	KAN	O11-C8-C9	3.24	115.52	107.17
2	D	301	KAN	O5-C5-C6	3.24	112.43	106.10
2	I	301	KAN	O11-C8-C9	3.31	115.72	107.17
2	F	301	KAN	O11-C8-C9	3.35	115.82	107.17
2	L	301	KAN	O11-C8-C9	3.36	115.84	107.17
2	G	301	KAN	O5-C5-C6	3.48	112.89	106.10
2	B	301	KAN	O11-C8-C9	3.57	116.39	107.17
7	H	306	PEG	O2-C2-C1	3.72	127.54	110.43
2	H	301	KAN	C13-C14-C15	3.76	115.45	110.40
7	H	306	PEG	O2-C3-C4	3.99	128.79	110.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

24 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	0J9	5	0
5	A	304	ACT	1	0
3	B	302	0J9	4	0
5	B	305	ACT	1	0
3	C	302	0J9	4	0
3	C	303	0J9	4	0
7	D	306	PEG	1	0
7	D	307	PEG	1	0
3	E	302	0J9	5	0
5	E	306	ACT	1	0
3	F	302	0J9	5	0
5	F	305	ACT	1	0
3	G	302	0J9	4	0
3	H	302	0J9	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	305	ACT	1	0
7	H	306	PEG	1	0
3	I	302	0J9	5	0
3	J	302	0J9	5	0
2	K	301	KAN	1	0
3	K	302	0J9	4	0
5	K	307	ACT	1	0
3	L	302	0J9	4	0
5	L	304	ACT	2	0
5	L	307	ACT	1	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	248/272 (91%)	-0.07	4 (1%) 74 74	29, 38, 62, 106	0
1	B	261/272 (95%)	0.10	11 (4%) 40 37	30, 42, 94, 114	0
1	C	261/272 (95%)	0.12	16 (6%) 25 23	29, 39, 100, 143	0
1	D	259/272 (95%)	0.52	29 (11%) 7 6	32, 50, 106, 140	0
1	E	255/272 (93%)	0.06	10 (3%) 43 40	27, 37, 68, 130	0
1	F	264/272 (97%)	0.12	16 (6%) 25 23	29, 42, 94, 122	0
1	G	260/272 (95%)	0.12	21 (8%) 15 14	30, 44, 107, 141	0
1	H	249/272 (91%)	0.00	8 (3%) 51 48	30, 40, 69, 98	0
1	I	260/272 (95%)	0.06	13 (5%) 32 31	29, 39, 93, 141	0
1	J	260/272 (95%)	0.66	39 (15%) 3 3	33, 57, 106, 148	0
1	K	262/272 (96%)	0.21	24 (9%) 11 11	28, 43, 106, 147	0
1	L	248/272 (91%)	-0.05	1 (0%) 93 92	28, 39, 64, 97	0
All	All	3087/3264 (94%)	0.16	192 (6%) 24 22	27, 42, 95, 148	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4	ILE	16.7
1	J	22	ASP	14.7
1	J	4	ILE	13.3
1	K	33	VAL	10.1
1	K	36	SER	9.8
1	G	17	SER	9.6
1	D	24	TYR	8.8
1	K	16	ASN	8.2
1	J	23	LEU	8.0
1	K	21	ALA	8.0
1	K	24	TYR	7.9

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Mol	Chain	Res	Type	RSRZ
1	J	2	SER	7.7
1	E	16	ASN	7.5
1	B	23	LEU	7.5
1	K	28	TRP	7.4
1	F	33	VAL	7.4
1	C	14	ARG	7.2
1	G	24	TYR	6.9
1	G	19	LEU	6.8
1	D	21	ALA	6.2
1	B	19	LEU	6.1
1	K	19	LEU	5.9
1	H	17	SER	5.9
1	K	31	ASP	5.7
1	D	48	ASN	5.6
1	G	16	ASN	5.6
1	E	12	ARG	5.3
1	D	16	ASN	5.3
1	D	20	ASP	5.3
1	G	28	TRP	5.3
1	B	24	TYR	5.3
1	G	29	ALA	5.2
1	F	32	ASN	5.2
1	E	17	SER	5.2
1	F	24	TYR	5.1
1	E	11	SER	5.0
1	D	22	ASP	4.9
1	C	12	ARG	4.8
1	G	30	ARG	4.8
1	E	14	ARG	4.7
1	D	45	GLY	4.6
1	E	15	LEU	4.6
1	F	35	GLN	4.6
1	B	45	GLY	4.6
1	C	17	SER	4.6
1	I	33	VAL	4.5
1	E	186	LEU	4.5
1	K	17	SER	4.5
1	G	20	ASP	4.4
1	D	49	ALA	4.4
1	I	21	ALA	4.4
1	I	14	ARG	4.3
1	C	33	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	G	45	GLY	4.3
1	J	17	SER	4.2
1	I	16	ASN	4.2
1	J	107	PHE	4.1
1	D	3	HIS	4.1
1	D	28	TRP	4.1
1	I	7	GLU	4.1
1	I	8	THR	4.0
1	K	44	TYR	4.0
1	K	22	ASP	4.0
1	K	48	ASN	4.0
1	D	41	TYR	4.0
1	C	32	ASN	4.0
1	D	14	ARG	4.0
1	K	14	ARG	4.0
1	G	25	GLY	3.9
1	D	17	SER	3.9
1	J	110	LEU	3.9
1	G	44	TYR	3.9
1	J	44	TYR	3.9
1	D	6	ARG	3.9
1	I	6	ARG	3.8
1	K	23	LEU	3.7
1	G	23	LEU	3.7
1	A	18	ASN	3.7
1	I	18	ASN	3.7
1	A	36	SER	3.7
1	C	5	GLN	3.6
1	J	19	LEU	3.6
1	B	4	ILE	3.6
1	C	6	ARG	3.6
1	C	23	LEU	3.5
1	D	15	LEU	3.5
1	K	29	ALA	3.5
1	D	116	SER	3.5
1	J	45	GLY	3.5
1	D	43	LEU	3.5
1	K	32	ASN	3.5
1	D	18	ASN	3.4
1	F	45	GLY	3.4
1	J	3	HIS	3.4
1	K	27	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	186	LEU	3.3
1	C	7	GLU	3.3
1	D	19	LEU	3.2
1	E	13	PRO	3.2
1	J	49	ALA	3.2
1	F	4	ILE	3.1
1	J	6	ARG	3.1
1	J	14	ARG	3.1
1	J	42	ARG	3.1
1	J	5	GLN	3.1
1	G	18	ASN	3.1
1	L	19	LEU	3.0
1	J	28	TRP	3.0
1	J	241	PRO	3.0
1	D	9	SER	3.0
1	J	24	TYR	3.0
1	C	19	LEU	2.9
1	C	190	PRO	2.9
1	A	186	LEU	2.9
1	I	19	LEU	2.9
1	D	5	GLN	2.9
1	G	47	PRO	2.8
1	J	206	PHE	2.8
1	H	172	GLY	2.8
1	K	49	ALA	2.8
1	I	15	LEU	2.7
1	J	204	LEU	2.7
1	J	50	PRO	2.7
1	J	8	THR	2.7
1	H	160	LEU	2.7
1	K	15	LEU	2.7
1	A	34	GLY	2.7
1	F	34	GLY	2.7
1	G	21	ALA	2.7
1	G	27	ARG	2.7
1	H	157	ASN	2.7
1	G	31	ASP	2.7
1	B	35	GLN	2.7
1	I	17	SER	2.6
1	J	101	ILE	2.6
1	J	48	ASN	2.6
1	C	13	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	190	PRO	2.6
1	F	19	LEU	2.5
1	H	18	ASN	2.5
1	D	25	GLY	2.5
1	J	25	GLY	2.5
1	I	9	SER	2.5
1	B	49	ALA	2.5
1	C	9	SER	2.4
1	F	28	TRP	2.4
1	J	27	ARG	2.4
1	J	41	TYR	2.4
1	C	15	LEU	2.4
1	K	20	ASP	2.4
1	D	29	ALA	2.4
1	J	51	GLU	2.4
1	J	18	ASN	2.4
1	J	29	ALA	2.4
1	F	31	ASP	2.3
1	D	47	PRO	2.3
1	J	32	ASN	2.3
1	J	208	GLU	2.3
1	K	43	LEU	2.3
1	F	27	ARG	2.3
1	F	16	ASN	2.2
1	G	15	LEU	2.2
1	B	28	TRP	2.2
1	C	22	ASP	2.2
1	F	23	LEU	2.2
1	J	119	ASN	2.2
1	J	106	ALA	2.2
1	C	20	ASP	2.2
1	K	46	LYS	2.2
1	G	26	TYR	2.2
1	G	32	ASN	2.1
1	K	50	PRO	2.1
1	B	44	TYR	2.1
1	K	30	ARG	2.1
1	J	16	ASN	2.1
1	J	43	LEU	2.1
1	E	187	PRO	2.1
1	B	16	ASN	2.1
1	F	20	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	48	ASN	2.1
1	J	53	PHE	2.1
1	E	34	GLY	2.1
1	F	36	SER	2.1
1	I	36	SER	2.1
1	D	50	PRO	2.1
1	G	14	ARG	2.1
1	B	22	ASP	2.1
1	D	46	LYS	2.0
1	D	12	ARG	2.0
1	D	44	TYR	2.0
1	H	154	SER	2.0
1	J	211	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
4	NA	F	304	1/1	0.97	0.21	19.70	41,41,41,41	0
4	NA	G	304	1/1	0.96	0.20	15.11	47,47,47,47	0
4	NA	K	304	1/1	0.99	0.21	9.15	43,43,43,43	0
5	ACT	D	305	4/4	0.68	0.29	6.76	64,85,93,106	0
5	ACT	A	304	4/4	0.88	0.18	6.28	74,75,88,89	0
3	0J9	B	302	24/24	0.81	0.23	6.02	36,54,92,106	24
5	ACT	E	304	4/4	0.91	0.16	5.77	36,37,38,83	0
5	ACT	H	304	4/4	0.88	0.17	5.71	44,44,75,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	ACT	K	306	4/4	0.86	0.18	5.64	40,57,69,100	0
5	ACT	C	306	4/4	0.87	0.21	5.31	59,71,79,111	0
3	0J9	G	302	24/24	0.79	0.35	4.48	38,76,106,128	24
5	ACT	K	307	4/4	0.91	0.25	4.25	45,61,75,109	0
5	ACT	L	306	4/4	0.87	0.17	4.02	52,70,83,83	0
5	ACT	I	306	4/4	0.85	0.16	3.53	63,74,91,92	0
7	PEG	D	306	7/7	0.80	0.18	3.49	51,76,102,118	0
4	NA	L	303	1/1	0.93	0.13	3.26	37,37,37,37	1
3	0J9	K	302	24/24	0.82	0.30	1.89	36,60,79,117	24
5	ACT	L	308	4/4	0.93	0.13	1.72	50,52,57,93	0
7	PEG	D	307	7/7	0.86	0.26	1.40	60,72,103,118	0
5	ACT	F	305	4/4	0.96	0.15	1.28	53,57,62,68	0
3	0J9	F	302	24/24	0.85	0.23	1.26	33,46,88,114	24
5	ACT	E	305	4/4	0.94	0.13	1.04	56,61,82,84	0
5	ACT	E	306	4/4	0.88	0.18	1.02	54,71,73,84	0
2	KAN	G	301	33/33	0.96	0.11	0.95	28,33,39,42	0
3	0J9	E	302	24/24	0.94	0.12	0.73	30,34,50,70	0
2	KAN	K	301	33/33	0.95	0.10	0.59	29,34,42,49	0
3	0J9	L	302	24/24	0.95	0.10	0.58	29,35,41,57	0
3	0J9	J	302	24/24	0.87	0.19	0.47	43,59,79,105	24
5	ACT	F	308	4/4	0.96	0.10	0.43	47,49,51,90	0
7	PEG	H	306	7/7	0.88	0.17	0.35	57,86,114,138	0
5	ACT	A	306	4/4	0.95	0.13	0.31	36,40,47,86	0
3	0J9	C	303	24/24	0.92	0.15	0.13	37,53,74,123	24
3	0J9	I	302	24/24	0.91	0.14	0.12	32,43,70,93	0
4	NA	B	304	1/1	0.98	0.10	0.05	51,51,51,51	0
2	KAN	C	301	33/33	0.94	0.13	0.04	30,37,52,57	0
5	ACT	C	308	4/4	0.91	0.11	0.04	49,77,89,106	0
2	KAN	D	301	33/33	0.95	0.10	-0.04	32,40,45,50	0
5	ACT	L	305	4/4	0.81	0.14	-0.08	53,63,78,126	0
5	ACT	B	306	4/4	0.91	0.12	-0.17	39,49,61,85	0
5	ACT	I	307	4/4	0.93	0.15	-0.22	51,84,91,99	0
3	0J9	H	302	24/24	0.94	0.10	-0.23	30,36,45,48	0
5	ACT	A	305	4/4	0.96	0.14	-0.24	48,51,53,91	0
5	ACT	D	302	4/4	0.97	0.10	-0.25	43,59,84,90	0
2	KAN	J	301	33/33	0.95	0.11	-0.27	37,46,53,57	0
3	0J9	C	302	24/24	0.91	0.11	-0.31	34,45,64,85	0
2	KAN	L	301	33/33	0.95	0.10	-0.38	32,42,47,48	0
2	KAN	I	301	33/33	0.95	0.10	-0.38	30,38,44,55	0
3	0J9	A	302	24/24	0.96	0.10	-0.39	29,34,53,59	0
5	ACT	L	304	4/4	0.78	0.13	-0.52	53,64,69,95	0
2	KAN	F	301	33/33	0.97	0.09	-0.55	25,32,37,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	KAN	E	301	33/33	0.95	0.09	-0.56	28,36,48,58	0
2	KAN	A	301	33/33	0.95	0.09	-0.60	26,37,48,55	0
2	KAN	B	301	33/33	0.98	0.09	-0.67	29,34,40,46	0
5	ACT	J	303	4/4	0.94	0.09	-0.76	45,57,57,71	0
2	KAN	H	301	33/33	0.96	0.08	-0.90	36,40,45,46	0
6	CL	C	305	1/1	0.95	0.10	-1.02	66,66,66,66	0
6	CL	I	304	1/1	0.89	0.10	-1.25	65,65,65,65	0
5	ACT	F	306	4/4	0.94	0.13	-	51,69,72,78	0
5	ACT	K	305	4/4	0.95	0.11	-	44,45,54,63	0
5	ACT	G	306	4/4	0.56	0.26	-	61,77,85,118	0
5	ACT	D	304	4/4	0.81	0.18	-	55,81,91,119	0
4	NA	E	303	1/1	0.97	0.06	-	53,53,53,53	0
4	NA	I	303	1/1	0.97	0.18	-	35,35,35,35	1
4	NA	F	303	1/1	0.90	0.08	-	33,33,33,33	1
4	NA	H	303	1/1	0.94	0.08	-	40,40,40,40	1
5	ACT	B	305	4/4	0.96	0.09	-	45,58,72,73	0
5	ACT	F	307	4/4	0.84	0.13	-	47,70,78,94	0
5	ACT	H	305	4/4	0.74	0.18	-	48,71,71,129	0
4	NA	C	304	1/1	0.98	0.20	-	43,43,43,43	1
4	NA	A	303	1/1	0.90	0.10	-	57,57,57,57	0
5	ACT	L	307	4/4	0.89	0.20	-	55,63,72,85	0
4	NA	B	303	1/1	0.93	0.12	-	39,39,39,39	1
5	ACT	C	307	4/4	0.78	0.20	-	46,63,66,128	0
5	ACT	D	303	4/4	0.80	0.28	-	71,71,80,84	0
4	NA	G	303	1/1	0.90	0.13	-	49,49,49,49	0
5	ACT	G	307	4/4	0.95	0.10	-	31,45,46,108	0
5	ACT	I	305	4/4	0.91	0.09	-	58,65,67,123	0
4	NA	K	303	1/1	0.93	0.07	-	41,41,41,41	1
5	ACT	G	305	4/4	0.88	0.16	-	43,48,79,88	0

6.5 Other polymers

There are no such residues in this entry.