



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:36 PM GMT

PDB ID : 4FEW  
Title : Crystal structure of the aminoglycoside phosphotransferase APH(3')-Ia, with substrate kanamycin and small molecule inhibitor pyrazolopyrimidine PP2  
Authors : Stogios, P.J.; Evdokimova, E.; Wawrzak, Z.; Minasov, G.; Egorova, O.; Di Leo, R.; Shakya, T.; Spanogiannopoulos, P.; Wright, G.D.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2012-05-30  
Resolution : 1.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

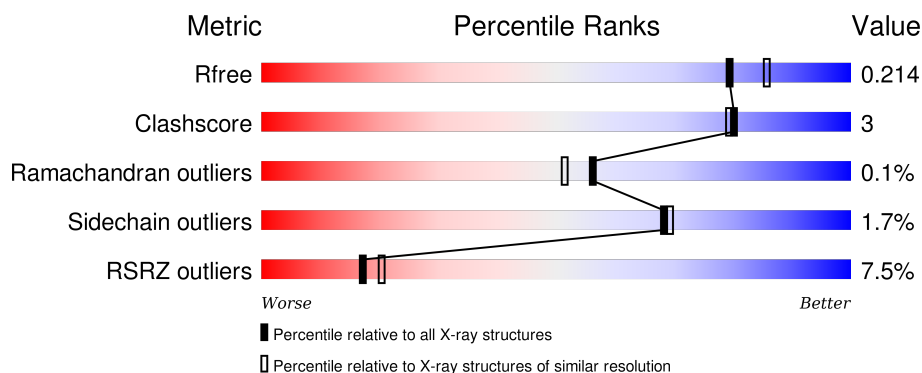
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	272	<div> <div>7%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>••</div> </div> </div>
1	B	272	<div> <div>11%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>6%</div> </div> </div>
1	C	272	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>7%</div> </div> </div>
1	D	272	<div> <div>7%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>•</div> </div> </div>
1	E	272	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>5%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	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	PP2	F	302	-	-	-	X
7	PEG	C	303	-	-	-	X
7	PEG	F	306	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14307 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.

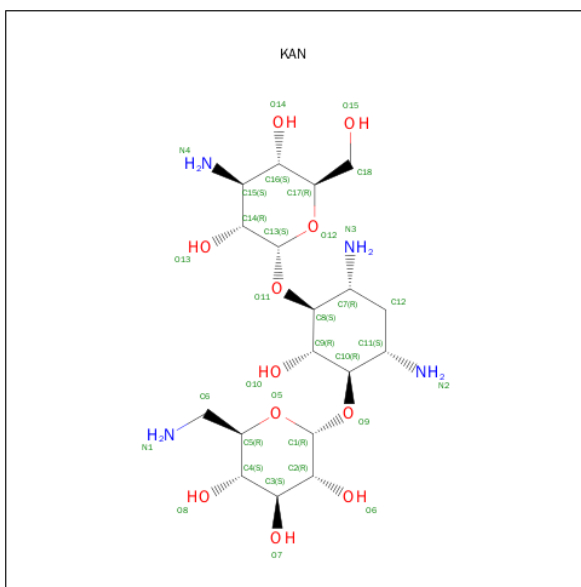
- Molecule 1 is a protein called Aminoglycoside 3'-phosphotransferase AphA1-IAB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	Se	0	1	0
			2143	1365	371	396	5	6			
1	B	256	Total	C	N	O	S	Se	0	0	0
			2071	1323	359	378	5	6			
1	C	254	Total	C	N	O	S	Se	0	5	0
			2081	1331	358	382	4	6			
1	D	266	Total	C	N	O	S	Se	0	5	0
			2176	1385	378	401	5	7			
1	E	254	Total	C	N	O	S	Se	0	4	0
			2077	1326	358	383	4	6			
1	F	266	Total	C	N	O	S	Se	0	4	0
			2178	1387	384	395	5	7			

There are 6 discrepancies between the modelled and reference sequences:

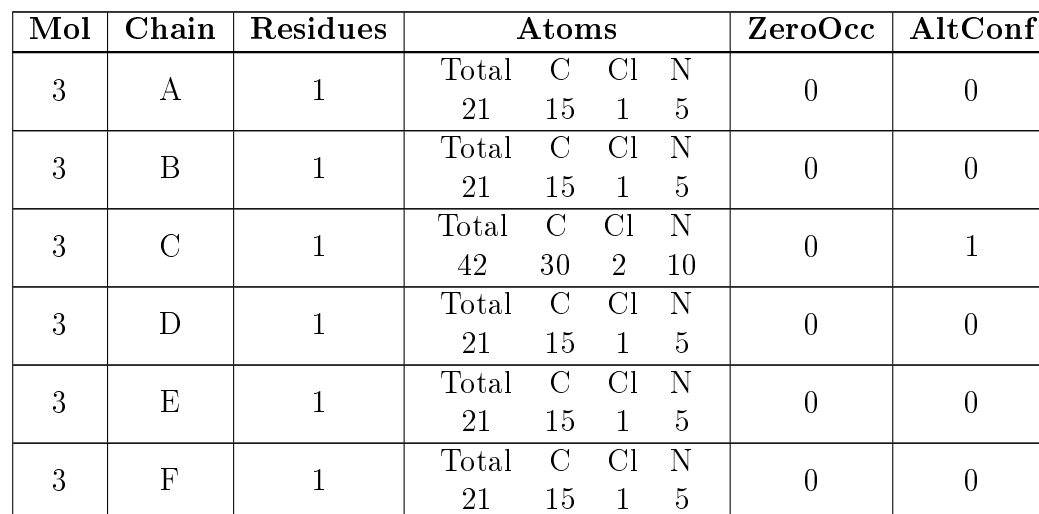
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP B0VD92
B	0	GLY	-	EXPRESSION TAG	UNP B0VD92
C	0	GLY	-	EXPRESSION TAG	UNP B0VD92
D	0	GLY	-	EXPRESSION TAG	UNP B0VD92
E	0	GLY	-	EXPRESSION TAG	UNP B0VD92
F	0	GLY	-	EXPRESSION TAG	UNP B0VD92

- Molecule 2 is KANAMYCIN A (three-letter code: KAN) (formula:  $C_{18}H_{36}N_4O_{11}$ ).



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		

- Molecule 3 is 1-TERT-BUTYL-3-(4-CHLORO-PHENYL)-1H-PYRAZOLO[3,4-D]PYRIMIDIN-4-YLAMINE (three-letter code: PP2) (formula: C<sub>15</sub>H<sub>17</sub>ClN<sub>5</sub>).

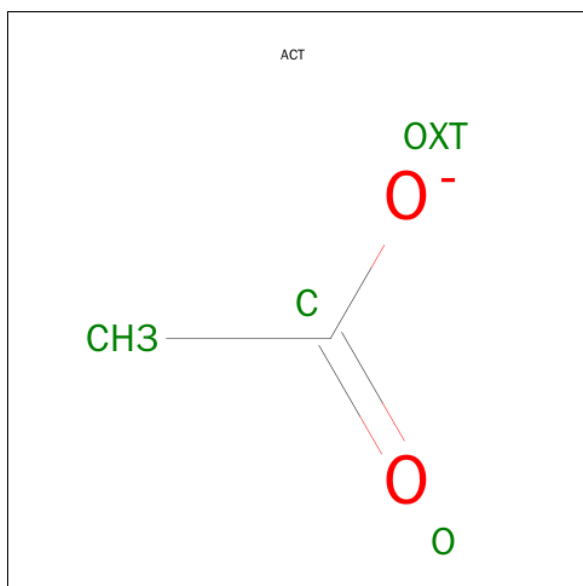


- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 4   | B     | 1        | Total Na<br>1 1 | 0       | 0       |
| 4   | A     | 1        | Total Na<br>1 1 | 0       | 0       |
| 4   | D     | 2        | Total Na<br>2 2 | 0       | 0       |
| 4   | F     | 2        | Total Na<br>2 2 | 0       | 0       |
| 4   | E     | 1        | Total Na<br>1 1 | 0       | 0       |

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

- Molecule 8 is water.

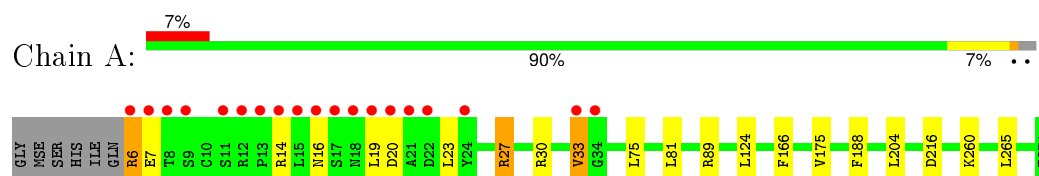
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	231	Total	O	0	6
			237	237		
8	B	139	Total	O	0	3
			142	142		
8	C	193	Total	O	0	1
			194	194		
8	D	214	Total	O	0	3
			217	217		
8	E	189	Total	O	0	2
			191	191		
8	F	204	Total	O	0	5
			209	209		



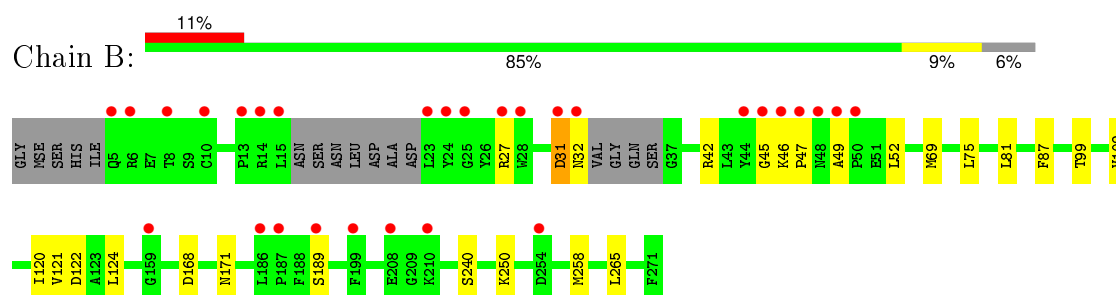
### 3 Residue-property plots [i](#)

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.

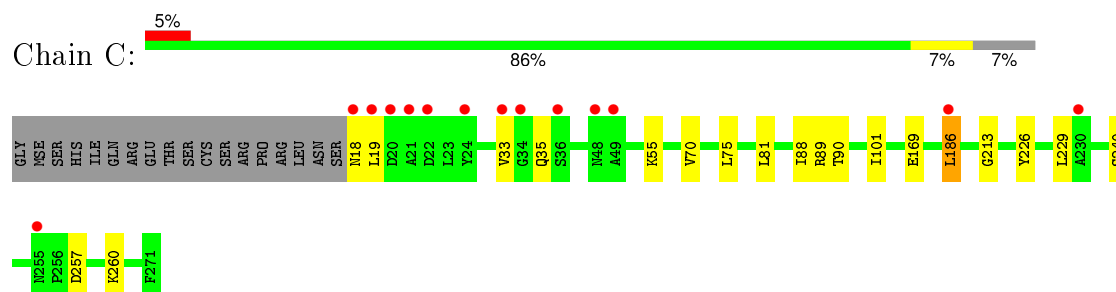
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



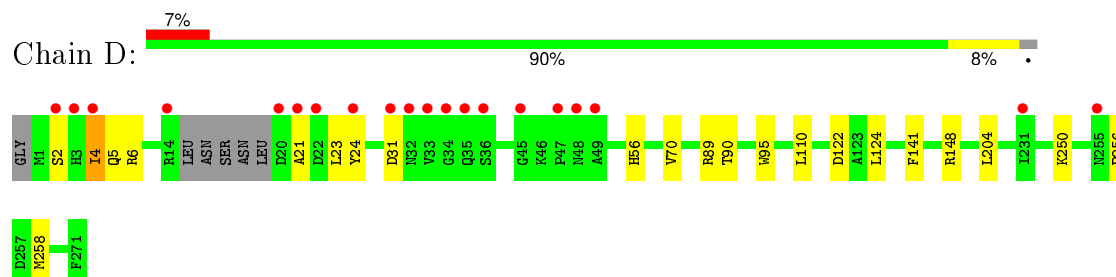
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB




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

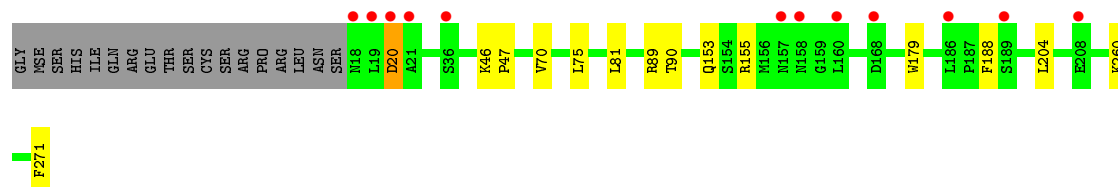


- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB




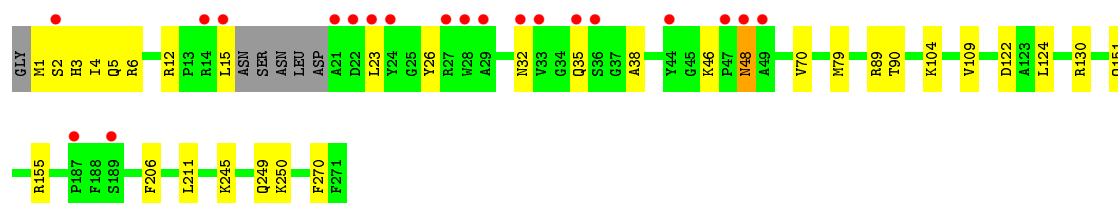
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB

Chain E: 



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

Chain F: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.28Å 93.58Å 96.40Å 61.22° 73.18° 87.35°	Depositor
Resolution (Å)	23.90 – 1.98 23.90 – 1.97	Depositor EDS
% Data completeness (in resolution range)	92.2 (23.90-1.98) 77.1 (23.90-1.97)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 1.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.157 , 0.216 0.158 , 0.214	Depositor DCC
$R_{free}$ test set	5631 reflections (5.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.7	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 59.9	EDS
Estimated twinning fraction	0.004 for -h,-k,-h-k+l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 115199 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	14307	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NA, KAN, PP2, 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	0.37	0/2195	0.52	0/2969
1	B	0.33	0/2118	0.49	0/2860
1	C	0.38	0/2135	0.53	0/2888
1	D	0.38	0/2234	0.53	1/3017 (0.0%)
1	E	0.37	0/2128	0.53	1/2878 (0.0%)
1	F	0.39	0/2232	0.53	0/3010
All	All	0.37	0/13042	0.52	2/17622 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	204	LEU	CA-CB-CG	-5.95	101.62	115.30
1	D	110	LEU	CA-CB-CG	5.60	128.17	115.30

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	2143	0	2082	13	0
1	B	2071	0	2013	16	0
1	C	2081	0	2023	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2176	0	2117	14	0
1	E	2077	0	2011	8	0
1	F	2178	0	2133	18	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
3	A	21	0	17	2	0
3	B	21	0	17	2	0
3	C	42	0	34	6	0
3	D	21	0	17	2	0
3	E	21	0	17	3	0
3	F	21	0	17	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
4	F	2	0	0	0	0
5	A	1	0	0	0	0
6	A	4	0	3	0	0
6	B	4	0	3	0	0
6	D	8	0	6	0	0
6	E	4	0	3	0	0
6	F	4	0	3	0	0
7	C	7	0	8	0	0
7	F	7	0	8	0	0
8	A	237	0	0	2	0
8	B	142	0	0	1	0
8	C	194	0	0	0	0
8	D	217	0	0	1	0
8	E	191	0	0	0	0
8	F	209	0	0	0	0
All	All	14307	0	12748	89	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 3.

All (89) 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:C:302[A]:PP2:H3	3:C:302[A]:PP2:H12	1.10	1.16
3:D:302:PP2:H12	3:D:302:PP2:H3	1.05	1.15
3:A:302:PP2:H12	3:A:302:PP2:H3	1.05	1.12
3:F:302:PP2:H3	3:F:302:PP2:H12	1.01	1.11
3:C:302[B]:PP2:H12	3:C:302[B]:PP2:H3	1.11	1.11
3:B:302:PP2:H3	3:B:302:PP2:H12	1.09	1.08
3:E:302:PP2:H12	3:E:302:PP2:H3	1.15	1.06
3:F:302:PP2:H12	3:F:302:PP2:N25	1.82	0.94
3:D:302:PP2:H12	3:D:302:PP2:N25	1.85	0.91
3:A:302:PP2:H12	3:A:302:PP2:N25	1.88	0.88
3:C:302[B]:PP2:H12	3:C:302[B]:PP2:N25	1.91	0.86
3:B:302:PP2:N25	3:B:302:PP2:H12	1.92	0.85
3:C:302[A]:PP2:H12	3:C:302[A]:PP2:N25	1.91	0.84
3:E:302:PP2:H12	3:E:302:PP2:N25	1.92	0.84
1:F:89[A]:ARG:NH1	1:F:90:THR:O	2.21	0.74
1:D:256:PRO:HB2	1:D:258:MSE:HE3	1.72	0.72
3:E:302:PP2:H3	3:E:302:PP2:C12	2.00	0.69
1:E:89[B]:ARG:NH1	1:E:90:THR:O	2.27	0.67
1:C:89[A]:ARG:NH1	1:C:90:THR:O	2.28	0.66
1:C:19:LEU:HD22	1:C:88:ILE:HD12	1.82	0.61
1:C:186:LEU:H	1:C:186:LEU:HD23	1.67	0.60
1:F:79:MSE:SE	1:F:130:ARG:HG2	2.52	0.60
1:F:32:ASN:HB2	1:F:35:GLN:HB2	1.84	0.60
1:B:46:LYS:HD2	1:B:47:PRO:HD2	1.82	0.60
1:F:155[A]:ARG:NH1	1:F:270:PHE:O	2.35	0.59
1:B:27:ARG:HG3	1:B:45:GLY:HA3	1.85	0.57
1:A:30:ARG:NH1	8:A:599:HOH:O	2.30	0.57
1:F:151:GLN:O	1:F:155[A]:ARG:HG3	2.06	0.55
1:A:124:LEU:HD22	1:A:204:LEU:HD13	1.88	0.55
1:E:70:VAL:HG11	1:F:70:VAL:HG11	1.88	0.55
1:D:4:ILE:HG23	1:D:6:ARG:HG3	1.89	0.54
1:E:20:ASP:OD1	1:E:20:ASP:N	2.40	0.54
1:F:124:LEU:HD23	1:F:211:LEU:HD11	1.90	0.53
1:A:166:PHE:HZ	1:A:175[B]:VAL:HG12	1.75	0.52
1:C:75:LEU:HB3	1:C:81:LEU:HD11	1.90	0.52
1:A:6:ARG:HB3	1:A:6:ARG:HH11	1.75	0.52
1:A:7:GLU:OE2	1:B:42:ARG:NH1	2.41	0.51
1:F:109:VAL:HG21	1:F:206:PHE:HB2	1.93	0.51
1:A:6:ARG:HB3	1:A:6:ARG:NH1	2.25	0.51
1:C:70[A]:VAL:HG11	1:D:70[A]:VAL:HG11	1.92	0.51
1:F:122:ASP:OD1	1:F:250:LYS:HG3	2.11	0.49
1:D:256:PRO:HB2	1:D:258:MSE:CE	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:302[A]:PP2:H15	1:D:5:GLN:OE1	2.12	0.48
1:D:124:LEU:HD22	1:D:204:LEU:HD13	1.95	0.48
1:A:188:PHE:CD1	1:A:260:LYS:HE2	2.49	0.48
1:C:169:GLU:HA	1:F:1:MSE:HE3	1.96	0.48
1:D:122:ASP:OD1	1:D:250:LYS:HG3	2.13	0.47
1:F:12:ARG:HH21	1:F:15:LEU:HD11	1.79	0.47
1:E:75:LEU:HB3	1:E:81:LEU:HD11	1.96	0.47
1:D:89:ARG:NH1	1:D:90:THR:O	2.46	0.46
1:D:258:MSE:HE2	1:D:258:MSE:HA	1.96	0.46
1:E:188:PHE:CD1	1:E:260:LYS:HE2	2.50	0.46
1:A:175[A]:VAL:HG23	8:A:411:HOH:O	2.15	0.46
1:B:52:LEU:HD23	1:B:99:THR:HA	1.98	0.46
1:D:56:HIS:HB2	1:D:95:TRP:CZ3	2.51	0.46
1:A:27:ARG:HB3	1:A:27:ARG:HE	1.30	0.46
1:F:12:ARG:NH2	1:F:15:LEU:HD11	2.31	0.45
1:D:21:ALA:HA	1:D:24:TYR:CZ	2.51	0.45
1:D:148:ARG:HD2	8:D:600:HOH:O	2.16	0.45
1:B:69:MSE:HG3	1:B:87:PHE:CG	2.51	0.44
1:A:19:LEU:O	1:A:23:LEU:HG	2.17	0.44
1:F:26:TYR:CE2	1:F:46:LYS:HD3	2.53	0.44
1:D:70[B]:VAL:HG12	1:D:141:PHE:HZ	1.83	0.43
1:B:121:VAL:HA	1:B:124:LEU:HD12	2.00	0.43
1:C:101:ILE:HD13	1:C:213:GLY:HA3	2.01	0.43
1:B:31:ASP:HA	1:B:32:ASN:HA	1.72	0.42
1:F:245:LYS:HE2	1:F:249:GLN:NE2	2.34	0.42
1:A:75:LEU:HB3	1:A:81:LEU:HD11	2.01	0.42
1:C:257:ASP:CG	1:C:260:LYS:HG3	2.40	0.42
1:F:32:ASN:ND2	1:F:38:ALA:O	2.33	0.42
1:B:122:ASP:OD1	1:B:250:LYS:HG3	2.19	0.42
1:E:155:ARG:HH21	1:E:271:PHE:HA	1.85	0.42
1:C:55:LYS:HE3	3:C:302[B]:PP2:H15	2.01	0.41
1:B:265:LEU:HA	1:B:265:LEU:HD23	1.79	0.41
1:E:46:LYS:HA	1:E:47:PRO:HD2	1.95	0.41
1:B:46:LYS:HG2	1:B:49:ALA:HB3	2.02	0.41
1:D:23:LEU:HA	1:D:23:LEU:HD12	1.82	0.41
1:B:69:MSE:HB3	1:B:69:MSE:HE3	1.96	0.41
1:F:4:ILE:HG23	1:F:6[B]:ARG:HG3	2.02	0.41
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.92	0.41
1:B:168:ASP:O	1:B:171:ASN:HB2	2.21	0.41
1:B:75:LEU:HB3	1:B:81:LEU:HD11	2.03	0.41
1:B:258:MSE:HE3	8:B:520:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:GLN:HB2	1:E:179:TRP:CH2	2.55	0.41
1:F:2:SER:HB2	1:F:3:HIS:CD2	2.56	0.41
1:B:109:VAL:HG12	1:B:120:ILE:HD11	2.03	0.41
1:A:89:ARG:HB3	1:B:87:PHE:HB3	2.03	0.40
1:F:48:ASN:OD1	1:F:48:ASN:N	2.54	0.40
1:C:226:TYR:HA	1:C:229:LEU:HB2	2.04	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	265/272 (97%)	257 (97%)	7 (3%)	1 (0%)	39	31
1	B	250/272 (92%)	247 (99%)	3 (1%)	0	100	100
1	C	257/272 (94%)	251 (98%)	6 (2%)	0	100	100
1	D	267/272 (98%)	263 (98%)	4 (2%)	0	100	100
1	E	256/272 (94%)	246 (96%)	10 (4%)	0	100	100
1	F	266/272 (98%)	260 (98%)	6 (2%)	0	100	100
All	All	1561/1632 (96%)	1524 (98%)	36 (2%)	1 (0%)	56	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	VAL

### 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	234/231 (101%)	227 (97%)	7 (3%)	48	44
1	B	225/231 (97%)	222 (99%)	3 (1%)	76	77
1	C	226/231 (98%)	221 (98%)	5 (2%)	60	59
1	D	238/231 (103%)	235 (99%)	3 (1%)	76	77
1	E	225/231 (97%)	224 (100%)	1 (0%)	93	95
1	F	237/231 (103%)	233 (98%)	4 (2%)	68	69
All	All	1385/1386 (100%)	1362 (98%)	23 (2%)	68	69

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	14	ARG
1	A	16	ASN
1	A	20	ASP
1	A	27	ARG
1	A	33	VAL
1	A	216	ASP
1	B	31	ASP
1	B	189	SER
1	B	240	SER
1	C	18	ASN
1	C	33	VAL
1	C	35	GLN
1	C	186	LEU
1	C	240	SER
1	D	2	SER
1	D	4	ILE
1	D	31	ASP
1	E	20	ASP
1	F	5	GLN
1	F	23	LEU
1	F	48	ASN
1	F	104	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 29 ligands modelled in this entry, 8 are monoatomic - leaving 21 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	0.84	2 (5%)	44,52,52	1.23	4 (9%)
3	PP2	A	302	-	20,23,23	3.52	2 (10%)	23,35,35	2.34	2 (8%)
6	ACT	A	305	4	1,3,3	1.17	0	0,3,3	0.00	-
2	KAN	B	301	-	35,35,35	0.61	0	44,52,52	1.35	5 (11%)
3	PP2	B	302	-	20,23,23	3.45	2 (10%)	23,35,35	2.34	3 (13%)
6	ACT	B	304	4	1,3,3	1.30	0	0,3,3	0.00	-
2	KAN	C	301	-	35,35,35	0.79	1 (2%)	44,52,52	1.39	8 (18%)
3	PP2	C	302[A]	-	20,23,23	3.51	2 (10%)	23,35,35	2.48	4 (17%)
3	PP2	C	302[B]	-	20,23,23	3.48	2 (10%)	23,35,35	2.47	3 (13%)
7	PEG	C	303	-	6,6,6	1.11	0	5,5,5	1.40	0
2	KAN	D	301	-	35,35,35	0.80	1 (2%)	44,52,52	1.41	6 (13%)
3	PP2	D	302	-	20,23,23	3.34	2 (10%)	23,35,35	2.44	3 (13%)
6	ACT	D	305	-	1,3,3	1.83	0	0,3,3	0.00	-
6	ACT	D	306	4	1,3,3	1.39	0	0,3,3	0.00	-
2	KAN	E	301	-	35,35,35	0.89	1 (2%)	44,52,52	1.51	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PP2	E	302	-	20,23,23	3.34	3 (15%)	23,35,35	2.35	2 (8%)
6	ACT	E	304	4	1,3,3	0.92	0	0,3,3	0.00	-
2	KAN	F	301	-	35,35,35	0.86	1 (2%)	44,52,52	1.44	5 (11%)
3	PP2	F	302	-	20,23,23	3.43	2 (10%)	23,35,35	2.54	3 (13%)
6	ACT	F	305	4	1,3,3	1.27	0	0,3,3	0.00	-
7	PEG	F	306	-	6,6,6	1.04	0	5,5,5	1.56	0

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	PP2	A	302	-	-	0/10/10/10	0/3/3/3
6	ACT	A	305	4	-	0/0/0/0	0/0/0/0
2	KAN	B	301	-	-	0/12/72/72	0/3/3/3
3	PP2	B	302	-	-	0/10/10/10	0/3/3/3
6	ACT	B	304	4	-	0/0/0/0	0/0/0/0
2	KAN	C	301	-	-	0/12/72/72	0/3/3/3
3	PP2	C	302[A]	-	-	0/10/10/10	0/3/3/3
3	PP2	C	302[B]	-	-	0/10/10/10	0/3/3/3
7	PEG	C	303	-	-	0/4/4/4	0/0/0/0
2	KAN	D	301	-	-	0/12/72/72	0/3/3/3
3	PP2	D	302	-	-	0/10/10/10	0/3/3/3
6	ACT	D	305	-	-	0/0/0/0	0/0/0/0
6	ACT	D	306	4	-	0/0/0/0	0/0/0/0
2	KAN	E	301	-	-	0/12/72/72	0/3/3/3
3	PP2	E	302	-	-	0/10/10/10	0/3/3/3
6	ACT	E	304	4	-	0/0/0/0	0/0/0/0
2	KAN	F	301	-	-	0/12/72/72	0/3/3/3
3	PP2	F	302	-	-	0/10/10/10	0/3/3/3
6	ACT	F	305	4	-	0/0/0/0	0/0/0/0
7	PEG	F	306	-	-	0/4/4/4	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	PP2	N9-N10	-13.40	1.23	1.37
3	C	302[A]	PP2	N9-N10	-13.33	1.23	1.37
3	F	302	PP2	N9-N10	-13.25	1.23	1.37
3	A	302	PP2	N9-N10	-13.16	1.24	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302[B]	PP2	N9-N10	-13.09	1.24	1.37
3	E	302	PP2	N9-N10	-13.09	1.24	1.37
3	D	302	PP2	N9-N10	-13.05	1.24	1.37
3	A	302	PP2	C11-C8	-8.03	1.39	1.49
3	C	302[B]	PP2	C11-C8	-7.88	1.40	1.49
3	C	302[A]	PP2	C11-C8	-7.74	1.40	1.49
3	F	302	PP2	C11-C8	-7.21	1.40	1.49
3	B	302	PP2	C11-C8	-7.03	1.41	1.49
3	D	302	PP2	C11-C8	-6.81	1.41	1.49
3	E	302	PP2	C11-C8	-6.50	1.41	1.49
2	F	301	KAN	C14-C15	-2.62	1.50	1.53
2	D	301	KAN	C16-C15	-2.19	1.50	1.53
3	E	302	PP2	C8-N9	-2.11	1.33	1.35
2	C	301	KAN	O5-C1	2.14	1.47	1.41
2	A	301	KAN	O5-C5	2.21	1.49	1.44
2	A	301	KAN	O11-C13	2.23	1.47	1.41
2	E	301	KAN	O5-C1	2.40	1.48	1.41

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	302	PP2	N2-C3-N4	-10.64	120.75	128.89
3	C	302[B]	PP2	N2-C3-N4	-10.38	120.94	128.89
3	C	302[A]	PP2	N2-C3-N4	-10.27	121.03	128.89
3	A	302	PP2	N2-C3-N4	-10.05	121.20	128.89
3	B	302	PP2	N2-C3-N4	-9.97	121.26	128.89
3	D	302	PP2	N2-C3-N4	-9.84	121.36	128.89
3	E	302	PP2	N2-C3-N4	-9.69	121.47	128.89
2	D	301	KAN	C6-C5-C4	-4.40	104.85	113.17
2	F	301	KAN	C6-C5-C4	-4.04	105.53	113.17
2	B	301	KAN	C6-C5-C4	-3.34	106.85	113.17
2	E	301	KAN	C6-C5-C4	-3.29	106.96	113.17
2	C	301	KAN	C6-C5-C4	-3.23	107.06	113.17
2	D	301	KAN	C18-C17-C16	-2.97	105.70	113.02
2	A	301	KAN	C6-C5-C4	-2.91	107.66	113.17
2	D	301	KAN	O14-C16-C15	-2.45	106.17	110.31
2	B	301	KAN	C1-O9-C10	-2.40	111.75	118.01
2	F	301	KAN	C14-C15-N4	-2.28	106.63	110.86
3	C	302[A]	PP2	C16-C11-C8	-2.22	117.13	120.70
2	C	301	KAN	O11-C13-C14	-2.18	102.81	108.10
2	E	301	KAN	C14-C15-N4	-2.04	107.07	110.86
2	C	301	KAN	O13-C14-C13	-2.04	105.55	110.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302[B]	PP2	C16-C11-C8	-2.03	117.43	120.70
3	C	302[A]	PP2	C8-C6-C1	-2.02	102.75	106.55
2	C	301	KAN	O9-C10-C9	2.04	112.44	107.17
2	D	301	KAN	C10-C9-C8	2.05	113.20	109.06
3	A	302	PP2	C11-C8-N9	2.06	123.37	120.71
2	C	301	KAN	O13-C14-C15	2.11	113.87	110.31
3	F	302	PP2	C15-C14-CL	2.14	122.86	119.35
3	D	302	PP2	C15-C14-CL	2.15	122.87	119.35
2	B	301	KAN	O5-C5-C6	2.15	110.31	106.10
3	B	302	PP2	C12-C11-C8	2.23	124.29	120.70
2	D	301	KAN	C13-C14-C15	2.26	113.44	110.40
3	B	302	PP2	C11-C8-N9	2.29	123.66	120.71
2	F	301	KAN	C10-C9-C8	2.38	113.86	109.06
2	A	301	KAN	O5-C5-C6	2.47	110.92	106.10
2	A	301	KAN	O12-C17-C18	2.51	112.69	106.36
2	C	301	KAN	C13-C14-C15	2.51	113.77	110.40
3	C	302[A]	PP2	C11-C8-N9	2.62	124.10	120.71
2	B	301	KAN	C13-C14-C15	2.75	114.10	110.40
3	C	302[B]	PP2	C11-C8-N9	2.85	124.39	120.71
2	E	301	KAN	C13-C14-C15	2.95	114.36	110.40
2	F	301	KAN	O5-C5-C6	2.98	111.93	106.10
3	E	302	PP2	C11-C8-N9	3.06	124.66	120.71
2	B	301	KAN	O11-C8-C9	3.19	115.39	107.17
2	F	301	KAN	O11-C8-C9	3.26	115.60	107.17
2	C	301	KAN	O11-C8-C9	3.28	115.63	107.17
3	D	302	PP2	C11-C8-N9	3.29	124.96	120.71
2	C	301	KAN	O5-C5-C6	3.30	112.55	106.10
2	E	301	KAN	O11-C8-C9	3.39	115.93	107.17
3	F	302	PP2	C11-C8-N9	3.40	125.11	120.71
2	A	301	KAN	O11-C8-C9	3.41	115.96	107.17
2	D	301	KAN	O11-C8-C9	3.53	116.29	107.17
2	E	301	KAN	O5-C5-C6	5.01	115.89	106.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	PP2	2	0
3	B	302	PP2	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	302[A]	PP2	3	0
3	C	302[B]	PP2	3	0
3	D	302	PP2	2	0
3	E	302	PP2	3	0
3	F	302	PP2	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	260/272 (95%)	0.07	19 (7%) 18 21	15, 29, 87, 112	0
1	B	250/272 (91%)	0.45	29 (11%) 6 8	20, 39, 87, 121	0
1	C	248/272 (91%)	-0.02	14 (5%) 28 32	17, 27, 60, 104	0
1	D	259/272 (95%)	0.14	20 (7%) 16 19	17, 30, 80, 121	0
1	E	248/272 (91%)	-0.00	12 (4%) 34 38	16, 30, 57, 109	0
1	F	259/272 (95%)	0.14	20 (7%) 16 19	17, 29, 79, 116	0
All	All	1524/1632 (93%)	0.13	114 (7%) 17 20	15, 30, 75, 121	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	24	TYR	7.8
1	B	14	ARG	7.7
1	C	36	SER	7.7
1	F	24	TYR	7.0
1	D	24	TYR	6.9
1	A	16	ASN	6.6
1	D	4	ILE	6.2
1	B	6	ARG	6.1
1	B	48	ASN	5.9
1	A	17	SER	5.7
1	C	34	GLY	5.3
1	D	36	SER	5.3
1	B	45	GLY	5.2
1	F	22	ASP	5.2
1	D	32	ASN	5.2
1	A	18	ASN	5.1
1	A	6	ARG	5.1
1	B	5	GLN	5.0
1	F	23	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	47	PRO	4.7
1	F	28	TRP	4.5
1	A	8	THR	4.5
1	F	48	ASN	4.5
1	D	14	ARG	4.4
1	B	32	ASN	4.4
1	B	8	THR	4.4
1	B	49	ALA	4.3
1	F	33	VAL	4.3
1	E	18	ASN	4.2
1	D	45	GLY	4.2
1	C	48	ASN	4.2
1	E	36	SER	4.2
1	D	22	ASP	4.2
1	D	2	SER	4.1
1	A	14	ARG	4.0
1	B	15	LEU	4.0
1	F	44	TYR	4.0
1	C	18	ASN	4.0
1	F	36	SER	3.9
1	F	47	PRO	3.8
1	C	33	VAL	3.7
1	B	44	TYR	3.7
1	F	32	ASN	3.6
1	D	33	VAL	3.6
1	A	13	PRO	3.6
1	F	35	GLN	3.6
1	C	20	ASP	3.6
1	B	25	GLY	3.5
1	D	48	ASN	3.5
1	C	19	LEU	3.5
1	F	14	ARG	3.4
1	F	2	SER	3.4
1	A	34	GLY	3.4
1	A	12	ARG	3.4
1	B	27	ARG	3.3
1	A	21	ALA	3.3
1	B	47	PRO	3.3
1	D	3	HIS	3.2
1	A	11	SER	3.2
1	D	20	ASP	3.2
1	C	22	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	27	ARG	3.0
1	D	49	ALA	3.0
1	A	33	VAL	3.0
1	A	9	SER	3.0
1	C	49	ALA	3.0
1	A	19	LEU	2.9
1	B	186	LEU	2.8
1	F	21	ALA	2.8
1	B	189	SER	2.8
1	F	15	LEU	2.8
1	D	35	GLN	2.8
1	C	24	TYR	2.8
1	D	34	GLY	2.7
1	F	29	ALA	2.7
1	E	160	LEU	2.7
1	D	21	ALA	2.7
1	D	255	ASN	2.7
1	E	19	LEU	2.7
1	F	49	ALA	2.7
1	B	199	PHE	2.7
1	E	168	ASP	2.6
1	C	21	ALA	2.6
1	F	187	PRO	2.5
1	E	189	SER	2.5
1	E	158	ASN	2.5
1	B	254	ASP	2.4
1	E	208	GLU	2.4
1	A	22	ASP	2.4
1	A	24	TYR	2.4
1	A	7	GLU	2.4
1	A	15	LEU	2.3
1	B	187	PRO	2.3
1	B	13	PRO	2.3
1	B	31	ASP	2.3
1	E	186	LEU	2.3
1	E	21	ALA	2.3
1	C	255	ASN	2.2
1	B	28	TRP	2.2
1	B	208	GLU	2.2
1	A	20	ASP	2.2
1	E	157	ASN	2.2
1	B	210	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	230	ALA	2.1
1	B	46	LYS	2.1
1	F	189	SER	2.1
1	C	186	LEU	2.1
1	B	159	GLY	2.1
1	D	231	ILE	2.0
1	B	23	LEU	2.0
1	B	10	CYS	2.0
1	B	50	PRO	2.0
1	D	31	ASP	2.0
1	E	20	ASP	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	PEG	C	303	7/7	0.89	0.18	5.31	38,60,89,127	0
3	PP2	F	302	21/21	0.87	0.16	2.56	16,38,75,133	21
7	PEG	F	306	7/7	0.91	0.13	2.40	35,42,68,114	0
3	PP2	B	302	21/21	0.91	0.13	1.61	19,37,63,143	21
5	CL	A	304	1/1	0.95	0.10	1.24	45,45,45,45	0
6	ACT	D	305	4/4	0.89	0.12	1.00	32,38,46,75	0
4	NA	D	303	1/1	0.96	0.08	0.85	22,22,22,22	1
3	PP2	E	302	21/21	0.93	0.13	0.56	11,20,39,60	21
3	PP2	C	302[A]	21/21	0.95	0.12	0.41	3,22,47,104	21
3	PP2	D	302	21/21	0.93	0.13	0.26	10,24,51,82	21

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PP2	C	302[B]	21/21	0.95	0.12	0.16	0,21,75,103	21
2	KAN	B	301	33/33	0.95	0.10	0.08	25,28,36,38	0
3	PP2	A	302	21/21	0.94	0.13	0.05	15,30,81,115	21
2	KAN	E	301	33/33	0.94	0.10	-0.45	30,33,37,38	0
2	KAN	D	301	33/33	0.97	0.07	-0.52	17,21,25,25	0
2	KAN	C	301	33/33	0.97	0.07	-0.64	22,25,35,38	0
2	KAN	A	301	33/33	0.96	0.08	-0.79	17,23,33,36	0
2	KAN	F	301	33/33	0.97	0.07	-0.82	13,19,26,27	0
4	NA	F	303	1/1	0.99	0.04	-3.33	23,23,23,23	1
4	NA	E	303	1/1	0.96	0.12	-	35,35,35,35	0
4	NA	F	304	1/1	0.94	0.14	-	37,37,37,37	0
4	NA	D	304	1/1	0.94	0.10	-	40,40,40,40	0
4	NA	A	303	1/1	0.95	0.14	-	32,32,32,32	0
6	ACT	B	304	4/4	0.90	0.21	-	31,59,67,91	0
6	ACT	F	305	4/4	0.80	0.23	-	61,75,101,107	0
6	ACT	E	304	4/4	0.92	0.18	-	37,47,51,99	0
6	ACT	D	306	4/4	0.81	0.20	-	44,60,61,66	0
6	ACT	A	305	4/4	0.89	0.15	-	27,40,47,49	0
4	NA	B	303	1/1	0.91	0.19	-	44,44,44,44	0

## 6.5 Other polymers

There are no such residues in this entry.