



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:30 am GMT

PDB ID : 4FEV
Title : Crystal structure of the aminoglycoside phosphotransferase APH(3')-Ia, with substrate kanamycin and small molecule inhibitor pyrazolopyrimidine PP1
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 : 1.89 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

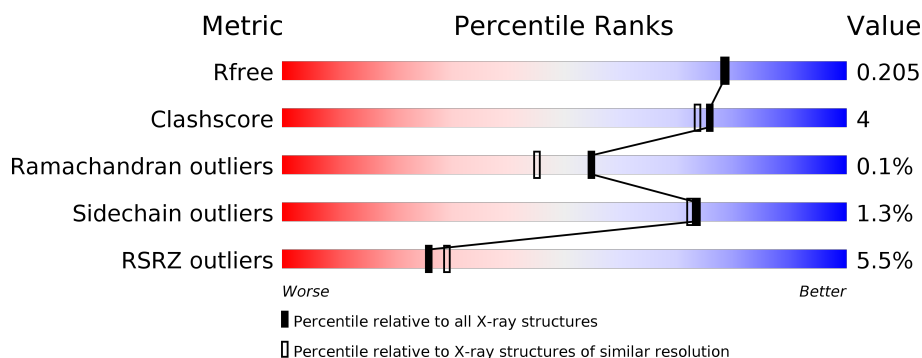
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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}	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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>4%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div>•</div> </div> </div>
1	B	272	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>•</div> <div>7%</div> </div> </div>
1	C	272	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>•</div> <div>7%</div> </div> </div>
1	D	272	<div> <div>9%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
1	E	272	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>5%</div> <div>•</div> </div> </div>
1	F	272	<div> <div>8%</div> <div> <div></div> <div>85%</div> <div>7%</div> <div>•</div> <div>7%</div> </div> </div>

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	PP1	F	302	-	-	-	X
4	NA	B	303	-	-	-	X
4	NA	E	303	-	-	-	X
4	NA	F	303	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14518 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.

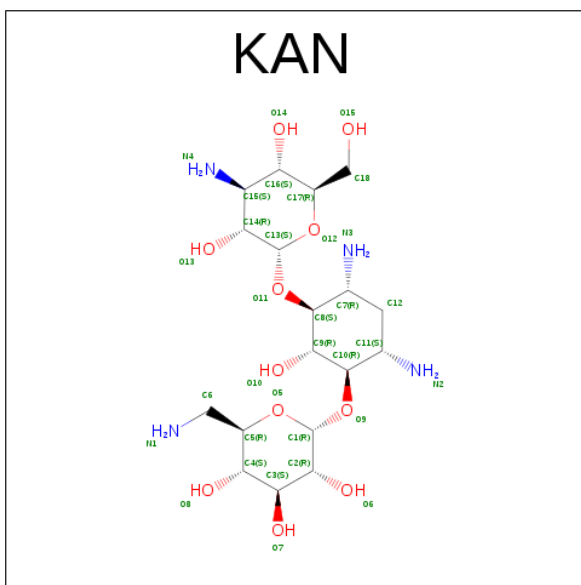
- Molecule 1 is a protein called Aminoglycoside 3'-phosphotransferase AphA1-IAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	4	0
			2144	1367	371	395	11			
1	B	254	Total	C	N	O	S	0	2	0
			2066	1318	361	376	11			
1	C	254	Total	C	N	O	S	0	4	0
			2070	1325	353	382	10			
1	D	271	Total	C	N	O	S	0	9	0
			2249	1430	393	414	12			
1	E	268	Total	C	N	O	S	0	4	0
			2181	1391	379	400	11			
1	F	252	Total	C	N	O	S	0	1	0
			2040	1304	350	376	10			

There are 6 discrepancies between the modelled and reference sequences:

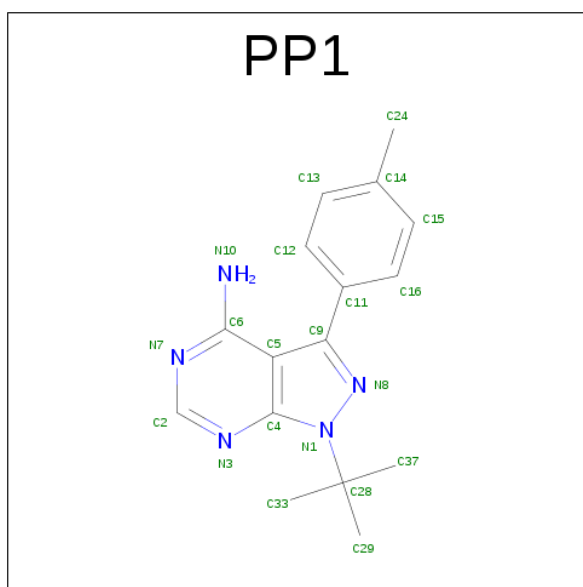
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP B0VD92
B	0	GLY	-	EXPRESSION TAG	UNP B0VD92
C	0	GLY	-	EXPRESSION TAG	UNP B0VD92
D	0	GLY	-	EXPRESSION TAG	UNP B0VD92
E	0	GLY	-	EXPRESSION TAG	UNP B0VD92
F	0	GLY	-	EXPRESSION TAG	UNP B0VD92

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



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

- Molecule 3 is 1-TER-BUTYL-3-P-TOLYL-1H-PYRAZOLO[3,4-D]PYRIMIDIN-4-YLAMIN E (three-letter code: PP1) (formula: C₁₆H₁₉N₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			21	16	5		
3	B	1	Total	C	N	0	0
			21	16	5		
3	C	1	Total	C	N	0	1
			42	32	10		
3	D	1	Total	C	N	0	0
			21	16	5		
3	E	1	Total	C	N	0	0
			21	16	5		
3	F	1	Total	C	N	0	0
			21	16	5		

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

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

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



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

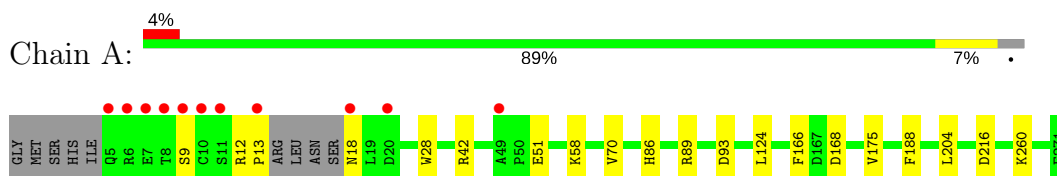
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	279	Total	O	0	1
			280	280		
6	B	178	Total	O	0	1
			179	179		
6	C	248	Total	O	0	2
			250	250		
6	D	244	Total	O	0	0
			244	244		
6	E	238	Total	O	0	1
			239	239		
6	F	217	Total	O	0	3
			220	220		

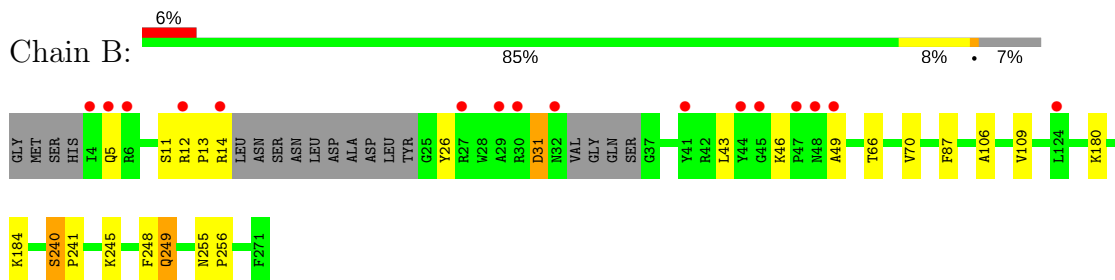
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

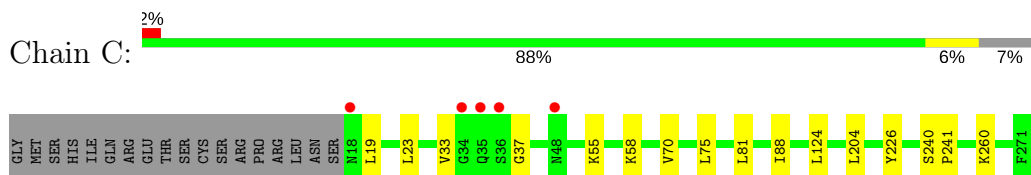
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



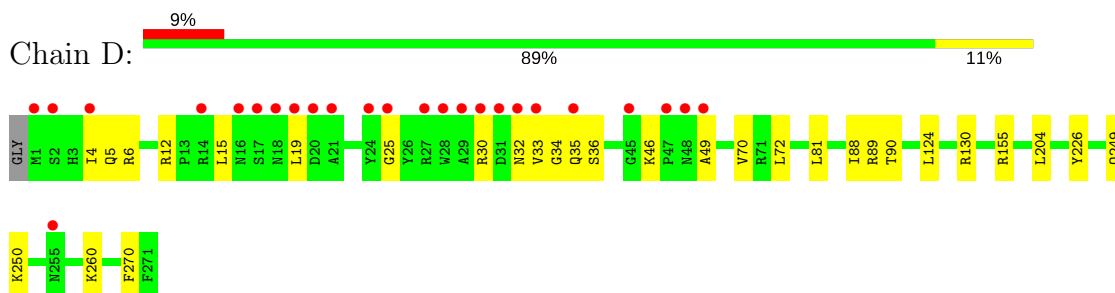
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



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

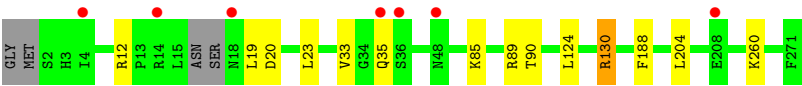


- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB

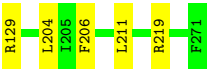
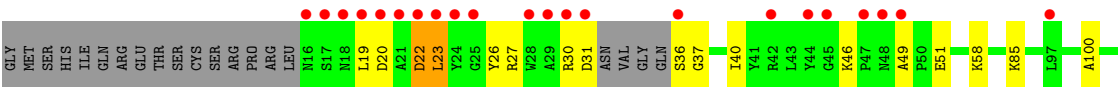
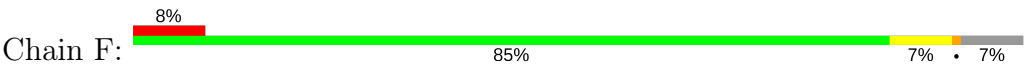


- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB





● 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	57.57Å 94.22Å 96.88Å 61.12° 73.09° 87.44°	Depositor
Resolution (Å)	19.97 – 1.89 19.97 – 1.89	Depositor EDS
% Data completeness (in resolution range)	94.6 (19.97-1.89) 79.5 (19.97-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 1.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1066)	Depositor
R, R_{free}	0.154 , 0.204 0.155 , 0.205	Depositor DCC
R_{free} test set	2039 reflections (1.54%)	DCC
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,-h-k+l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14518	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 4.60% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PP1, KAN, ACT

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	0/2204	0.52	0/2989
1	B	0.33	0/2121	0.49	0/2873
1	C	0.37	0/2127	0.53	0/2888
1	D	0.35	0/2317	0.52	0/3140
1	E	0.37	0/2245	0.52	0/3044
1	F	0.37	0/2093	0.52	0/2839
All	All	0.36	0/13107	0.52	0/17773

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	2144	0	2084	16	0
1	B	2066	0	2015	17	0
1	C	2070	0	2008	13	0
1	D	2249	0	2196	22	0
1	E	2181	0	2129	9	0
1	F	2040	0	1973	12	0
2	A	33	0	36	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	19	2	0
3	B	21	0	19	2	0
3	C	42	0	38	7	0
3	D	21	0	19	2	0
3	E	21	0	19	2	0
3	F	21	0	19	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	D	4	0	3	0	0
6	A	280	0	0	1	0
6	B	179	0	0	4	0
6	C	250	0	0	1	0
6	D	244	0	0	2	0
6	E	239	0	0	3	0
6	F	220	0	0	1	0
All	All	14518	0	12757	93	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 (93) 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:D:302:PP1:HC16	3:D:302:PP1:H101	1.04	1.17
3:C:302[B]:PP1:H101	3:C:302[B]:PP1:HC16	1.04	1.17
3:E:302:PP1:HC16	3:E:302:PP1:H101	1.06	1.16
3:F:302:PP1:HC12	3:F:302:PP1:H101	1.10	1.12
3:B:302:PP1:HC12	3:B:302:PP1:H101	1.12	1.11
3:A:302:PP1:HC12	3:A:302:PP1:H101	1.13	1.09
3:C:302[A]:PP1:HC16	3:C:302[A]:PP1:H101	1.16	1.07
1:C:70:VAL:HG11	1:D:70[B]:VAL:HG21	1.38	1.05
1:A:70:VAL:HG11	1:B:70[B]:VAL:HG21	1.40	1.02
3:C:302[B]:PP1:N10	3:C:302[B]:PP1:HC16	1.85	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:302:PP1:HC16	3:D:302:PP1:N10	1.87	0.88
3:E:302:PP1:N10	3:E:302:PP1:HC16	1.88	0.88
3:F:302:PP1:N10	3:F:302:PP1:HC12	1.92	0.84
3:B:302:PP1:HC12	3:B:302:PP1:N10	1.95	0.81
3:A:302:PP1:HC12	3:A:302:PP1:N10	1.94	0.80
1:A:70:VAL:HG11	1:B:70[A]:VAL:HG11	1.64	0.80
3:C:302[A]:PP1:HC16	3:C:302[A]:PP1:N10	1.95	0.79
1:E:33:VAL:HG23	1:E:35:GLN:HG2	1.73	0.69
3:C:302[B]:PP1:HC13	1:D:5:GLN:NE2	2.08	0.69
1:C:58:LYS:NZ	6:C:541:HOH:O	2.28	0.66
1:A:168:ASP:OD2	1:D:6:ARG:NH1	2.29	0.65
1:A:18:ASN:HB3	1:A:86:HIS:CE1	2.32	0.65
1:A:124:LEU:HD22	1:A:204:LEU:HD13	1.79	0.63
1:A:18:ASN:HB3	1:A:86:HIS:HE1	1.64	0.62
3:C:302[A]:PP1:H101	3:C:302[A]:PP1:C16	2.02	0.60
1:A:12:ARG:HD3	1:A:13:PRO:HD2	1.82	0.60
1:F:219:ARG:NH1	6:F:550:HOH:O	2.30	0.59
1:A:166:PHE:HZ	1:A:175[B]:VAL:HG12	1.67	0.59
1:F:46:LYS:HG2	1:F:49:ALA:HB3	1.86	0.57
1:E:124:LEU:HD22	1:E:204:LEU:HD13	1.87	0.57
1:B:184:LYS:NZ	6:B:499:HOH:O	2.38	0.56
1:D:12:ARG:HH21	1:D:15:LEU:HD11	1.70	0.56
1:F:51:GLU:HG3	1:F:100:ALA:HB3	1.88	0.56
1:C:70:VAL:HG11	1:D:70[A]:VAL:HG11	1.87	0.56
1:D:30:ARG:HD2	1:D:33:VAL:HG22	1.89	0.56
1:C:55:LYS:HE3	3:C:302[A]:PP1:HC13	1.88	0.54
1:E:12:ARG:NH2	6:E:512:HOH:O	2.40	0.53
1:A:188:PHE:CD1	1:A:260:LYS:HE2	2.43	0.53
1:F:20:ASP:HA	1:F:23:LEU:HB2	1.91	0.53
1:D:249[B]:GLN:HE21	1:D:250:LYS:HE2	1.74	0.52
1:C:124:LEU:HD22	1:C:204[A]:LEU:HD13	1.92	0.52
1:E:130:ARG:NH1	6:E:599:HOH:O	2.41	0.51
1:E:188:PHE:CD1	1:E:260:LYS:HE2	2.45	0.51
1:C:33:VAL:HG12	1:D:5:GLN:HG2	1.91	0.51
1:B:249:GLN:HG2	6:B:537:HOH:O	2.10	0.50
1:D:124:LEU:HD22	1:D:204:LEU:HD13	1.94	0.50
1:F:26:TYR:CE1	1:F:46:LYS:HD3	2.46	0.49
1:E:89[A]:ARG:NH1	1:E:90:THR:O	2.44	0.49
1:C:75:LEU:HB3	1:C:81:LEU:HD11	1.93	0.48
1:D:19:LEU:HB2	1:D:88:ILE:HD11	1.95	0.48
1:C:19:LEU:HG	1:C:23:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:LEU:O	1:E:23:LEU:HG	2.15	0.47
1:E:33:VAL:HG23	1:E:35:GLN:CG	2.41	0.47
1:D:25:GLY:O	1:D:46:LYS:HG2	2.15	0.46
1:B:66:THR:O	1:B:70[B]:VAL:HG23	2.15	0.46
1:C:19:LEU:O	1:C:23:LEU:HG	2.15	0.46
1:C:70:VAL:CG1	1:D:70[B]:VAL:HG21	2.28	0.46
1:D:46:LYS:HB3	1:D:49:ALA:HB3	1.98	0.46
1:D:72[B]:LEU:HD12	1:D:81:LEU:HD13	1.98	0.45
1:C:19:LEU:HD22	1:C:88:ILE:HD12	1.98	0.45
1:A:175[A]:VAL:HG23	6:A:629:HOH:O	2.16	0.45
1:B:26:TYR:CD1	1:B:43:LEU:HB3	2.52	0.45
1:D:32:ASN:HB3	1:D:35:GLN:HB2	1.98	0.45
1:C:226:TYR:CD1	1:C:260:LYS:HE3	2.52	0.44
1:F:30:ARG:HA	1:F:40:ILE:O	2.17	0.44
1:F:36:SER:HA	1:F:37:GLY:HA2	1.62	0.44
1:D:33:VAL:HA	1:D:34:GLY:HA2	1.64	0.44
1:D:130[B]:ARG:NH2	6:D:616:HOH:O	2.22	0.44
1:D:89[B]:ARG:NH1	1:D:90:THR:O	2.51	0.43
1:E:85:LYS:NZ	6:E:519:HOH:O	2.44	0.43
1:D:155:ARG:HD3	1:D:270:PHE:O	2.18	0.43
1:F:129[B]:ARG:HA	1:F:129[B]:ARG:HD3	1.81	0.43
1:A:70:VAL:HG11	1:B:70[B]:VAL:CG2	2.30	0.43
1:F:206:PHE:CE1	1:F:211:LEU:HD13	2.54	0.43
1:B:248:PHE:CG	1:B:256:PRO:HG3	2.54	0.43
1:A:58:LYS:HD2	1:A:93:ASP:OD2	2.19	0.42
1:D:72[B]:LEU:HG	6:D:409:HOH:O	2.20	0.42
1:F:19:LEU:O	1:F:23:LEU:HG	2.20	0.42
1:A:28:TRP:CZ3	1:B:13:PRO:HD2	2.54	0.42
1:B:245:LYS:NZ	6:B:532:HOH:O	2.46	0.42
1:B:240:SER:HA	1:B:241:PRO:HD3	1.93	0.42
1:A:89:ARG:HB3	1:B:87:PHE:HB3	2.02	0.42
1:B:106:ALA:HA	1:B:109:VAL:HG22	2.01	0.42
1:A:70:VAL:CG1	1:B:70[A]:VAL:HG11	2.43	0.41
1:A:42:ARG:NH2	1:A:51:GLU:OE2	2.41	0.41
1:B:31:ASP:N	1:B:31:ASP:OD1	2.54	0.41
1:F:204:LEU:HB3	1:F:211:LEU:HD11	2.03	0.41
1:D:226:TYR:CD1	1:D:260:LYS:HE3	2.56	0.41
1:B:5:GLN:NE2	6:B:449:HOH:O	2.53	0.41
1:D:4:ILE:O	1:D:5:GLN:HG3	2.21	0.41
1:C:240:SER:HA	1:C:241:PRO:HD3	1.95	0.41
1:B:46:LYS:HB3	1:B:49:ALA:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:LYS:HE2	1:F:58:LYS:HB3	1.84	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	263/272 (97%)	255 (97%)	8 (3%)	0	100	100
1	B	250/272 (92%)	246 (98%)	4 (2%)	0	100	100
1	C	256/272 (94%)	251 (98%)	4 (2%)	1 (0%)	38	26
1	D	278/272 (102%)	270 (97%)	8 (3%)	0	100	100
1	E	268/272 (98%)	261 (97%)	7 (3%)	0	100	100
1	F	249/272 (92%)	241 (97%)	7 (3%)	1 (0%)	38	26
All	All	1564/1632 (96%)	1524 (97%)	38 (2%)	2 (0%)	55	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	22	ASP
1	C	37	GLY

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	234/238 (98%)	232 (99%)	2 (1%)	82	82
1	B	225/238 (94%)	217 (96%)	8 (4%)	40	29
1	C	225/238 (94%)	225 (100%)	0	100	100
1	D	247/238 (104%)	246 (100%)	1 (0%)	93	93
1	E	239/238 (100%)	237 (99%)	2 (1%)	85	85
1	F	221/238 (93%)	216 (98%)	5 (2%)	56	49
All	All	1391/1428 (97%)	1373 (99%)	18 (1%)	73	72

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	216	ASP
1	B	11	SER
1	B	12	ARG
1	B	14	ARG
1	B	31	ASP
1	B	180	LYS
1	B	240	SER
1	B	249	GLN
1	B	255	ASN
1	D	36	SER
1	E	20	ASP
1	E	130	ARG
1	F	22	ASP
1	F	23	LEU
1	F	27	ARG
1	F	31	ASP
1	F	85	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	HIS
1	A	262	GLN
1	D	5	GLN
1	D	138	ASN
1	E	153	GLN
1	F	16	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 21 ligands modelled in this entry, 7 are monoatomic - leaving 14 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	0.68	0	46,52,52	1.46	4 (8%)
3	PP1	A	302	-	20,23,23	3.34	2 (10%)	23,35,35	2.22	3 (13%)
2	KAN	B	301	-	35,35,35	0.67	1 (2%)	46,52,52	1.46	7 (15%)
3	PP1	B	302	-	20,23,23	3.44	2 (10%)	23,35,35	2.03	2 (8%)
2	KAN	C	301	-	35,35,35	0.81	1 (2%)	46,52,52	1.70	7 (15%)
3	PP1	C	302[A]	-	20,23,23	3.18	2 (10%)	23,35,35	2.37	5 (21%)
3	PP1	C	302[B]	-	20,23,23	3.33	2 (10%)	23,35,35	2.27	3 (13%)
2	KAN	D	301	-	35,35,35	0.83	2 (5%)	46,52,52	1.58	6 (13%)
3	PP1	D	302	-	20,23,23	3.28	2 (10%)	23,35,35	2.15	2 (8%)
5	ACT	D	305	-	1,3,3	1.36	0	0,3,3	0.00	-
2	KAN	E	301	-	35,35,35	0.84	1 (2%)	46,52,52	1.56	5 (10%)
3	PP1	E	302	-	20,23,23	3.30	3 (15%)	23,35,35	2.11	2 (8%)
2	KAN	F	301	-	35,35,35	0.81	2 (5%)	46,52,52	1.60	7 (15%)
3	PP1	F	302	-	20,23,23	3.30	2 (10%)	23,35,35	2.04	2 (8%)

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	PP1	A	302	-	-	0/10/10/10	0/3/3/3
2	KAN	B	301	-	-	0/12/72/72	0/3/3/3
3	PP1	B	302	-	-	0/10/10/10	0/3/3/3
2	KAN	C	301	-	-	0/12/72/72	0/3/3/3
3	PP1	C	302[A]	-	-	0/10/10/10	0/3/3/3
3	PP1	C	302[B]	-	-	0/10/10/10	0/3/3/3
2	KAN	D	301	-	-	0/12/72/72	0/3/3/3
3	PP1	D	302	-	-	0/10/10/10	0/3/3/3
5	ACT	D	305	-	-	0/0/0/0	0/0/0/0
2	KAN	E	301	-	-	0/12/72/72	0/3/3/3
3	PP1	E	302	-	-	0/10/10/10	0/3/3/3
2	KAN	F	301	-	-	0/12/72/72	0/3/3/3
3	PP1	F	302	-	-	0/10/10/10	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	PP1	N8-N1	-13.46	1.23	1.37
3	E	302	PP1	N8-N1	-13.18	1.24	1.37
3	C	302[B]	PP1	N8-N1	-13.00	1.24	1.37
3	F	302	PP1	N8-N1	-12.97	1.24	1.37
3	D	302	PP1	N8-N1	-12.92	1.24	1.37
3	A	302	PP1	N8-N1	-12.90	1.24	1.37
3	C	302[A]	PP1	N8-N1	-12.44	1.24	1.37
3	A	302	PP1	C11-C9	-7.04	1.40	1.49
3	B	302	PP1	C11-C9	-6.91	1.40	1.49
3	C	302[B]	PP1	C11-C9	-6.79	1.40	1.49
3	D	302	PP1	C11-C9	-6.60	1.41	1.49
3	C	302[A]	PP1	C11-C9	-6.47	1.41	1.49
3	F	302	PP1	C11-C9	-6.42	1.41	1.49
3	E	302	PP1	C11-C9	-5.64	1.42	1.49
3	E	302	PP1	C9-N8	-2.31	1.33	1.35
2	F	301	KAN	C14-C15	-2.11	1.50	1.53
2	D	301	KAN	C14-C15	-2.09	1.50	1.53
2	B	301	KAN	O5-C1	2.01	1.46	1.41
2	D	301	KAN	O5-C1	2.06	1.46	1.41
2	E	301	KAN	O5-C1	2.12	1.47	1.41
2	F	301	KAN	O5-C1	2.24	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	KAN	O5-C1	2.55	1.48	1.41

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302[A]	PP1	N3-C2-N7	-9.39	120.68	128.86
3	A	302	PP1	N3-C2-N7	-9.23	120.82	128.86
3	C	302[B]	PP1	N3-C2-N7	-9.21	120.84	128.86
3	D	302	PP1	N3-C2-N7	-8.86	121.14	128.86
3	E	302	PP1	N3-C2-N7	-8.76	121.23	128.86
3	F	302	PP1	N3-C2-N7	-8.62	121.35	128.86
3	B	302	PP1	N3-C2-N7	-8.44	121.51	128.86
2	C	301	KAN	C6-C5-C4	-5.48	103.22	113.30
2	F	301	KAN	C6-C5-C4	-5.45	103.27	113.30
2	A	301	KAN	C6-C5-C4	-5.27	103.60	113.30
2	D	301	KAN	C6-C5-C4	-5.17	103.79	113.30
2	E	301	KAN	C6-C5-C4	-4.88	104.31	113.30
2	B	301	KAN	C6-C5-C4	-3.79	106.33	113.30
2	C	301	KAN	C17-C16-C15	-3.48	106.47	110.35
2	F	301	KAN	C17-C16-C15	-3.08	106.91	110.35
2	D	301	KAN	C17-C16-C15	-2.71	107.33	110.35
3	C	302[A]	PP1	C16-C15-C14	-2.62	117.92	121.39
2	F	301	KAN	C14-C15-N4	-2.50	105.92	111.00
2	B	301	KAN	C17-C16-C15	-2.48	107.58	110.35
3	C	302[B]	PP1	C16-C15-C14	-2.32	118.32	121.39
2	C	301	KAN	O13-C14-C13	-2.30	105.22	110.03
2	C	301	KAN	O11-C13-C14	-2.26	103.01	108.11
2	A	301	KAN	C16-C15-C14	-2.13	106.43	111.06
2	B	301	KAN	O13-C14-C13	-2.13	105.57	110.03
2	B	301	KAN	C16-C15-C14	-2.09	106.51	111.06
2	F	301	KAN	O5-C1-C2	-2.07	106.31	110.30
3	C	302[A]	PP1	C12-C11-C9	-2.01	117.24	120.64
3	A	302	PP1	C12-C11-C9	2.01	124.05	120.64
2	F	301	KAN	C10-C9-C8	2.05	113.28	109.01
3	F	302	PP1	C11-C9-N8	2.05	124.26	120.82
3	D	302	PP1	C11-C9-N8	2.13	124.39	120.82
3	A	302	PP1	C2-N7-C6	2.18	122.58	118.77
3	B	302	PP1	C12-C11-C9	2.24	124.43	120.64
3	E	302	PP1	C11-C9-N8	2.36	124.77	120.82
2	D	301	KAN	C10-C9-C8	2.39	113.99	109.01
2	D	301	KAN	C13-C14-C15	2.42	113.65	110.40
2	B	301	KAN	C13-C14-C15	2.51	113.77	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	KAN	C13-C14-C15	2.64	113.94	110.40
3	C	302[B]	PP1	C11-C9-N8	2.66	125.28	120.82
2	E	301	KAN	O12-C17-C18	2.68	112.83	106.41
3	C	302[A]	PP1	C16-C11-C9	2.68	125.18	120.64
3	C	302[A]	PP1	C11-C9-N8	2.80	125.51	120.82
2	C	301	KAN	C13-C14-C15	2.86	114.24	110.40
2	A	301	KAN	O11-C8-C9	2.92	114.22	107.19
2	B	301	KAN	O11-C8-C9	3.04	114.51	107.19
2	D	301	KAN	O5-C5-C6	3.10	111.89	106.01
2	C	301	KAN	O11-C8-C9	3.20	114.89	107.19
2	E	301	KAN	O11-C8-C9	3.35	115.25	107.19
2	F	301	KAN	O11-C8-C9	3.47	115.54	107.19
2	F	301	KAN	O5-C5-C6	3.57	112.78	106.01
2	D	301	KAN	O11-C8-C9	3.62	115.91	107.19
2	A	301	KAN	O5-C5-C6	3.83	113.26	106.01
2	B	301	KAN	O5-C5-C6	3.85	113.31	106.01
2	E	301	KAN	O5-C5-C6	3.95	113.48	106.01
2	C	301	KAN	O5-C5-C6	4.39	114.32	106.01

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	PP1	2	0
3	B	302	PP1	2	0
3	C	302[A]	PP1	4	0
3	C	302[B]	PP1	3	0
3	D	302	PP1	2	0
3	E	302	PP1	2	0
3	F	302	PP1	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, 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	263/272 (96%)	-0.17	11 (4%) 37 40	4, 16, 59, 101	0
1	B	254/272 (93%)	0.15	16 (6%) 21 24	10, 27, 71, 84	0
1	C	254/272 (93%)	-0.27	5 (1%) 65 69	7, 16, 43, 80	0
1	D	271/272 (99%)	0.05	25 (9%) 10 11	7, 19, 68, 79	0
1	E	268/272 (98%)	-0.16	7 (2%) 56 60	6, 19, 45, 86	0
1	F	252/272 (92%)	0.25	22 (8%) 11 12	6, 19, 81, 107	0
All	All	1562/1632 (95%)	-0.03	86 (5%) 26 29	4, 19, 66, 107	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	24	TYR	9.6
1	F	21	ALA	8.8
1	B	4	ILE	7.3
1	D	24	TYR	6.8
1	F	22	ASP	6.5
1	D	33	VAL	6.4
1	F	19	LEU	6.3
1	F	48	ASN	5.9
1	F	36	SER	5.8
1	D	32	ASN	5.6
1	C	36	SER	5.6
1	F	18	ASN	5.6
1	A	6	ARG	5.5
1	F	44	TYR	5.5
1	A	8	THR	5.3
1	F	16	ASN	5.2
1	A	5	GLN	5.0
1	B	49	ALA	5.0
1	F	17	SER	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	11	SER	4.7
1	A	7	GLU	4.6
1	F	25	GLY	4.5
1	D	1	MET	4.5
1	E	14	ARG	4.4
1	F	28	TRP	4.3
1	F	47	PRO	4.3
1	E	36	SER	4.1
1	B	32	ASN	4.1
1	B	6	ARG	4.0
1	F	20	ASP	3.9
1	B	48	ASN	3.8
1	F	45	GLY	3.8
1	A	13	PRO	3.7
1	D	45	GLY	3.7
1	F	29	ALA	3.6
1	D	4	ILE	3.5
1	D	14	ARG	3.5
1	A	18	ASN	3.4
1	B	124	LEU	3.4
1	B	27	ARG	3.3
1	B	29	ALA	3.3
1	D	17	SER	3.3
1	B	5	GLN	3.3
1	B	45	GLY	3.2
1	A	9	SER	3.0
1	F	23	LEU	2.9
1	B	44	TYR	2.9
1	F	49	ALA	2.9
1	D	48	ASN	2.9
1	D	20	ASP	2.8
1	C	18	ASN	2.7
1	D	31	ASP	2.7
1	F	97	LEU	2.7
1	D	28	TRP	2.7
1	E	4	ILE	2.6
1	E	35	GLN	2.6
1	D	19	LEU	2.6
1	D	16	ASN	2.6
1	D	21	ALA	2.6
1	D	49	ALA	2.6
1	C	35	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	31	ASP	2.5
1	D	30	ARG	2.5
1	F	30	ARG	2.5
1	D	35	GLN	2.5
1	A	49	ALA	2.4
1	D	255	ASN	2.4
1	F	42	ARG	2.4
1	E	208	GLU	2.4
1	D	29	ALA	2.4
1	C	48	ASN	2.3
1	B	14	ARG	2.3
1	D	47	PRO	2.3
1	E	18	ASN	2.2
1	D	27	ARG	2.2
1	A	20	ASP	2.2
1	D	18	ASN	2.2
1	B	47	PRO	2.2
1	A	10	CYS	2.2
1	B	12	ARG	2.1
1	C	34	GLY	2.1
1	D	25	GLY	2.1
1	E	48	ASN	2.1
1	B	41	TYR	2.1
1	B	30	ARG	2.0
1	D	2	SER	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(Å ²)	Q<0.9
4	NA	B	303	1/1	0.95	0.33	13.88	37,37,37,37	0
4	NA	E	303	1/1	0.95	0.19	8.41	25,25,25,25	1
4	NA	F	303	1/1	0.98	0.14	5.26	13,13,13,13	1
3	PP1	F	302	21/21	0.86	0.17	2.64	19,34,71,78	21
3	PP1	C	302[B]	21/21	0.94	0.15	1.57	0,10,47,60	21
3	PP1	C	302[A]	21/21	0.94	0.15	1.47	0,8,43,66	21
3	PP1	B	302	21/21	0.94	0.11	1.01	18,31,70,131	21
2	KAN	F	301	33/33	0.94	0.09	0.58	6,10,20,20	0
3	PP1	A	302	21/21	0.96	0.13	0.30	6,16,68,75	0
2	KAN	D	301	33/33	0.95	0.09	0.19	6,9,19,22	0
2	KAN	B	301	33/33	0.94	0.11	0.05	15,22,26,28	0
3	PP1	D	302	21/21	0.94	0.11	-0.13	5,16,79,86	21
3	PP1	E	302	21/21	0.96	0.10	-0.31	8,12,62,113	0
2	KAN	A	301	33/33	0.94	0.09	-0.35	6,17,23,27	0
2	KAN	C	301	33/33	0.95	0.08	-0.56	9,19,26,29	0
2	KAN	E	301	33/33	0.96	0.08	-0.71	14,22,26,27	0
4	NA	D	303	1/1	0.94	0.06	-0.91	19,19,19,19	1
5	ACT	D	305	4/4	0.89	0.14	-	34,43,46,119	0
4	NA	A	303	1/1	0.94	0.27	-	30,30,30,30	1
4	NA	F	304	1/1	0.96	0.14	-	32,32,32,32	0
4	NA	D	304	1/1	0.86	0.19	-	32,32,32,32	1

6.5 Other polymers [i](#)

There are no such residues in this entry.