Full wwPDB X-ray Structure Validation Report (i)

May 15, 2020 – 02:03 pm BST

PDB ID : 1YGK

Title : Crystal Structure of Pyridoxal Kinase in Complex with Roscovitine and Derivatives

Authors : Tang, L.; Li, M.-H.; Cao, P.; Wang, F.; Chang, W.-R.; Bach, S.; Reinhardt, J.; Ferandin, Y.; Koken, M.; Galons, H.; Wan, Y.; Gray, N.; Meijer, L.; Jiang, T.; Liang, D.-C.

Deposited on : 2005-01-05

Resolution : 2.60 Å(reported)

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

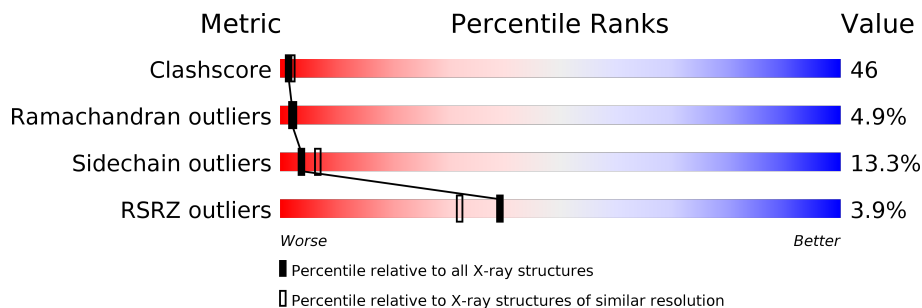|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	Percentile Ranks	Value
Clashscore		46
Ramachandran outliers		4.9%
Sidechain outliers		13.3%
RSRZ outliers		3.9%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	312	4% 37% 50% 11% ••

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2624 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 Pyridoxal kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2414	1517	424	457	16			

- Molecule 2 is R-ROSCOVITINE (three-letter code: RRC) (formula: $C_{19}H_{26}N_6O$).

RRC
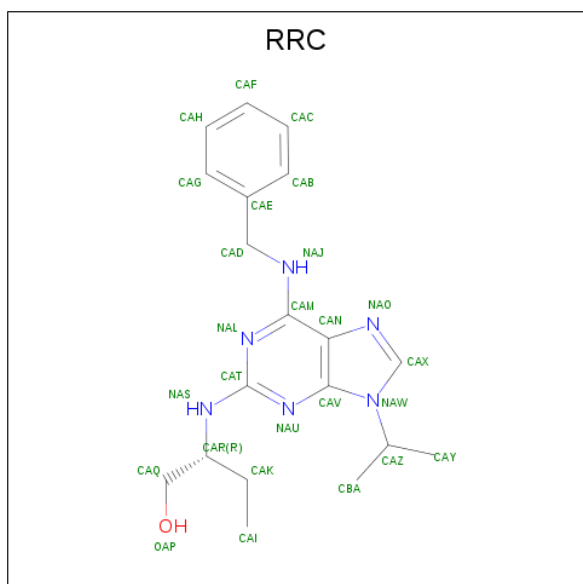
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	19	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	184	Total	O	0	0
			184	184		

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: Pyridoxal kinase
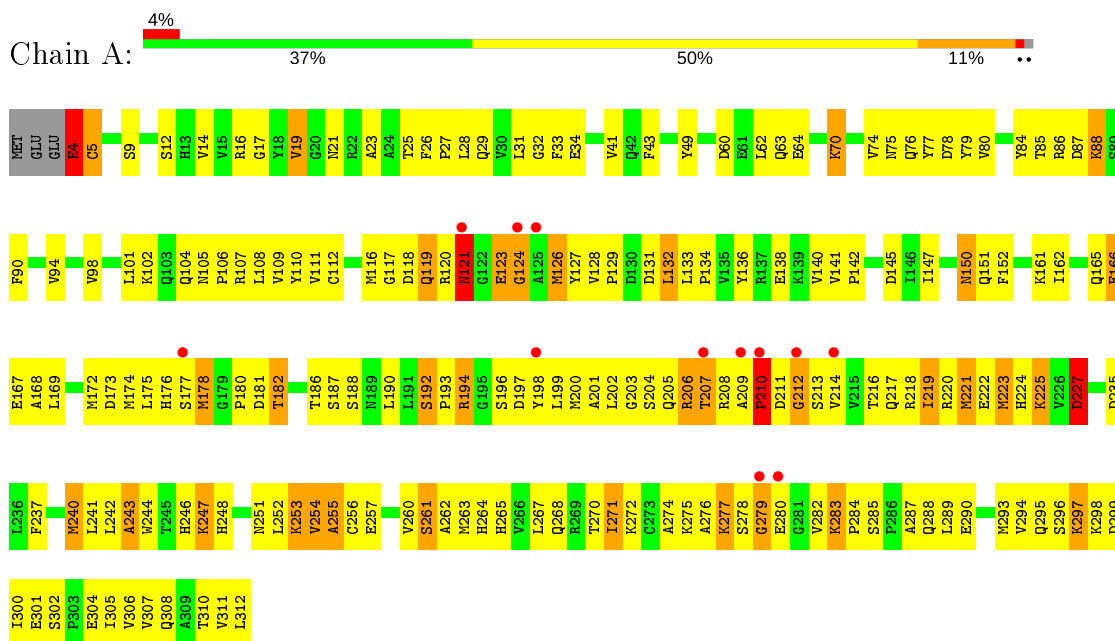
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	102.83Å 102.83Å 58.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.60 9.96 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.60) 98.6 (9.96-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.36 (at 2.60Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.271 0.231 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	43.5	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 67.0	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	2624	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.17% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: RRC

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	0.67	1/2459 (0.0%)	1.09	10/3333 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	GLU	C-O	7.24	1.37	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	GLY	N-CA-C	-10.49	86.88	113.10
1	A	132	LEU	CA-CB-CG	6.81	130.97	115.30
1	A	127	TYR	CB-CA-C	-6.31	97.79	110.40
1	A	227	ASP	N-CA-C	5.82	126.71	111.00
1	A	127	TYR	CA-CB-CG	5.73	124.29	113.40
1	A	211	ASP	CB-CA-C	5.73	121.86	110.40
1	A	5	CYS	N-CA-C	5.59	126.10	111.00
1	A	280	GLU	N-CA-C	-5.37	96.51	111.00
1	A	124	GLY	N-CA-C	5.09	125.84	113.10
1	A	121	ASN	N-CA-C	5.02	124.56	111.00

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	2414	0	2418	226	0
2	A	26	0	26	4	0
3	A	184	0	0	7	0
All	All	2624	0	2444	226	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 46.

All (226) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:GLU:HG3	1:A:5:CYS:N	1.31	1.26
1:A:251:ASN:HB3	1:A:254:VAL:HG23	1.24	1.18
1:A:4:GLU:CG	1:A:5:CYS:H	1.57	1.17
1:A:70:LYS:HA	1:A:75:ASN:HD22	1.10	1.09
1:A:192:SER:HB2	1:A:222:GLU:OE2	1.60	1.02
1:A:70:LYS:HA	1:A:75:ASN:ND2	1.76	0.99
1:A:251:ASN:HB3	1:A:254:VAL:CG2	1.95	0.96
1:A:240:MET:HE3	1:A:300:ILE:HG23	1.46	0.96
1:A:253:LYS:O	1:A:257:GLU:HG3	1.66	0.95
1:A:4:GLU:CG	1:A:5:CYS:N	2.21	0.94
1:A:31:LEU:HD12	1:A:243:ALA:HB1	1.49	0.92
1:A:197:ASP:O	1:A:225:LYS:HB2	1.70	0.90
1:A:78:ASP:O	1:A:108:LEU:HD12	1.73	0.89
1:A:201:ALA:HB3	1:A:221:MET:HE2	1.54	0.88
1:A:94:VAL:O	1:A:98:VAL:HG23	1.73	0.87
1:A:297:LYS:O	1:A:301:GLU:HG3	1.76	0.86
1:A:268:GLN:O	1:A:272:LYS:HG2	1.75	0.85
1:A:169:LEU:HD22	1:A:218:ARG:HD3	1.59	0.85
1:A:220:ARG:HG2	1:A:220:ARG:O	1.77	0.82
1:A:4:GLU:HG3	1:A:5:CYS:H	0.76	0.82
1:A:194:ARG:HD2	1:A:198:TYR:CE2	2.16	0.81
1:A:31:LEU:HD12	1:A:243:ALA:CB	2.10	0.81
1:A:223:MET:HG2	1:A:260:VAL:HG11	1.62	0.80
1:A:193:PRO:O	1:A:194:ARG:HG3	1.81	0.80
1:A:78:ASP:O	1:A:108:LEU:CD1	2.31	0.79
1:A:107:ARG:NH1	1:A:107:ARG:HB2	1.99	0.78
1:A:295:GLN:N	1:A:295:GLN:OE1	2.14	0.78
1:A:151:GLN:OE1	1:A:188:SER:HB2	1.84	0.77
1:A:243:ALA:O	1:A:246:HIS:HB3	1.84	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLY:HA3	1:A:126:MET:HB3	1.68	0.76
1:A:193:PRO:O	1:A:194:ARG:CG	2.33	0.76
1:A:109:VAL:HG13	1:A:145:ASP:HB2	1.69	0.74
1:A:181:ASP:O	1:A:205:GLN:HG3	1.88	0.73
1:A:263:MET:O	1:A:267:LEU:HG	1.89	0.73
1:A:306:VAL:HG12	1:A:306:VAL:O	1.87	0.73
1:A:107:ARG:HH11	1:A:107:ARG:HB2	1.53	0.72
1:A:194:ARG:HD2	1:A:198:TYR:HE2	1.54	0.72
1:A:306:VAL:CG1	1:A:306:VAL:O	2.37	0.72
1:A:116:MET:O	1:A:126:MET:HB2	1.89	0.72
1:A:111:VAL:HG21	1:A:242:LEU:HD12	1.72	0.70
1:A:105:ASN:HD21	1:A:107:ARG:HH12	1.37	0.70
1:A:207:THR:HG22	1:A:208:ARG:H	1.57	0.70
1:A:102:LYS:HG2	1:A:108:LEU:HD23	1.73	0.70
1:A:247:LYS:C	1:A:248:HIS:HD1	1.94	0.70
1:A:147:ILE:HD11	1:A:175:LEU:HD13	1.72	0.70
1:A:204:SER:HA	1:A:217:GLN:O	1.91	0.70
1:A:253:LYS:HD2	1:A:311:VAL:CG2	2.23	0.69
1:A:275:LYS:O	1:A:277:LYS:N	2.25	0.69
1:A:62:LEU:HD11	3:A:1146:HOH:O	1.93	0.68
1:A:275:LYS:C	1:A:277:LYS:H	1.96	0.68
1:A:256:CYS:O	1:A:260:VAL:HG23	1.93	0.68
1:A:174:MET:O	1:A:178:MET:HG2	1.94	0.68
1:A:128:VAL:HB	1:A:132:LEU:HD12	1.77	0.67
1:A:181:ASP:O	1:A:205:GLN:CG	2.42	0.67
1:A:88:LYS:HE3	1:A:131:ASP:OD1	1.95	0.67
1:A:5:CYS:O	1:A:34:GLU:N	2.28	0.66
1:A:198:TYR:CE1	1:A:224:HIS:HD2	2.14	0.66
1:A:275:LYS:HB2	1:A:275:LYS:NZ	2.12	0.65
1:A:133:LEU:HB3	1:A:134:PRO:HD3	1.78	0.65
1:A:136:TYR:O	1:A:141:VAL:HG23	1.96	0.65
1:A:246:HIS:CD2	1:A:247:LYS:HD2	2.32	0.64
1:A:295:GLN:H	1:A:295:GLN:CD	1.98	0.64
1:A:224:HIS:O	1:A:225:LYS:O	2.16	0.64
1:A:31:LEU:CD1	1:A:243:ALA:HB1	2.26	0.63
1:A:270:THR:O	1:A:274:ALA:HB2	1.99	0.63
1:A:162:ILE:HA	1:A:167:GLU:HG2	1.80	0.62
1:A:223:MET:HG2	1:A:260:VAL:CG1	2.29	0.62
1:A:227:ASP:O	1:A:227:ASP:OD1	2.17	0.62
1:A:192:SER:O	1:A:194:ARG:N	2.33	0.61
1:A:172:MET:O	1:A:175:LEU:HB2	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:GLN:HB2	1:A:252:LEU:HD22	1.83	0.61
1:A:214:VAL:HG23	1:A:214:VAL:O	2.01	0.60
1:A:219:ILE:HA	1:A:310:THR:O	2.00	0.60
1:A:86:ARG:HD3	2:A:1001:RRC:HAF	1.84	0.60
1:A:60:ASP:O	1:A:63:GLN:HB3	2.01	0.60
1:A:176:HIS:NE2	1:A:204:SER:OG	2.33	0.60
1:A:247:LYS:HB2	1:A:248:HIS:ND1	2.17	0.60
1:A:70:LYS:HE2	3:A:1160:HOH:O	2.00	0.60
1:A:218:ARG:HB2	1:A:312:LEU:HD23	1.84	0.59
1:A:218:ARG:O	1:A:219:ILE:HG23	2.02	0.59
1:A:136:TYR:HA	1:A:140:VAL:HB	1.83	0.59
1:A:206:ARG:HD3	1:A:216:THR:OG1	2.01	0.59
1:A:247:LYS:HB2	1:A:248:HIS:CE1	2.38	0.59
1:A:75:ASN:OD1	1:A:75:ASN:O	2.21	0.58
1:A:248:HIS:HB3	1:A:251:ASN:HB2	1.85	0.58
1:A:105:ASN:HD21	1:A:107:ARG:NH1	2.02	0.58
1:A:221:MET:HE3	1:A:260:VAL:HG21	1.86	0.58
1:A:262:ALA:HA	1:A:265:HIS:HD2	1.69	0.57
1:A:284:PRO:HB2	1:A:289:LEU:HD21	1.84	0.57
1:A:198:TYR:HE1	1:A:224:HIS:HD2	1.52	0.57
1:A:243:ALA:O	1:A:246:HIS:CB	2.51	0.57
1:A:200:MET:HE3	1:A:202:LEU:HD11	1.85	0.57
1:A:129:PRO:HB2	1:A:131:ASP:OD2	2.04	0.57
1:A:175:LEU:O	1:A:178:MET:HB2	2.05	0.56
1:A:246:HIS:HD2	1:A:247:LYS:CD	2.17	0.56
1:A:165:GLN:O	1:A:168:ALA:HB3	2.05	0.56
1:A:244:TRP:HA	1:A:244:TRP:CE3	2.40	0.56
1:A:275:LYS:C	1:A:277:LYS:N	2.56	0.56
1:A:302:SER:HA	3:A:1015:HOH:O	2.05	0.56
1:A:306:VAL:HG13	3:A:1154:HOH:O	2.05	0.56
1:A:80:VAL:HG23	1:A:108:LEU:HD11	1.88	0.56
1:A:304:GLU:O	1:A:306:VAL:HG23	2.05	0.55
1:A:205:GLN:HB2	1:A:252:LEU:CD2	2.37	0.55
1:A:203:GLY:O	1:A:218:ARG:HA	2.06	0.55
1:A:257:GLU:O	1:A:261:SER:OG	2.22	0.55
1:A:85:THR:HG22	1:A:87:ASP:H	1.70	0.55
1:A:174:MET:O	1:A:178:MET:CG	2.54	0.55
1:A:219:ILE:HG21	1:A:253:LYS:HG3	1.89	0.54
1:A:246:HIS:CD2	1:A:247:LYS:CD	2.90	0.54
1:A:175:LEU:HA	1:A:178:MET:HG3	1.90	0.54
1:A:270:THR:O	1:A:274:ALA:CB	2.57	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:PRO:HG2	1:A:220:ARG:HH12	1.73	0.53
1:A:12:SER:HB2	1:A:41:VAL:HG22	1.91	0.53
1:A:285:SER:O	1:A:288:GLN:N	2.41	0.52
1:A:49:TYR:OH	1:A:290:GLU:OE1	2.25	0.52
1:A:4:GLU:HB2	1:A:246:HIS:CE1	2.44	0.52
1:A:193:PRO:HG2	1:A:220:ARG:NH1	2.24	0.52
1:A:298:LYS:O	1:A:301:GLU:HB2	2.09	0.52
1:A:253:LYS:HD2	1:A:311:VAL:HG23	1.89	0.52
1:A:264:HIS:NE2	1:A:268:GLN:OE1	2.42	0.52
1:A:294:VAL:O	1:A:297:LYS:N	2.43	0.52
1:A:70:LYS:CA	1:A:75:ASN:HD22	2.02	0.52
1:A:194:ARG:CD	1:A:198:TYR:HE2	2.23	0.52
1:A:205:GLN:HE21	1:A:252:LEU:HB2	1.75	0.52
1:A:84:TYR:HB2	2:A:1001:RRC:HAY2	1.92	0.52
1:A:23:ALA:O	1:A:293:MET:HE1	2.10	0.52
1:A:284:PRO:HA	1:A:288:GLN:NE2	2.25	0.51
1:A:244:TRP:C	1:A:246:HIS:H	2.13	0.51
1:A:79:TYR:HD2	1:A:109:VAL:HB	1.75	0.51
1:A:235:ASP:OD2	2:A:1001:RRC:HBA3	2.10	0.51
1:A:216:THR:HG21	1:A:218:ARG:HH21	1.76	0.51
1:A:218:ARG:O	1:A:311:VAL:HA	2.10	0.51
1:A:109:VAL:CG1	1:A:145:ASP:HB2	2.39	0.51
1:A:247:LYS:HD2	1:A:247:LYS:N	2.25	0.51
1:A:296:SER:O	1:A:297:LYS:C	2.50	0.51
1:A:198:TYR:CE1	1:A:224:HIS:CD2	2.99	0.50
1:A:26:PHE:HB3	1:A:27:PRO:HD3	1.93	0.50
1:A:271:ILE:HA	1:A:274:ALA:HB3	1.94	0.50
1:A:180:PRO:C	1:A:182:THR:H	2.15	0.50
1:A:199:LEU:HD11	3:A:1166:HOH:O	2.11	0.50
1:A:176:HIS:CE1	1:A:204:SER:O	2.65	0.50
1:A:172:MET:O	1:A:175:LEU:N	2.45	0.50
1:A:126:MET:N	1:A:126:MET:SD	2.85	0.49
1:A:237:PHE:HA	1:A:263:MET:CE	2.43	0.49
1:A:25:THR:HB	3:A:1008:HOH:O	2.11	0.49
1:A:175:LEU:O	1:A:178:MET:N	2.41	0.49
1:A:268:GLN:O	1:A:272:LYS:CG	2.55	0.49
1:A:198:TYR:HE1	1:A:224:HIS:CD2	2.30	0.49
1:A:16:ARG:HH21	1:A:287:ALA:HB1	1.77	0.49
1:A:190:LEU:HB2	1:A:200:MET:HE1	1.95	0.49
1:A:254:VAL:HA	1:A:257:GLU:OE1	2.12	0.49
1:A:307:VAL:CG1	1:A:308:GLN:N	2.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:HIS:ND1	1:A:248:HIS:N	2.61	0.48
1:A:169:LEU:CD2	1:A:218:ARG:HD3	2.39	0.48
1:A:275:LYS:O	1:A:279:GLY:N	2.46	0.48
1:A:244:TRP:C	1:A:246:HIS:N	2.66	0.48
1:A:16:ARG:NH2	1:A:287:ALA:HB1	2.29	0.48
1:A:275:LYS:HB2	1:A:275:LYS:HZ3	1.79	0.48
1:A:76:GLN:O	1:A:76:GLN:CG	2.62	0.48
1:A:255:ALA:O	1:A:256:CYS:C	2.52	0.48
1:A:214:VAL:CG2	1:A:214:VAL:O	2.63	0.47
1:A:198:TYR:O	1:A:225:LYS:HG3	2.15	0.47
1:A:216:THR:HG21	1:A:218:ARG:NH2	2.29	0.47
1:A:243:ALA:O	1:A:246:HIS:N	2.42	0.47
1:A:85:THR:HG22	1:A:86:ARG:N	2.29	0.47
1:A:26:PHE:HD2	1:A:293:MET:HG3	1.80	0.47
1:A:77:TYR:HD1	1:A:101:LEU:HD22	1.80	0.47
1:A:176:HIS:HE1	1:A:204:SER:O	1.97	0.47
1:A:172:MET:CE	1:A:202:LEU:HB3	2.45	0.46
1:A:311:VAL:C	1:A:312:LEU:OXT	2.54	0.46
1:A:209:ALA:O	1:A:210:PRO:C	2.52	0.46
1:A:295:GLN:C	1:A:297:LYS:H	2.18	0.46
1:A:212:GLY:HA3	3:A:1182:HOH:O	2.16	0.46
1:A:252:LEU:O	1:A:252:LEU:HD12	2.15	0.46
1:A:119:GLN:HB3	1:A:152:PHE:HB2	1.98	0.46
1:A:248:HIS:N	1:A:248:HIS:HD1	2.14	0.45
1:A:251:ASN:CB	1:A:254:VAL:CG2	2.80	0.45
1:A:224:HIS:O	1:A:225:LYS:C	2.55	0.45
1:A:240:MET:CE	1:A:300:ILE:HG23	2.33	0.45
1:A:78:ASP:O	1:A:108:LEU:HD13	2.12	0.45
1:A:246:HIS:HD2	1:A:247:LYS:HE3	1.81	0.44
1:A:255:ALA:O	1:A:257:GLU:N	2.51	0.44
1:A:242:LEU:O	1:A:243:ALA:C	2.54	0.44
1:A:307:VAL:HG12	1:A:308:GLN:N	2.33	0.44
1:A:16:ARG:HG2	1:A:17:GLY:N	2.32	0.44
1:A:4:GLU:CB	1:A:246:HIS:CE1	3.00	0.44
1:A:175:LEU:O	1:A:178:MET:CB	2.64	0.44
1:A:190:LEU:HD12	1:A:200:MET:CE	2.48	0.44
1:A:271:ILE:O	1:A:274:ALA:HB3	2.18	0.44
1:A:310:THR:HG22	1:A:312:LEU:OXT	2.17	0.44
1:A:138:GLU:O	1:A:142:PRO:HG2	2.17	0.43
1:A:255:ALA:C	1:A:257:GLU:N	2.71	0.43
1:A:173:ASP:OD2	1:A:218:ARG:NH2	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ARG:HH21	1:A:287:ALA:CB	2.31	0.43
1:A:282:VAL:HG12	1:A:283:LYS:N	2.34	0.43
1:A:120:ARG:HG3	1:A:120:ARG:NH1	2.32	0.43
1:A:181:ASP:O	1:A:205:GLN:HG2	2.15	0.43
1:A:90:PHE:O	1:A:94:VAL:HG23	2.17	0.43
1:A:102:LYS:HD3	1:A:108:LEU:O	2.19	0.43
1:A:119:GLN:NE2	1:A:152:PHE:H	2.17	0.43
1:A:117:GLY:O	1:A:150:ASN:OD1	2.37	0.42
1:A:175:LEU:HA	1:A:175:LEU:HD23	1.87	0.42
1:A:28:LEU:O	1:A:33:PHE:HB2	2.18	0.42
1:A:299:ASP:O	1:A:300:ILE:C	2.58	0.42
1:A:311:VAL:O	1:A:312:LEU:OXT	2.38	0.42
1:A:182:THR:OG1	1:A:205:GLN:HG3	2.19	0.42
1:A:150:ASN:HD22	1:A:150:ASN:HA	1.61	0.42
1:A:118:ASP:OD2	1:A:119:GLN:N	2.48	0.42
1:A:79:TYR:OH	1:A:246:HIS:ND1	2.21	0.42
1:A:29:GLN:O	1:A:32:GLY:N	2.52	0.42
1:A:241:LEU:O	1:A:242:LEU:C	2.57	0.41
1:A:14:VAL:HA	1:A:43:PHE:O	2.20	0.41
1:A:128:VAL:CB	1:A:132:LEU:HD12	2.48	0.41
1:A:194:ARG:HD2	1:A:198:TYR:CD2	2.55	0.41
1:A:219:ILE:HG22	1:A:311:VAL:HA	2.03	0.41
1:A:9:SER:OG	1:A:21:ASN:ND2	2.53	0.41
1:A:247:LYS:CD	1:A:247:LYS:N	2.84	0.41
1:A:196:SER:O	1:A:225:LYS:HE3	2.21	0.41
1:A:76:GLN:HG3	1:A:76:GLN:O	2.19	0.41
1:A:110:TYR:CZ	1:A:112:CYS:HB2	2.56	0.41
1:A:19:VAL:HG22	2:A:1001:RRC:HBA2	2.03	0.41
1:A:166:GLU:HA	1:A:169:LEU:HD12	2.02	0.41
1:A:271:ILE:HG22	1:A:272:LYS:N	2.36	0.40
1:A:275:LYS:HB2	1:A:275:LYS:HZ2	1.83	0.40
1:A:165:GLN:O	1:A:168:ALA:N	2.51	0.40
1:A:246:HIS:HD2	1:A:247:LYS:CE	2.34	0.40

There are no symmetry-related clashes.

Full wwPDB X-ray Structure Validation Report

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	307/312 (98%)	246 (80%)	46 (15%)	15 (5%)	2 2

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	ARG
1	A	210	PRO
1	A	225	LYS
1	A	227	ASP
1	A	278	SER
1	A	305	ILE
1	A	123	GLU
1	A	124	GLY
1	A	243	ALA
1	A	276	ALA
1	A	121	ASN
1	A	255	ALA
1	A	279	GLY
1	A	206	ARG
1	A	219	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	270/273 (99%)	234 (87%)	36 (13%)	4 7

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	19	VAL
1	A	64	GLU
1	A	70	LYS
1	A	74	VAL
1	A	88	LYS
1	A	104	GLN
1	A	106	PRO
1	A	119	GLN
1	A	121	ASN
1	A	123	GLU
1	A	126	MET
1	A	150	ASN
1	A	161	LYS
1	A	166	GLU
1	A	177	SER
1	A	178	MET
1	A	182	THR
1	A	186	THR
1	A	187	SER
1	A	192	SER
1	A	207	THR
1	A	210	PRO
1	A	213	SER
1	A	221	MET
1	A	223	MET
1	A	227	ASP
1	A	240	MET
1	A	247	LYS
1	A	253	LYS
1	A	254	VAL
1	A	261	SER
1	A	271	ILE
1	A	277	LYS
1	A	283	LYS
1	A	297	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	45	ASN
1	A	75	ASN
1	A	119	GLN
1	A	150	ASN
1	A	189	ASN
1	A	205	GLN
1	A	224	HIS
1	A	265	HIS
1	A	308	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	RRC	A	1001	-	25,28,28	1.56	4 (16%)	27,38,38	3.76	9 (33%)

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	RRC	A	1001	-	-	5/17/17/17	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	RRC	CAM-NAL	3.73	1.37	1.32
2	A	1001	RRC	CAX-NAO	3.28	1.40	1.34
2	A	1001	RRC	CAT-NAS	2.51	1.37	1.34
2	A	1001	RRC	CAC-CAB	2.14	1.43	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	RRC	CAX-NAW-CAZ	12.75	137.94	125.42
2	A	1001	RRC	CAZ-NAW-CAV	-10.17	115.08	127.15
2	A	1001	RRC	NAU-CAT-NAL	-5.48	117.57	126.23
2	A	1001	RRC	CAT-NAU-CAV	4.66	120.56	115.28
2	A	1001	RRC	NAS-CAT-NAL	4.57	124.04	117.18
2	A	1001	RRC	CAK-CAR-CAQ	-3.03	106.84	111.72
2	A	1001	RRC	CAT-NAL-CAM	2.84	122.90	116.39
2	A	1001	RRC	CAT-NAS-CAR	2.66	128.81	124.31
2	A	1001	RRC	OAP-CAQ-CAR	-2.19	106.28	111.95

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	RRC	OAP-CAQ-CAR-CAK
2	A	1001	RRC	CAI-CAK-CAR-NAS
2	A	1001	RRC	CAN-CAM-NAJ-CAD
2	A	1001	RRC	NAL-CAM-NAJ-CAD
2	A	1001	RRC	OAP-CAQ-CAR-NAS

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	RRC	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand RRC A 1001
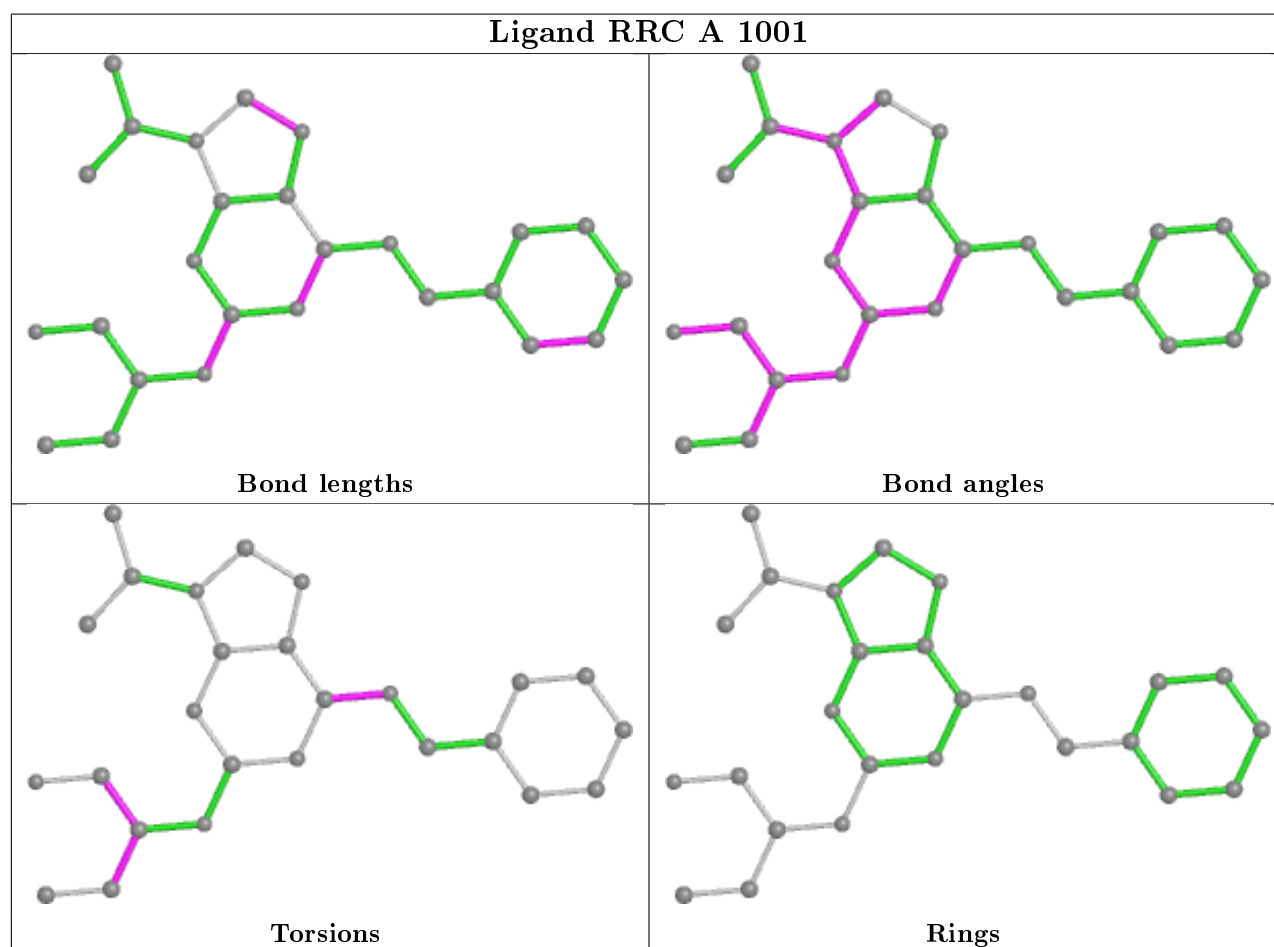
5.7 Other polymers (i)

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	309/312 (99%)	-0.10	12 (3%)	39	32	15, 42, 63, 63	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	214	VAL	3.8
1	A	280	GLU	3.5
1	A	121	ASN	3.3
1	A	124	GLY	2.6
1	A	279	GLY	2.6
1	A	125	ALA	2.5
1	A	177	SER	2.5
1	A	210	PRO	2.5
1	A	212	GLY	2.4
1	A	198	TYR	2.3
1	A	209	ALA	2.1
1	A	207	THR	2.1

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

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

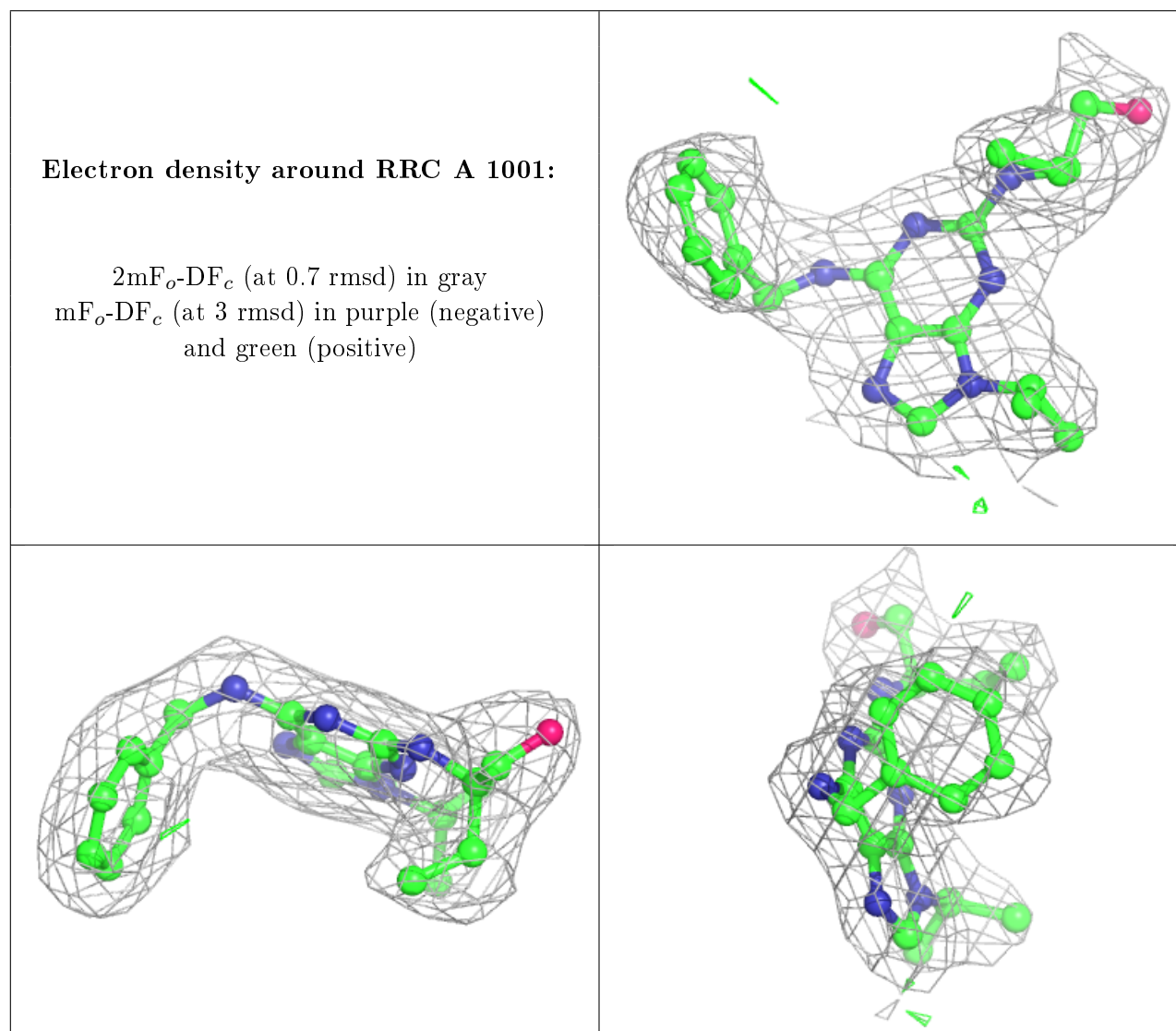## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	RRC	A	1001	26/26	0.92	0.14	34,37,41,47	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around RRC A 1001:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5　Other polymers ⓘ

There are no such residues in this entry.