Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 07:38 am GMT

PDB ID	:	6HKY
Title	:	Eg5-inhibitor complex
Authors	:	Talapatra, S.K.; Kozielski, F.
Deposited on	:	2018-09-09
Resolution	:	2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

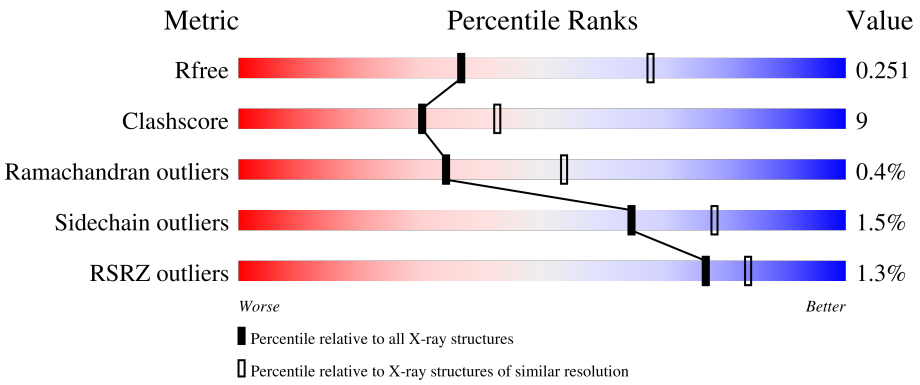
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.75 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	368	.% 74% 14% • 11%
1	B	368	2% 75% 13% • 12%
1	C	368	.% 67% 19% • 12%

2 Entry composition (i)

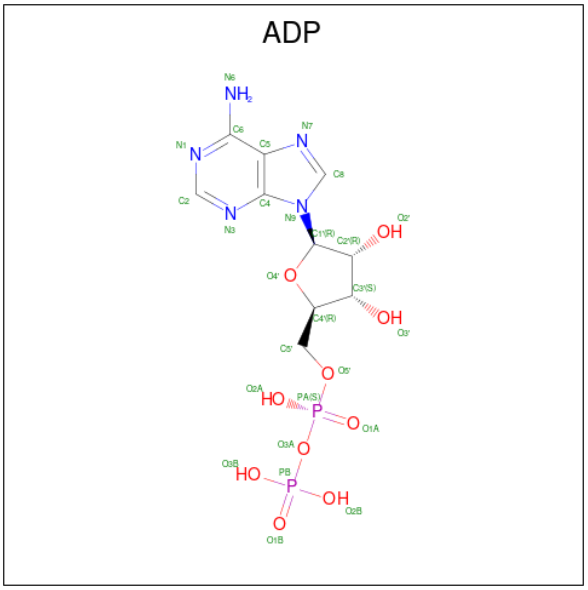
There are 5 unique types of molecules in this entry. The entry contains 8050 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Kinesin-like protein KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	328	2555	1602	448	495	10	0	1	0
1	B	325	2545	1597	443	495	10	0	3	0
1	C	324	2524	1583	431	500	10	0	2	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

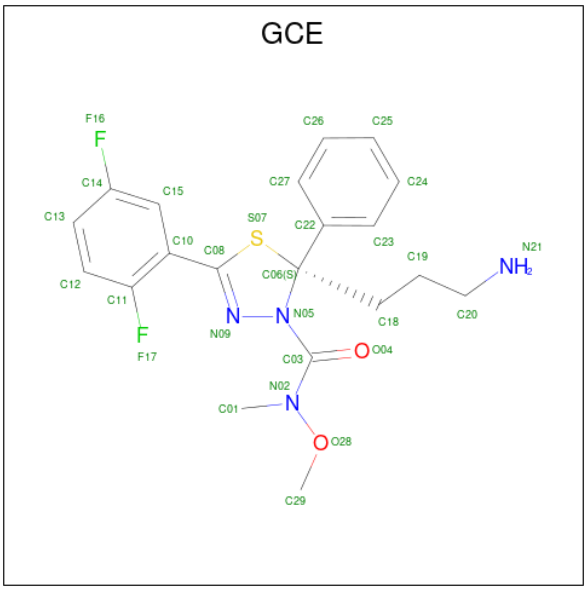


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	27	10	5	10	2	0	0
2	B	1	27	10	5	10	2	0	0
2	C	1	27	10	5	10	2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is (2 {S})-2-(3-azanylpropyl)-5-[2,5-bis(fluoranyl)phenyl]- {N}-methoxy- {N}-methyl-2-phenyl-1,3,4-thiadiazole-3-carboxamide (three-letter code: GCE) (formula: $C_{20}H_{22}F_2N_4O_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C F N O S 29 20 2 4 2 1	0	0
4	B	1	Total C F N O S 29 20 2 4 2 1	0	0
4	C	1	Total C F N O S 29 20 2 4 2 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	100	Total O 100 100	0	0
5	B	87	Total O 87 87	0	0

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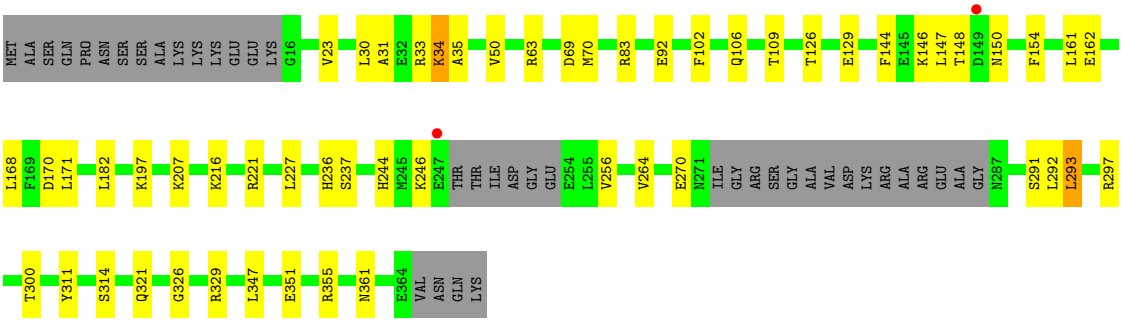
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	C	68	68	68	0	0

3 Residue-property plots (i)

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

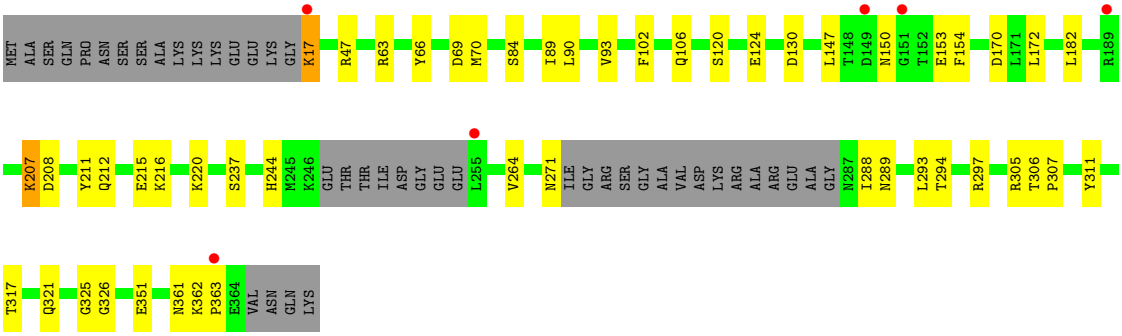
• Molecule 1: Kinesin-like protein KIF11

Chain A:



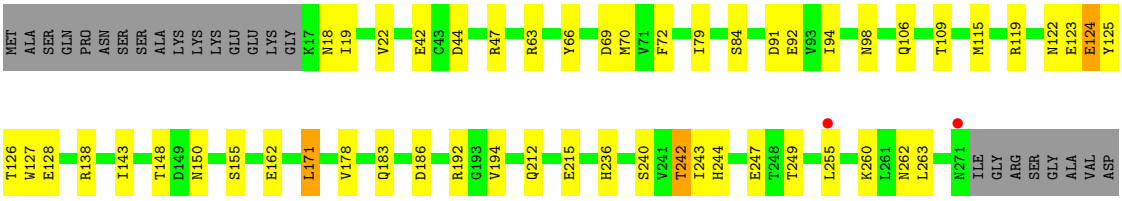
• Molecule 1: Kinesin-like protein KIF11

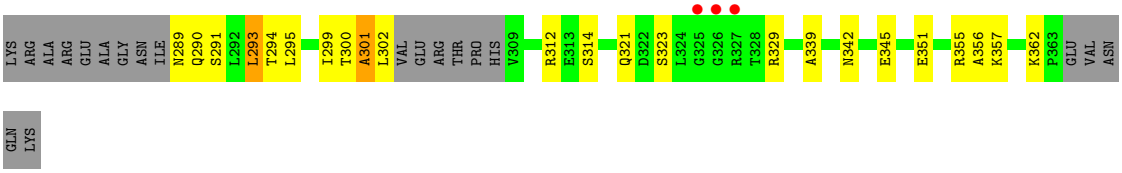
Chain B:



• Molecule 1: Kinesin-like protein KIF11

Chain C:




LYS
ARG
ALA
ARG
GLU
ALA
GLY
ASN
ILE
N289
Q290
S291
L292
L293
T294
L295
I299
T300
A301
L302
VAL
GLU
ARG
THR
PRO
HIS
V309
R312
E313
S314
Q321
D322
S323
L324
G325
G326
R327
T328
R329
A339
N342
E345
E351
R355
A356
K357
K362
P363
GLU
VAL
ASN

GLN
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	95.81Å 95.81Å 125.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.91 – 2.75 47.91 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.91-2.75) 100.0 (47.91-2.75)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.179 , 0.252 0.179 , 0.251	Depositor DCC
R_{free} test set	1689 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	41.0	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 51.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l 0.036 for h,-h-k,-l 0.021 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8050	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: ADP, GCE, MG

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	0.56	0/2596	0.76	1/3512 (0.0%)
1	B	0.60	0/2593	0.78	3/3510 (0.1%)
1	C	0.61	2/2566 (0.1%)	0.81	6/3473 (0.2%)
All	All	0.59	2/7755 (0.0%)	0.78	10/10495 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	124	GLU	CD-OE1	-8.73	1.16	1.25
1	C	124	GLU	CG-CD	-5.68	1.43	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	171	LEU	CA-CB-CG	-7.63	97.74	115.30
1	B	17	LYS	CD-CE-NZ	7.36	128.62	111.70
1	C	293	LEU	CA-CB-CG	7.20	131.87	115.30
1	B	212	GLN	N-CA-CB	6.70	122.66	110.60
1	B	212	GLN	CB-CA-C	-5.71	98.99	110.40
1	C	242	THR	OG1-CB-CG2	5.57	122.81	110.00
1	C	124	GLU	CB-CA-C	-5.51	99.37	110.40
1	C	63	ARG	CA-CB-CG	5.43	125.34	113.40
1	C	63	ARG	N-CA-CB	5.09	119.77	110.60
1	A	227	LEU	CB-CG-CD2	5.00	119.51	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	2555	0	2561	34	0
1	B	2545	0	2548	39	0
1	C	2524	0	2521	69	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	29	0	0	0	0
4	B	29	0	0	0	0
4	C	29	0	0	0	0
5	A	100	0	0	3	0
5	B	87	0	0	1	0
5	C	68	0	0	5	0
All	All	8050	0	7666	143	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (143) 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:C:162:GLU:HG3	1:C:171:LEU:HD13	1.57	0.87
1:A:126:THR:OG1	1:A:129:GLU:HG2	1.76	0.86
1:C:122:ASN:ND2	1:C:124:GLU:HG3	1.93	0.83
1:C:122:ASN:O	1:C:124:GLU:N	2.19	0.75
1:C:18:ASN:ND2	1:C:329:ARG:NH2	2.33	0.75
1:C:242:THR:HG23	1:C:260:LYS:HG3	1.69	0.75
1:A:162:GLU:HG3	1:A:171:LEU:HD13	1.70	0.74
1:C:122:ASN:ND2	1:C:124:GLU:CG	2.54	0.71
1:B:306:THR:O	5:B:501:HOH:O	2.09	0.70
1:C:92:GLU:OE1	1:C:329:ARG:HG2	1.91	0.70
1:A:270:GLU:O	5:A:501:HOH:O	2.11	0.69
1:A:102:PHE:HB3	1:A:264:VAL:HB	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:ALA:O	1:C:302:LEU:HG	1.92	0.69
1:B:293:LEU:HD11	1:B:297:ARG:CZ	2.23	0.69
1:B:102:PHE:HB3	1:B:264:VAL:HB	1.76	0.67
1:C:22:VAL:HG11	1:C:70:MET:HE2	1.78	0.65
1:C:192:ARG:HA	1:C:321:GLN:NE2	2.11	0.65
1:A:293:LEU:HD21	1:A:297:ARG:NH2	2.12	0.65
1:C:44:ASP:OD2	1:C:47:ARG:HG3	1.98	0.64
1:A:92:GLU:OE1	1:A:329:ARG:NH1	2.23	0.64
1:C:18:ASN:ND2	1:C:329:ARG:HH22	1.95	0.64
1:C:294:THR:HG21	1:C:314:SER:HB3	1.80	0.63
1:C:299:ILE:O	1:C:302:LEU:HD12	1.98	0.63
1:C:247:GLU:N	1:C:247:GLU:OE2	2.33	0.62
1:B:17:LYS:HE2	1:B:363:PRO:HG3	1.81	0.61
1:C:236:HIS:HE2	1:C:291:SER:HB2	1.65	0.61
1:C:79:ILE:HD12	1:C:138:ARG:HH12	1.66	0.61
1:C:192:ARG:HA	1:C:321:GLN:HE21	1.65	0.60
1:C:289:ASN:OD1	1:C:290:GLN:N	2.33	0.60
1:B:325:GLY:H	1:B:361:ASN:ND2	1.98	0.60
1:C:18:ASN:HD22	1:C:329:ARG:CZ	2.15	0.59
1:C:19:ILE:HD12	1:C:19:ILE:N	2.17	0.59
1:C:18:ASN:ND2	1:C:329:ARG:CZ	2.66	0.59
1:B:69:ASP:O	1:B:70:MET:HG3	2.02	0.59
1:A:30:LEU:HD13	1:A:33:ARG:NH1	2.18	0.59
1:A:83:ARG:HH11	1:A:83:ARG:HG2	1.68	0.58
1:C:122:ASN:HD22	1:C:124:GLU:CG	2.15	0.58
1:A:170:ASP:HB2	1:A:182:LEU:HD11	1.87	0.57
1:B:216:LYS:HZ2	1:B:220:LYS:HE3	1.69	0.57
1:A:293:LEU:HD21	1:A:297:ARG:HH22	1.69	0.57
1:C:124:GLU:HB2	1:C:125:TYR:CD1	2.39	0.57
1:B:271:ASN:HB3	1:B:289:ASN:OD1	2.05	0.56
1:B:293:LEU:HD11	1:B:297:ARG:NH2	2.21	0.56
1:C:186:ASP:HA	1:C:194:VAL:HA	1.88	0.56
1:A:311:TYR:CD1	1:A:321:GLN:HG3	2.41	0.55
1:C:18:ASN:HD22	1:C:329:ARG:NH2	2.01	0.55
1:B:70:MET:HE1	1:B:84:SER:HB3	1.87	0.55
1:B:288:ILE:HG23	1:B:289:ASN:ND2	2.21	0.55
1:B:70:MET:CE	1:B:84:SER:HB3	2.36	0.55
1:C:69:ASP:O	1:C:70:MET:HG3	2.06	0.55
1:C:183:GLN:NE2	5:C:502:HOH:O	2.23	0.55
1:B:172:LEU:HA	1:B:216:LYS:HE3	1.90	0.54
1:A:347:LEU:O	1:A:351:GLU:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ASP:O	1:C:94:ILE:HG13	2.07	0.54
1:C:192:ARG:CA	1:C:321:GLN:HE21	2.21	0.54
1:A:23:VAL:HG11	1:A:50:VAL:HG21	1.90	0.54
1:C:143:ILE:HD13	1:C:243:ILE:HD11	1.90	0.54
1:C:236:HIS:NE2	1:C:291:SER:HB2	2.23	0.53
1:A:34:LYS:HE3	1:A:35:ALA:HB2	1.89	0.53
1:C:242:THR:HG23	1:C:260:LYS:CG	2.39	0.53
1:C:212:GLN:HA	1:C:215:GLU:HB2	1.91	0.53
1:C:240:SER:OG	1:C:262:ASN:OD1	2.20	0.52
1:C:18:ASN:HD21	1:C:329:ARG:HH22	1.57	0.52
1:C:119:ARG:NH2	5:C:505:HOH:O	2.39	0.52
1:B:153:GLU:HA	1:B:153:GLU:OE1	2.09	0.52
1:C:119:ARG:HH21	1:C:127:TRP:HB3	1.75	0.52
1:C:178:VAL:HG12	1:C:178:VAL:O	2.11	0.51
1:B:154:PHE:HA	1:B:244:HIS:O	2.11	0.51
1:C:115:MET:CE	1:C:263:LEU:HB3	2.41	0.51
1:B:147:LEU:O	1:B:150:ASN:HB3	2.11	0.51
2:C:401:ADP:O2'	5:C:501:HOH:O	2.20	0.50
1:A:246:LYS:HA	1:A:256:VAL:HG12	1.92	0.50
1:A:144:PHE:O	1:A:148:THR:HG22	2.12	0.50
1:C:294:THR:CG2	1:C:314:SER:HB3	2.41	0.50
1:A:221:ARG:NH1	5:A:504:HOH:O	2.43	0.49
1:A:300:THR:OG1	1:A:355:ARG:NH1	2.45	0.49
1:B:288:ILE:HG23	1:B:289:ASN:HD22	1.76	0.49
1:C:106:GLN:HG2	1:C:109:THR:CG2	2.43	0.49
1:C:155:SER:OG	1:C:244:HIS:HB2	2.13	0.49
1:B:216:LYS:NZ	1:B:220:LYS:HE3	2.27	0.49
1:A:106:GLN:HG2	1:A:109:THR:CG2	2.43	0.49
1:B:207:LYS:NZ	1:B:208:ASP:OD2	2.46	0.48
1:A:161:LEU:C	1:A:161:LEU:HD12	2.33	0.48
1:B:325:GLY:HA2	1:B:361:ASN:HD22	1.78	0.48
1:B:325:GLY:CA	1:B:361:ASN:HD22	2.27	0.47
1:A:326:GLY:O	1:A:361:ASN:HB3	2.14	0.47
1:B:17:LYS:HG2	1:B:361:ASN:C	2.35	0.47
1:C:98:ASN:OD1	1:C:260:LYS:HB3	2.14	0.47
1:C:290:GLN:O	1:C:293:LEU:HD23	2.14	0.47
1:C:18:ASN:ND2	1:C:329:ARG:NH1	2.63	0.47
1:C:19:ILE:O	1:C:357:LYS:NZ	2.36	0.47
1:C:19:ILE:CD1	1:C:302:LEU:HD13	2.45	0.46
1:A:63:ARG:HD2	5:A:511:HOH:O	2.14	0.46
1:B:311:TYR:CG	1:B:321:GLN:HG3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ASP:O	1:A:70:MET:HG3	2.16	0.46
1:B:63:ARG:HG2	1:B:63:ARG:NH1	2.30	0.46
1:B:66:TYR:OH	1:B:351:GLU:OE2	2.26	0.46
1:A:146:LYS:O	1:A:150:ASN:HB2	2.16	0.45
1:B:90:LEU:HD12	1:B:90:LEU:HA	1.48	0.45
1:B:170:ASP:HB2	1:B:182:LEU:HD11	1.99	0.45
1:B:17:LYS:HE2	1:B:363:PRO:CG	2.46	0.45
1:B:63:ARG:HG2	1:B:63:ARG:HH11	1.82	0.45
1:C:66:TYR:OH	1:C:351:GLU:OE1	2.27	0.45
1:B:325:GLY:H	1:B:361:ASN:HD21	1.61	0.44
1:A:168:LEU:HB2	1:A:182:LEU:HB2	1.97	0.44
1:C:339:ALA:HB3	1:C:342:ASN:HD22	1.81	0.44
1:A:292:LEU:HD12	1:A:292:LEU:HA	1.73	0.44
1:B:89:ILE:O	1:B:93:VAL:HG23	2.18	0.44
1:C:70:MET:HE1	1:C:84:SER:OG	2.18	0.44
1:B:294:THR:HG22	1:B:317:THR:HG21	2.00	0.44
1:A:197:LYS:HD3	1:A:197:LYS:HA	1.74	0.44
1:B:326:GLY:O	1:B:361:ASN:HB3	2.19	0.43
1:C:70:MET:HE3	1:C:72:PHE:CZ	2.54	0.43
1:C:262:ASN:ND2	1:C:323:SER:OG	2.50	0.43
1:B:17:LYS:HD3	1:B:363:PRO:HG3	2.00	0.43
1:A:291:SER:HA	1:A:314:SER:HB2	2.01	0.43
1:C:290:GLN:HA	1:C:293:LEU:HD23	2.00	0.43
1:A:216:LYS:HB2	1:A:216:LYS:HE2	1.80	0.43
1:A:31:ALA:O	1:A:34:LYS:HG3	2.19	0.42
1:A:30:LEU:HD13	1:A:33:ARG:HH12	1.83	0.42
1:C:300:THR:O	1:C:302:LEU:N	2.52	0.42
1:C:128:GLU:OE1	1:C:128:GLU:N	2.47	0.42
1:C:295:LEU:O	1:C:299:ILE:HD12	2.20	0.42
1:A:147:LEU:O	1:A:150:ASN:HB3	2.20	0.42
1:A:154:PHE:HA	1:A:244:HIS:O	2.19	0.42
1:B:211:TYR:HE1	1:B:215:GLU:OE1	2.03	0.42
1:C:106:GLN:HG2	1:C:109:THR:HG23	2.01	0.42
1:A:236:HIS:NE2	1:A:292:LEU:HD13	2.34	0.42
1:C:345:GLU:HG2	5:C:556:HOH:O	2.20	0.42
1:C:70:MET:HE2	1:C:70:MET:HB2	1.75	0.42
1:C:148:THR:C	1:C:150:ASN:H	2.23	0.42
1:C:124:GLU:HB2	1:C:125:TYR:CE1	2.55	0.41
1:B:17:LYS:CE	1:B:363:PRO:HG3	2.48	0.41
1:B:124:GLU:O	1:B:124:GLU:HG2	2.21	0.41
1:C:294:THR:H	1:C:294:THR:HG23	1.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:ILE:HD12	1:C:19:ILE:H	1.86	0.41
1:B:120:SER:OG	1:B:130:ASP:OD1	2.28	0.40
1:C:126:THR:HB	1:C:128:GLU:OE1	2.21	0.40
1:B:17:LYS:HG3	1:B:361:ASN:H	1.86	0.40
1:C:47:ARG:NH2	1:C:362:LYS:O	2.54	0.40
1:C:115:MET:HE3	1:C:263:LEU:HB3	2.03	0.40
1:C:312:ARG:NH2	5:C:511:HOH:O	2.54	0.40
1:C:300:THR:HG22	1:C:355:ARG:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	323/368 (88%)	317 (98%)	6 (2%)	0	100	100
1	B	322/368 (88%)	317 (98%)	4 (1%)	1 (0%)	41	60
1	C	320/368 (87%)	309 (97%)	8 (2%)	3 (1%)	17	31
All	All	965/1104 (87%)	943 (98%)	18 (2%)	4 (0%)	34	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	123	GLU
1	C	356	ALA
1	C	301	ALA
1	B	307	PRO

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	284/322 (88%)	280 (99%)	4 (1%)	67	79
1	B	285/322 (88%)	279 (98%)	6 (2%)	53	71
1	C	283/322 (88%)	280 (99%)	3 (1%)	73	84
All	All	852/966 (88%)	839 (98%)	13 (2%)	65	78

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	207	LYS
1	A	237	SER
1	A	293	LEU
1	B	47	ARG
1	B	106	GLN
1	B	207	LYS
1	B	237	SER
1	B	305	ARG
1	B	362	LYS
1	C	42	GLU
1	C	249	THR
1	C	255	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	361	ASN
1	C	18	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
4	GCE	B	403	-	26,31,31	3.66	6 (23%)	30,44,44	3.20	11 (36%)
2	ADP	B	401	3	24,29,29	1.06	2 (8%)	29,45,45	1.34	5 (17%)
2	ADP	C	401	-	24,29,29	1.18	1 (4%)	29,45,45	1.46	8 (27%)
2	ADP	A	401	3	24,29,29	0.91	1 (4%)	29,45,45	1.60	6 (20%)
4	GCE	C	403	-	26,31,31	3.63	6 (23%)	30,44,44	2.68	9 (30%)
4	GCE	A	403	-	26,31,31	3.66	5 (19%)	30,44,44	3.24	7 (23%)

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
4	GCE	B	403	-	-	9/20/40/40	0/3/3/3
2	ADP	B	401	3	-	2/12/32/32	0/3/3/3
2	ADP	C	401	-	-	5/12/32/32	0/3/3/3
2	ADP	A	401	3	-	3/12/32/32	0/3/3/3
4	GCE	C	403	-	-	11/20/40/40	0/3/3/3
4	GCE	A	403	-	-	5/20/40/40	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	GCE	C08-N09	12.49	1.53	1.29
4	C	403	GCE	C08-N09	12.36	1.53	1.29
4	B	403	GCE	C08-N09	12.09	1.52	1.29
4	B	403	GCE	C08-S07	-10.92	1.59	1.77
4	A	403	GCE	C08-S07	-10.10	1.60	1.77
4	C	403	GCE	C08-S07	-9.45	1.61	1.77
4	A	403	GCE	N05-N09	7.36	1.55	1.39
4	B	403	GCE	N05-N09	7.18	1.54	1.39
4	C	403	GCE	N05-N09	7.17	1.54	1.39
4	C	403	GCE	C10-C08	4.57	1.54	1.47
4	A	403	GCE	C10-C08	3.96	1.53	1.47
4	C	403	GCE	C06-C22	3.64	1.57	1.51
2	C	401	ADP	C5-C4	3.17	1.49	1.40
4	A	403	GCE	C06-C22	2.86	1.56	1.51
4	B	403	GCE	C10-C08	2.82	1.51	1.47
2	B	401	ADP	C5-C4	2.63	1.47	1.40
4	B	403	GCE	C06-C22	2.47	1.55	1.51
4	B	403	GCE	O04-C03	-2.37	1.18	1.22
4	C	403	GCE	O04-C03	-2.18	1.18	1.22
2	B	401	ADP	C2-N3	2.09	1.35	1.32
2	A	401	ADP	C5-C4	2.03	1.46	1.40

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	403	GCE	S07-C08-N09	-14.57	107.09	115.82
4	B	403	GCE	S07-C08-N09	-13.55	107.70	115.82
4	C	403	GCE	S07-C08-N09	-11.45	108.96	115.82
4	B	403	GCE	C15-C10-C11	5.24	123.04	116.66
4	A	403	GCE	C03-N05-N09	5.23	127.68	120.08
4	A	403	GCE	C08-N09-N05	-5.05	108.14	112.86
4	B	403	GCE	C03-N05-N09	5.02	127.36	120.08
4	C	403	GCE	C03-N05-N09	4.13	126.08	120.08
4	B	403	GCE	C12-C11-C10	-3.78	118.99	123.11
2	A	401	ADP	N6-C6-N1	3.56	125.96	118.57
2	A	401	ADP	N3-C2-N1	-3.53	123.16	128.68
4	A	403	GCE	C15-C10-C11	3.33	120.71	116.66
2	A	401	ADP	C3'-C2'-C1'	3.32	105.97	100.98
4	B	403	GCE	C15-C10-C08	-3.28	114.89	120.09
4	C	403	GCE	C15-C10-C11	3.10	120.43	116.66
4	C	403	GCE	C15-C10-C08	-3.07	115.23	120.09
4	C	403	GCE	C12-C11-C10	-3.06	119.78	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	ADP	N3-C2-N1	-2.94	124.09	128.68
4	A	403	GCE	O28-N02-C01	2.90	119.20	114.33
4	C	403	GCE	C08-N09-N05	-2.90	110.15	112.86
2	C	401	ADP	PA-O3A-PB	-2.89	122.90	132.83
4	A	403	GCE	C12-C11-C10	-2.88	119.98	123.11
4	B	403	GCE	C12-C13-C14	2.50	120.95	118.36
2	A	401	ADP	C5-C6-N6	-2.49	116.56	120.35
2	B	401	ADP	N6-C6-N1	2.45	123.66	118.57
2	C	401	ADP	C4-C5-N7	-2.44	106.86	109.40
4	B	403	GCE	C23-C22-C06	-2.39	117.48	120.56
4	B	403	GCE	C08-N09-N05	-2.38	110.64	112.86
4	C	403	GCE	O28-N02-C03	2.37	121.57	116.37
2	C	401	ADP	N6-C6-N1	2.35	123.46	118.57
4	B	403	GCE	O28-N02-C01	2.35	118.26	114.33
4	C	403	GCE	C29-O28-N02	2.35	113.04	109.88
4	A	403	GCE	F16-C14-C15	2.31	121.56	118.25
2	B	401	ADP	C2-N1-C6	2.31	122.70	118.75
2	A	401	ADP	O3B-PB-O2B	2.30	116.42	107.64
2	B	401	ADP	C4-C5-N7	-2.30	107.01	109.40
2	B	401	ADP	C3'-C2'-C1'	2.22	104.33	100.98
2	A	401	ADP	PA-O3A-PB	-2.21	125.23	132.83
4	B	403	GCE	C13-C14-C15	-2.20	120.43	123.29
4	B	403	GCE	C18-C19-C20	2.16	116.23	112.35
2	C	401	ADP	C2'-C3'-C4'	2.15	106.82	102.64
4	C	403	GCE	C13-C14-C15	-2.12	120.53	123.29
2	C	401	ADP	C2-N1-C6	2.11	122.36	118.75
2	C	401	ADP	C5-C6-N1	-2.08	115.63	120.35
2	C	401	ADP	O3A-PB-O1B	-2.04	99.89	111.19
2	C	401	ADP	O5'-C5'-C4'	2.02	115.95	108.99

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ADP	PA-O3A-PB-O3B
2	B	401	ADP	PA-O3A-PB-O2B
2	C	401	ADP	C5'-O5'-PA-O3A
2	C	401	ADP	O4'-C4'-C5'-O5'
2	C	401	ADP	C3'-C4'-C5'-O5'
4	B	403	GCE	C01-N02-O28-C29
4	C	403	GCE	C22-C06-C18-C19
4	C	403	GCE	N05-C06-C18-C19

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Mol	Chain	Res	Type	Atoms
4	C	403	GCE	S07-C06-C18-C19
4	C	403	GCE	C01-N02-O28-C29
4	C	403	GCE	C03-N02-O28-C29
4	B	403	GCE	C18-C06-C22-C27
4	A	403	GCE	C03-N02-O28-C29
4	C	403	GCE	C18-C19-C20-N21
4	B	403	GCE	S07-C08-C10-C11
4	C	403	GCE	C18-C06-C22-C23
2	C	401	ADP	C5'-O5'-PA-O1A
4	C	403	GCE	N05-C06-C22-C27
4	B	403	GCE	C18-C19-C20-N21
4	A	403	GCE	C18-C06-C22-C23
4	A	403	GCE	C18-C06-C22-C27
4	B	403	GCE	C18-C06-C22-C23
4	C	403	GCE	C18-C06-C22-C27
4	B	403	GCE	C22-C06-C18-C19
2	A	401	ADP	PA-O3A-PB-O1B
2	A	401	ADP	PA-O3A-PB-O2B
2	B	401	ADP	PA-O3A-PB-O3B
2	C	401	ADP	PB-O3A-PA-O1A
4	A	403	GCE	N05-C06-C22-C27
4	B	403	GCE	N05-C06-C22-C23
4	B	403	GCE	N05-C06-C22-C27
4	C	403	GCE	N05-C06-C22-C23
4	A	403	GCE	O04-C03-N02-C01
4	B	403	GCE	O04-C03-N02-C01
4	C	403	GCE	O04-C03-N02-C01

There are no ring outliers.

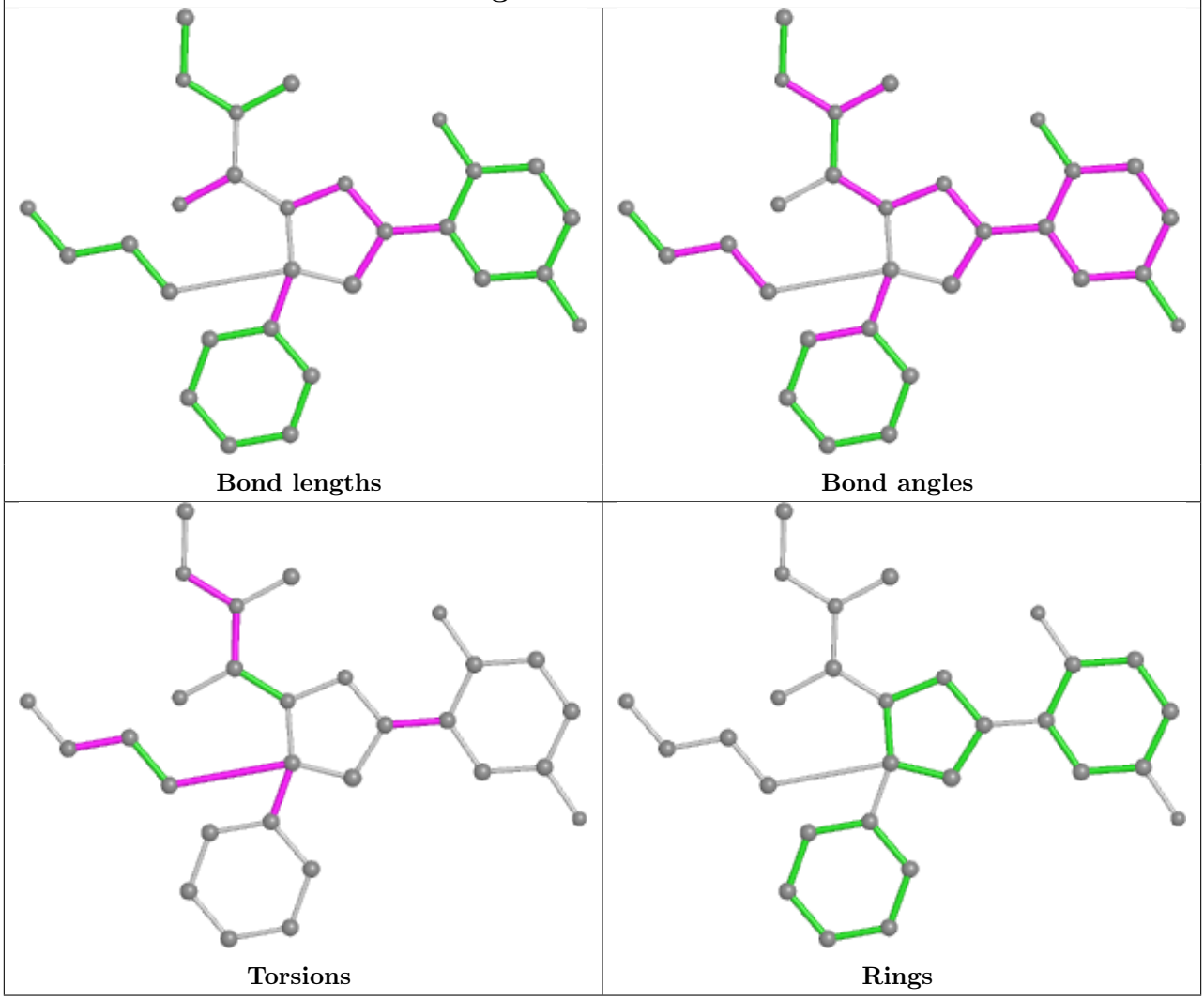
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	ADP	1	0

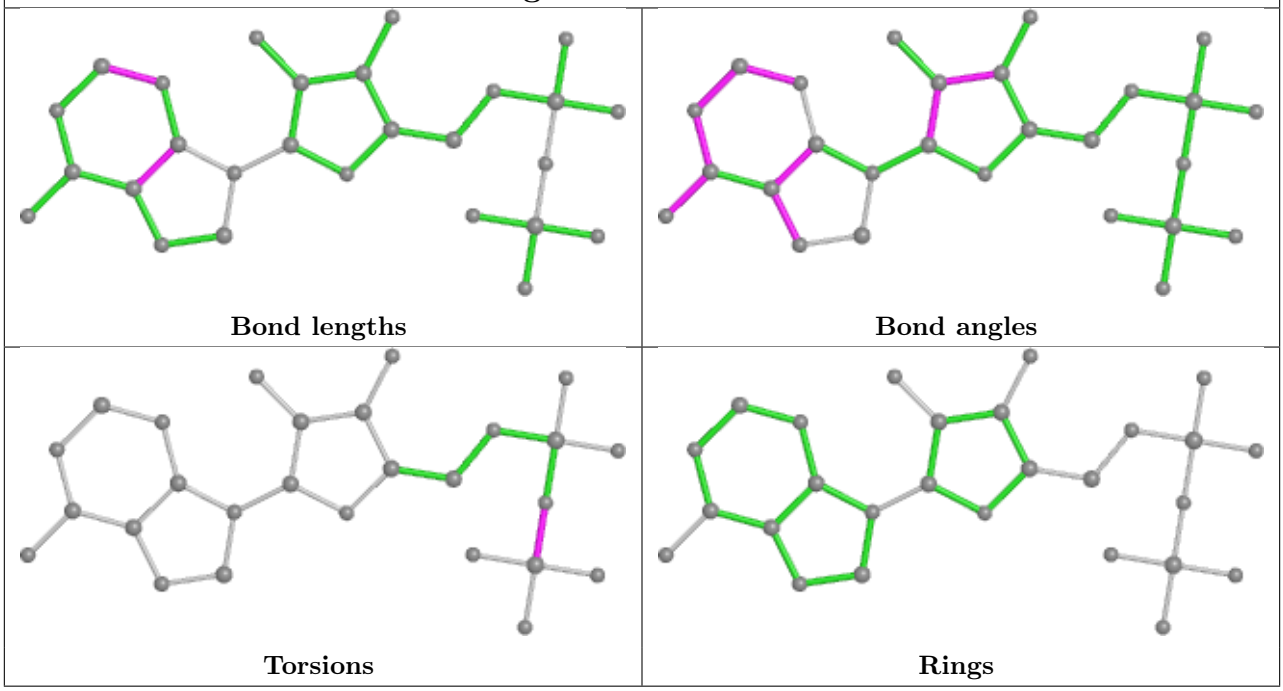
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

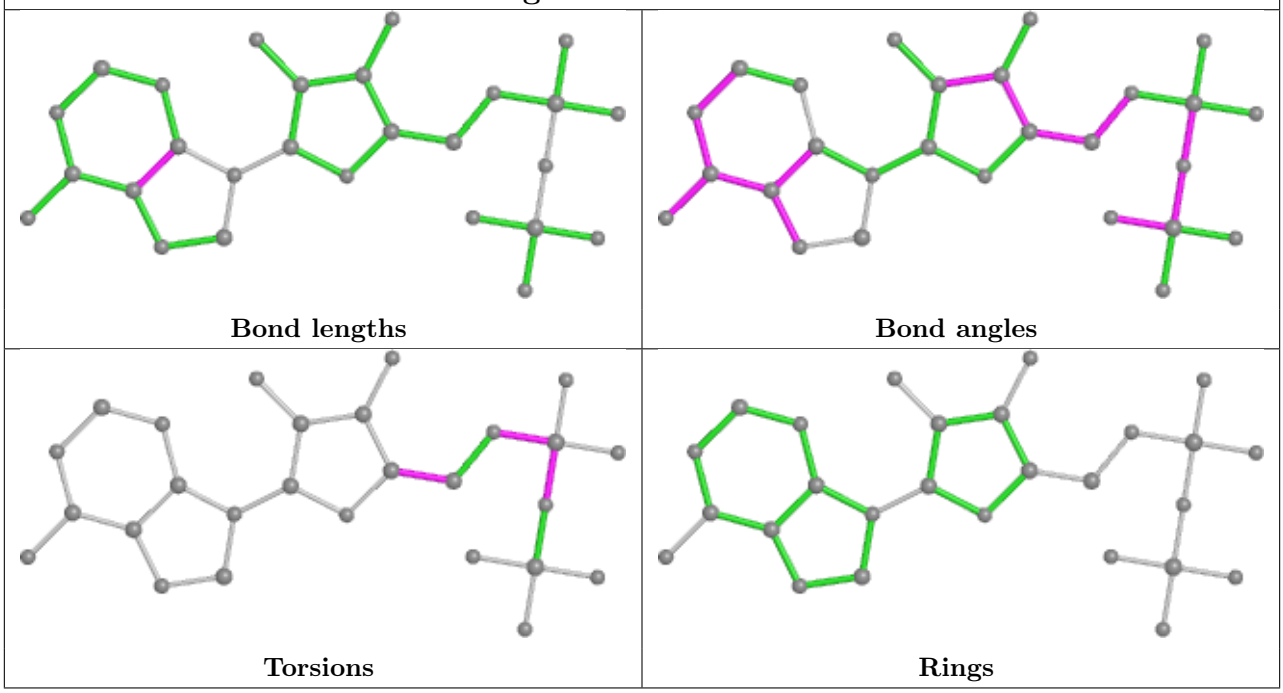
Ligand GCE B 403



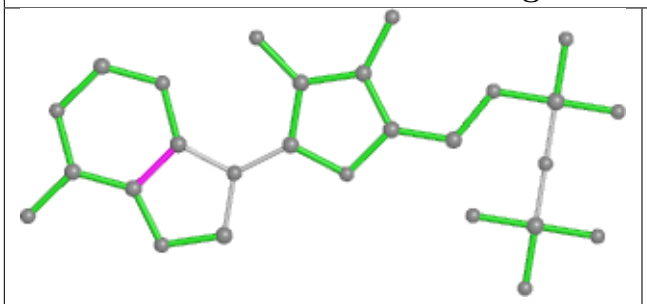
Ligand ADP B 401



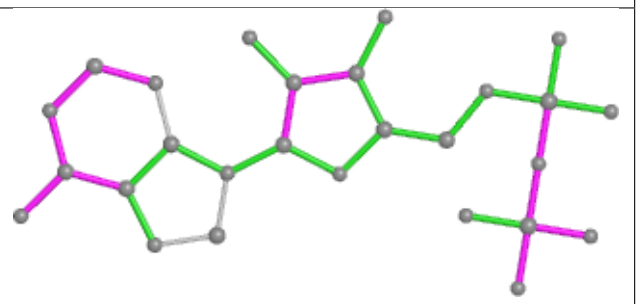
Ligand ADP C 401



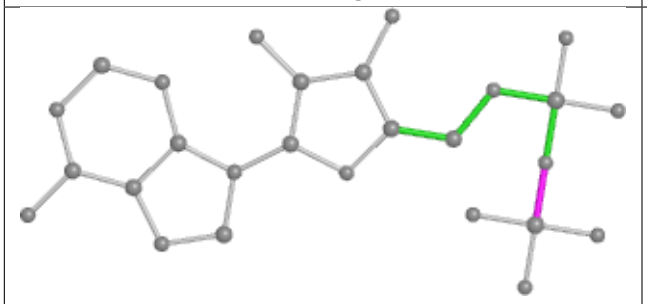
Ligand ADP A 401



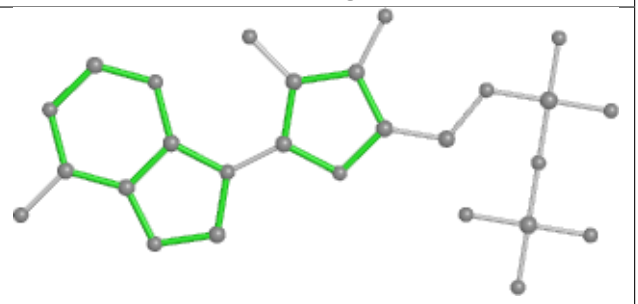
Bond lengths



Bond angles

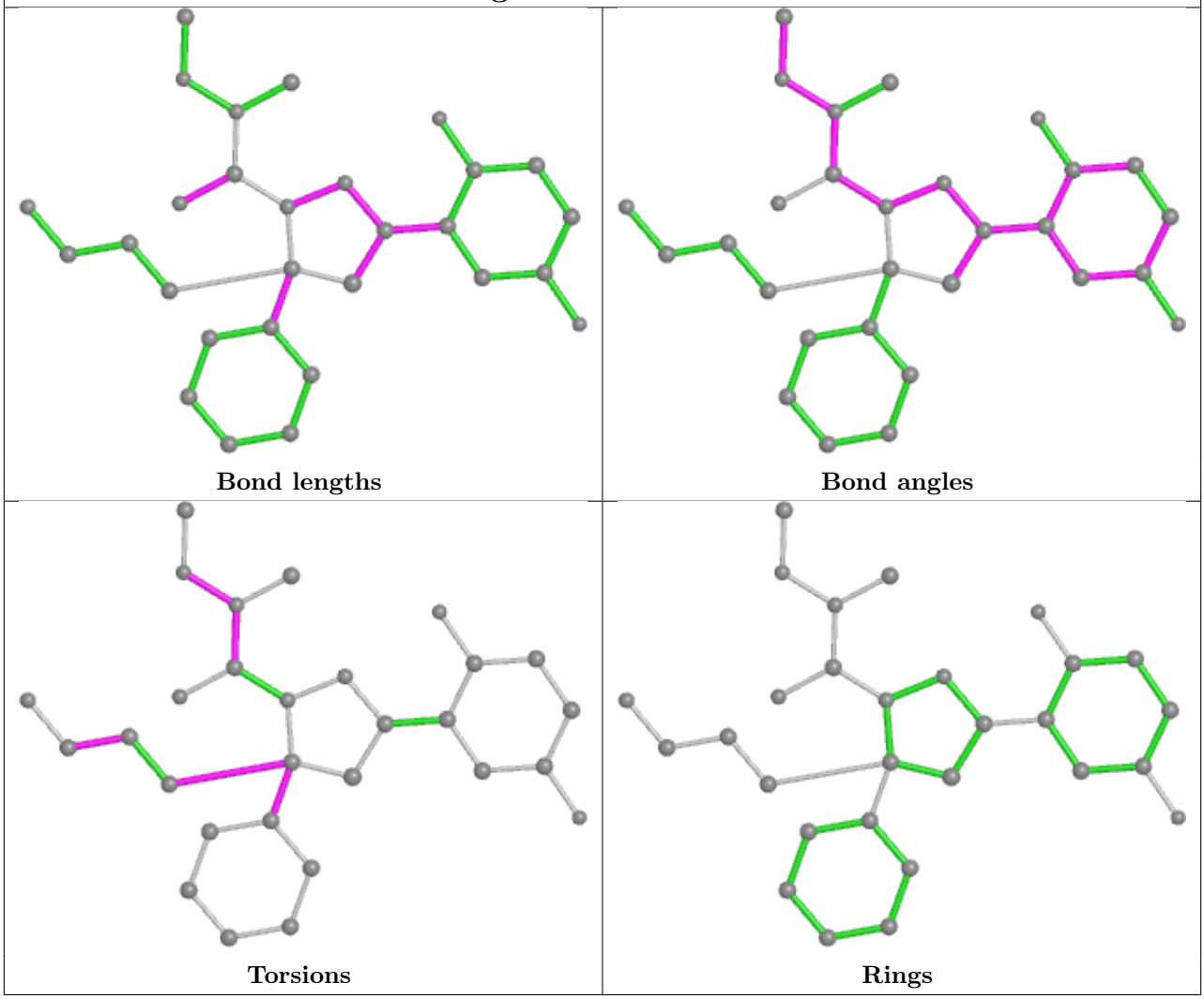


Torsions

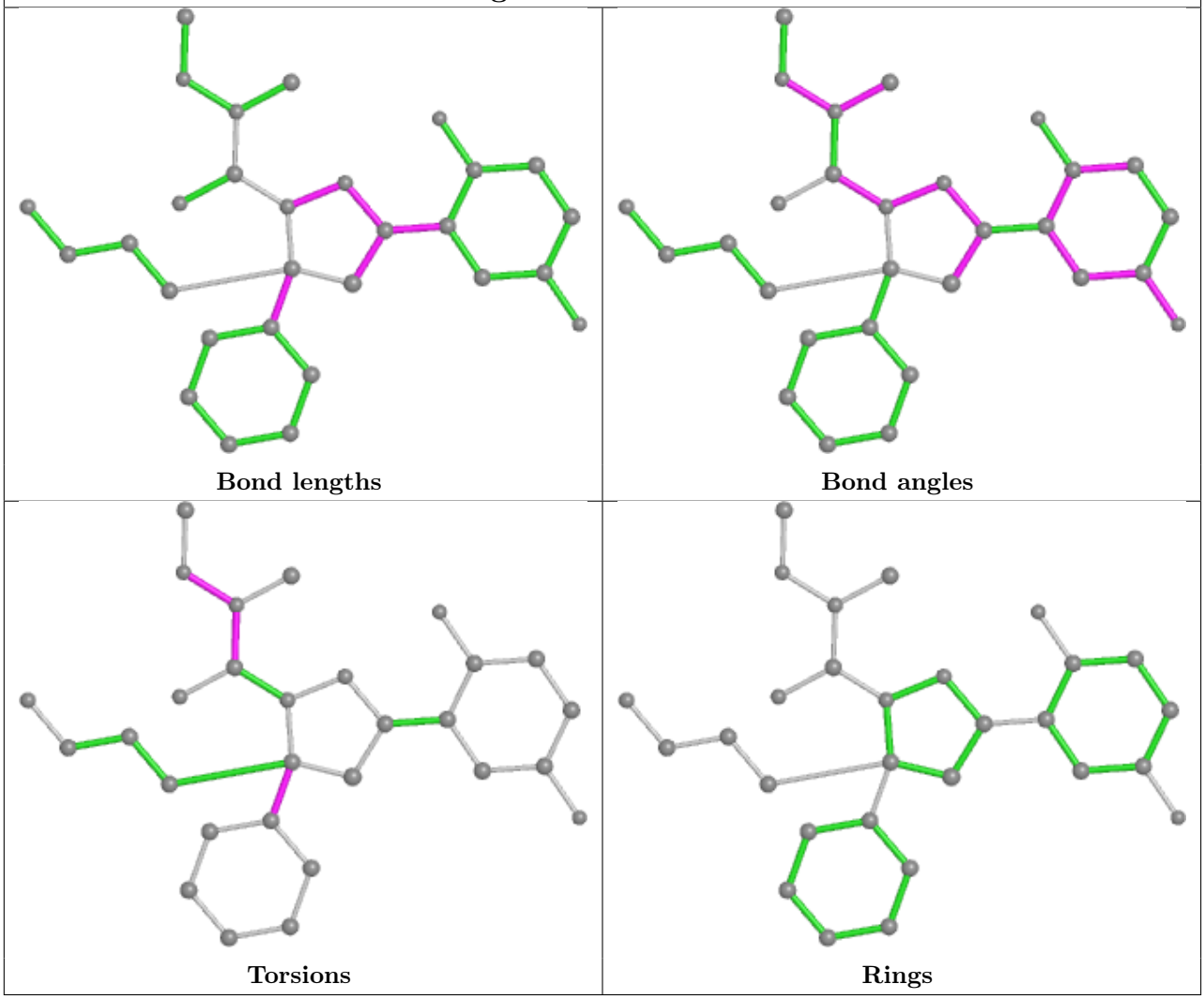


Rings

Ligand GCE C 403



Ligand GCE A 403



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	328/368 (89%)	-0.39	2 (0%)	89	92	13, 30, 58, 89	0
1	B	325/368 (88%)	-0.30	6 (1%)	68	76	14, 32, 70, 97	0
1	C	324/368 (88%)	-0.17	5 (1%)	73	81	20, 43, 76, 96	0
All	All	977/1104 (88%)	-0.29	13 (1%)	77	84	13, 34, 71, 97	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	149	ASP	5.1
1	B	363	PRO	4.4
1	B	255	LEU	4.3
1	B	17	LYS	3.6
1	C	255	LEU	3.5
1	A	149	ASP	3.4
1	C	326	GLY	3.2
1	C	271	ASN	3.2
1	B	189	ARG	3.0
1	C	327	ARG	2.4
1	A	247	GLU	2.4
1	C	325	GLY	2.3
1	B	151	GLY	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

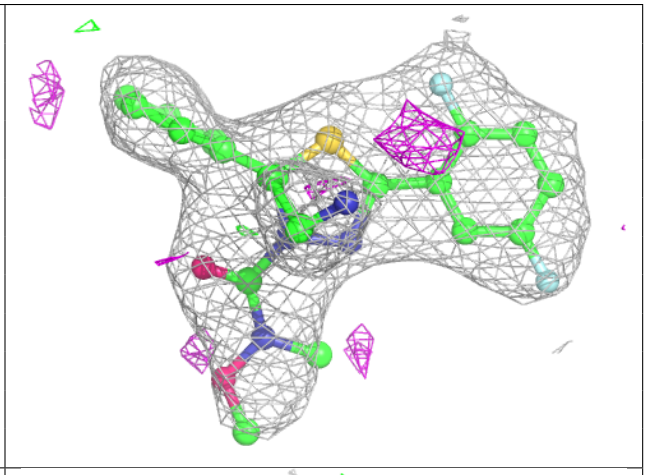
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

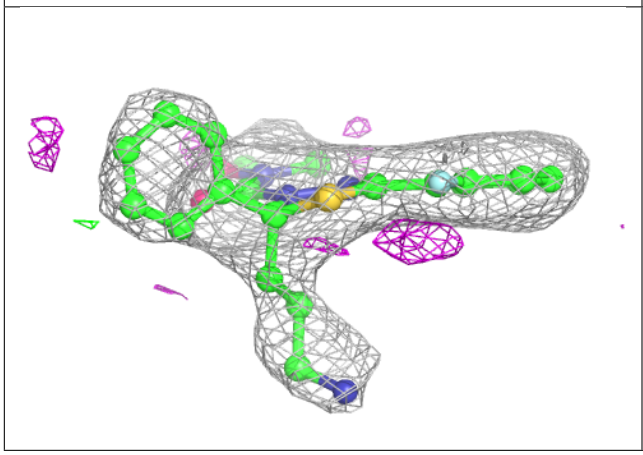
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	C	402	1/1	0.89	0.16	44,44,44,44	0
4	GCE	C	403	29/29	0.95	0.21	29,44,55,69	0
4	GCE	A	403	29/29	0.96	0.15	24,33,47,68	0
2	ADP	C	401	27/27	0.97	0.14	19,41,60,61	0
3	MG	A	402	1/1	0.97	0.10	36,36,36,36	0
4	GCE	B	403	29/29	0.97	0.17	19,29,38,61	0
3	MG	B	402	1/1	0.97	0.07	32,32,32,32	0
2	ADP	B	401	27/27	0.98	0.15	17,32,44,50	0
2	ADP	A	401	27/27	0.99	0.13	17,28,32,41	0

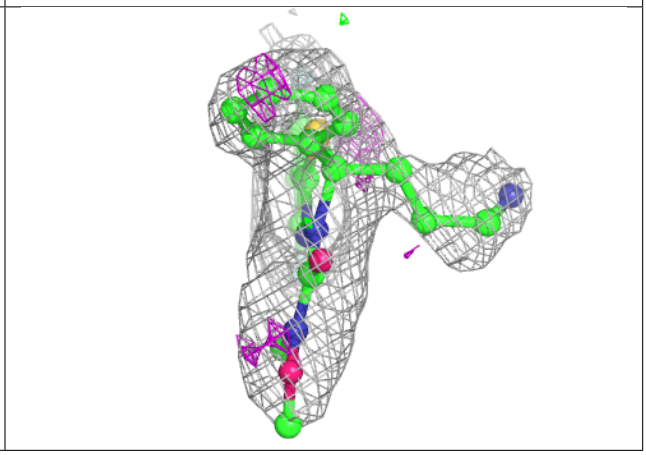
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GCE C 403:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

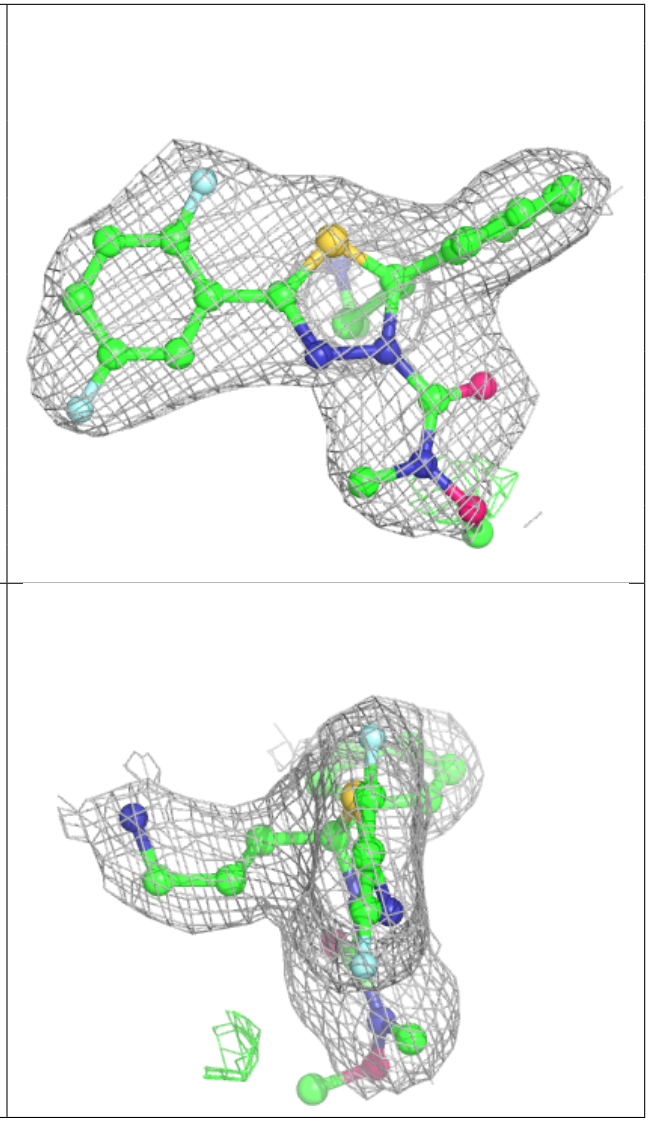






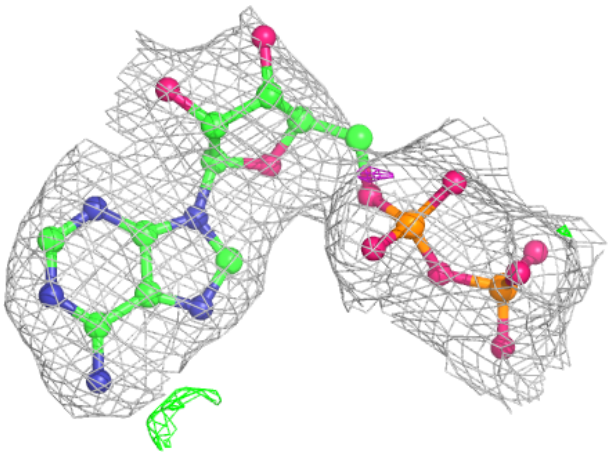
Electron density around GCE A 403:

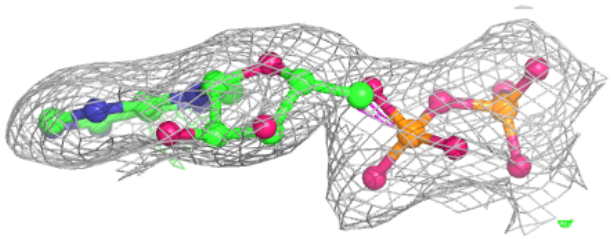
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

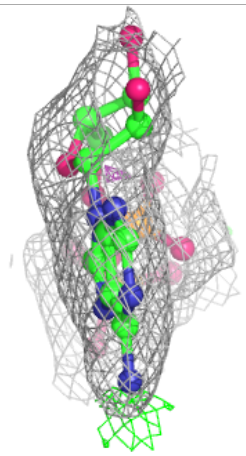


Electron density around ADP C 401:

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

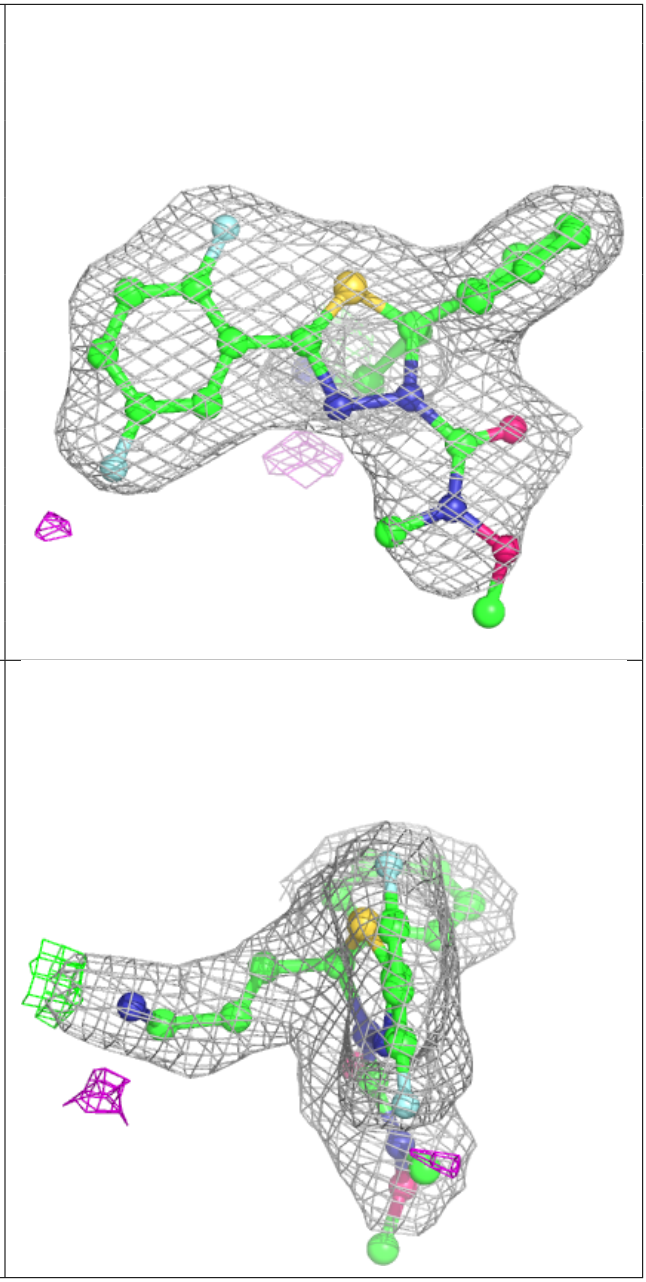






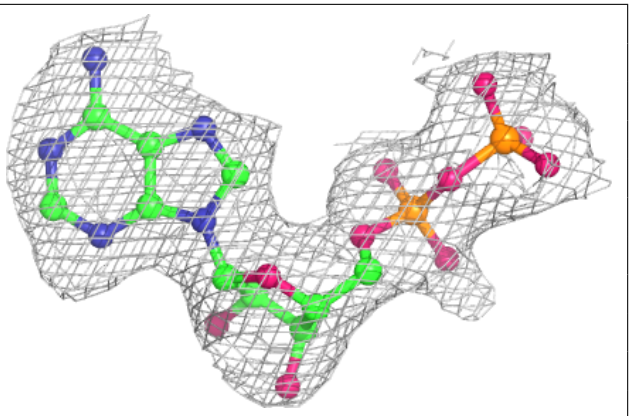
Electron density around GCE B 403:

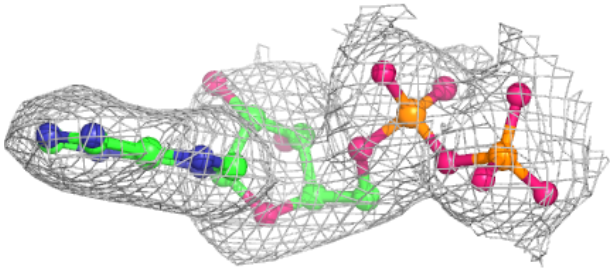
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

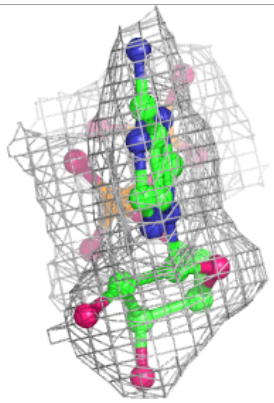


Electron density around ADP B 401:

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

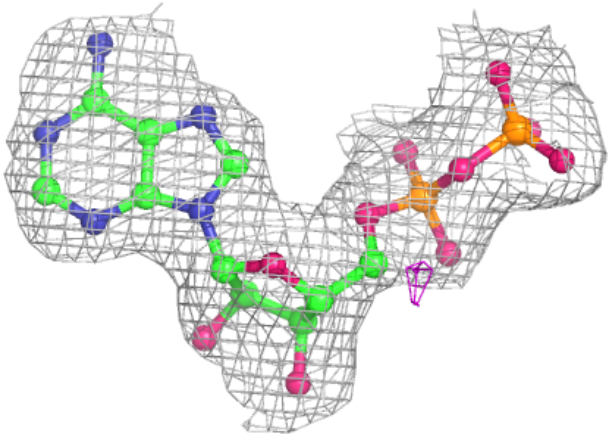


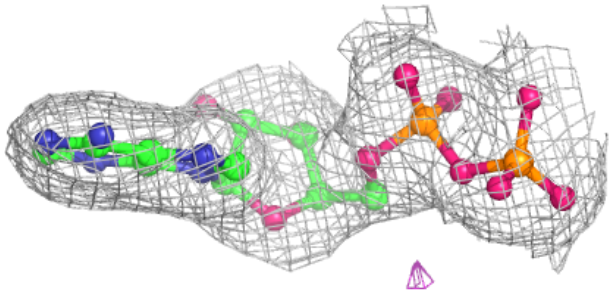


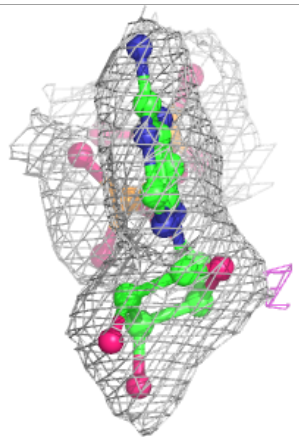


Electron density around ADP A 401:

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







6.5 Other polymers (i)

There are no such residues in this entry.