Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2025 – 08:04 AM EDT

PDB ID	:	9BAG / pdb_00009bag
Title	:	Crystal structure of Oryza sativa ketol-acid reductoisomerase in complex with Mg2+, and JK-5-114
Authors	:	Lin, X.; Guddat, L.W.
Deposited on	:	2024-04-04
Resolution	:	1.96 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 ⓘ 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 ⓘ) were used in the production of this report:

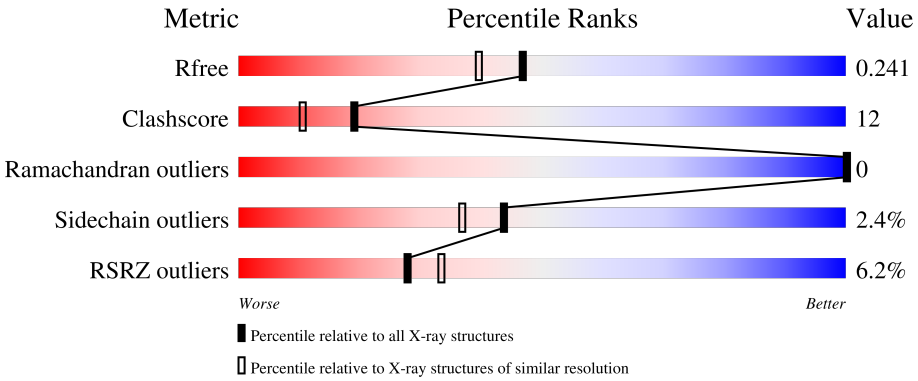
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 1.96 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}	164625	3187 (1.96-1.96)
Clashscore	180529	3412 (1.96-1.96)
Ramachandran outliers	177936	3390 (1.96-1.96)
Sidechain outliers	177891	3390 (1.96-1.96)
RSRZ outliers	164620	3186 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	525	5% 73% 17% • 9%
1	B	525	7% 72% 18% • 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7726 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.

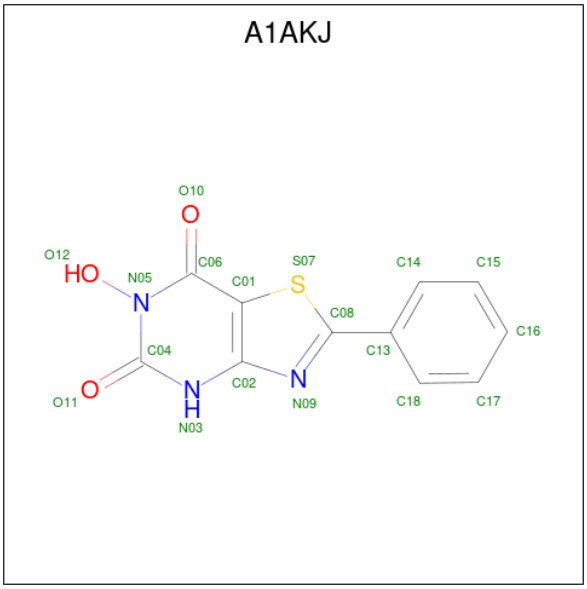
- Molecule 1 is a protein called Ketol-acid reductoisomerase, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	5	0
			3700	2351	619	712	18			
1	B	476	Total	C	N	O	S	0	6	0
			3689	2342	620	710	17			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		

- Molecule 3 is 6-hydroxy-2-phenyl[1,3]thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione (CCD ID: A1AKJ) (formula: $C_{11}H_7N_3O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			18	11	3	3	1		
3	B	1	Total	C	N	O	S	0	0
			18	11	3	3	1		

- Molecule 4 is water.

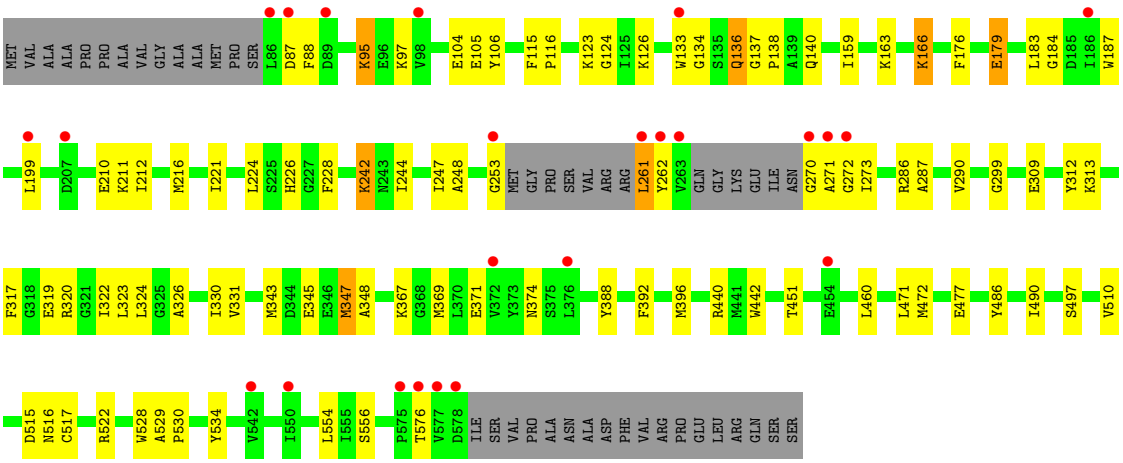
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	161	Total	O	0	0
			161	161		
4	B	136	Total	O	0	0
			136	136		

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.

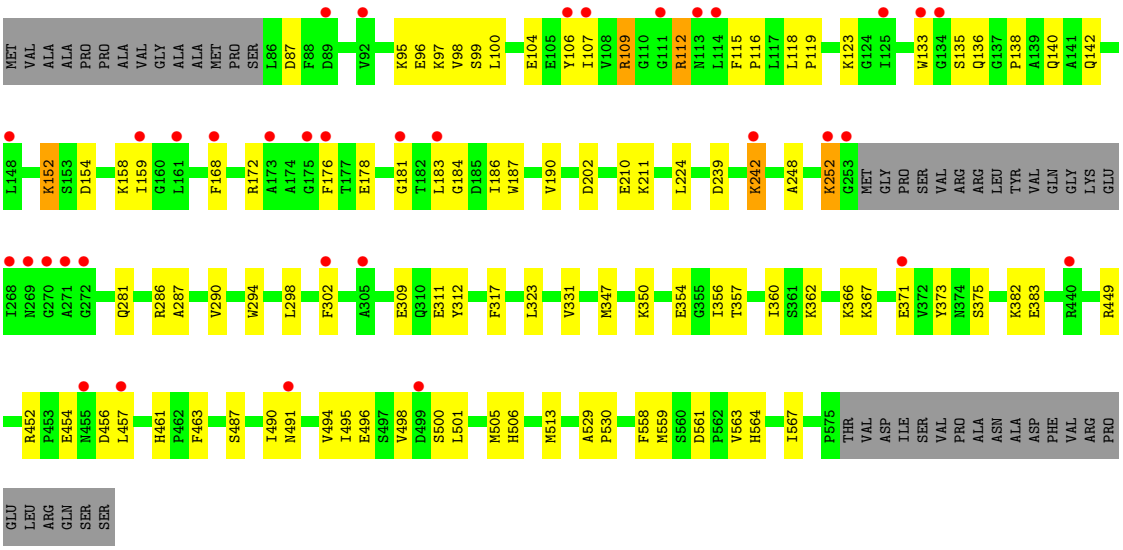
• Molecule 1: Ketol-acid reductoisomerase, chloroplastic

Chain A:



• Molecule 1: Ketol-acid reductoisomerase, chloroplastic

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	126.41Å 91.86Å 87.00Å 90.00° 101.37° 90.00°	Depositor
Resolution (Å)	45.93 – 1.96 45.93 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.93-1.96) 99.4 (45.93-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 1.97Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.213 , 0.238 0.214 , 0.241	Depositor DCC
R_{free} test set	67548 reflections (2.89%)	wwPDB-VP
Wilson B-factor (Å^2)	37.9	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 41.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7726	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1AKJ, 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	0.35	1/3789 (0.0%)	0.51	2/5122 (0.0%)
1	B	0.28	0/3781	0.54	2/5108 (0.0%)
All	All	0.32	1/7570 (0.0%)	0.52	4/10230 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	GLU	CG-CD	5.31	1.59	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	109	ARG	NE-CZ-NH2	14.39	127.50	120.30
1	B	109	ARG	NE-CZ-NH1	-8.81	115.90	120.30
1	A	179	GLU	CB-CA-C	5.78	121.96	110.40
1	A	179	GLU	N-CA-CB	-5.19	101.26	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3700	0	3645	83	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3689	0	3644	89	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	18	0	0	2	0
3	B	18	0	0	0	0
4	A	161	0	0	8	0
4	B	136	0	0	2	0
All	All	7726	0	7289	171	1

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 12.

All (171) 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:515:ASP:HA	1:A:522:ARG:HD3	1.35	1.04
1:A:309:GLU:HG2	1:A:313:LYS:HE3	1.53	0.89
1:A:242:LYS:H	1:A:242:LYS:HE2	1.39	0.84
1:A:261:LEU:HB3	1:A:272:GLY:N	1.94	0.82
1:A:187:TRP:CZ2	1:A:211:LYS:HD3	2.14	0.82
1:A:261:LEU:HB3	1:A:272:GLY:H	1.44	0.80
1:B:323:LEU:HG	1:B:501:LEU:HD12	1.68	0.76
1:B:178:GLU:OE1	1:B:178:GLU:N	2.15	0.76
1:A:261:LEU:O	1:A:271:ALA:HB1	1.86	0.75
1:B:202:ASP:OD2	4:B:701:HOH:O	2.06	0.73
1:A:97:LYS:HD2	1:A:104:GLU:OE1	1.90	0.72
1:B:168:PHE:O	1:B:172:ARG:HG3	1.91	0.71
1:A:210:GLU:OE2	4:A:701:HOH:O	2.10	0.70
1:B:501:LEU:C	1:B:513:MET:HE3	2.13	0.68
1:B:239:ASP:HB3	1:B:242[B]:LYS:HZ1	1.58	0.68
1:B:97:LYS:HD3	1:B:104:GLU:OE2	1.94	0.68
1:B:501:LEU:HB3	1:B:513:MET:HE3	1.75	0.67
1:B:152:LYS:O	1:B:152:LYS:HG2	1.94	0.67
1:B:456:ASP:C	1:B:457:LEU:HD23	2.16	0.66
1:B:187:TRP:CE2	1:B:211:LYS:HE2	2.30	0.66
1:B:286:ARG:O	1:B:290:VAL:HG12	1.95	0.66
1:B:133:TRP:CE2	1:B:138:PRO:HG3	2.31	0.65
1:A:95:LYS:HD2	1:A:106:TYR:CD1	2.30	0.65
1:B:311[B]:GLU:HG3	1:B:312:TYR:N	2.12	0.65
1:B:159:ILE:HD12	1:B:176:PHE:HB3	1.79	0.64
1:A:309:GLU:HG2	1:A:313:LYS:CE	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ILE:HD13	1:A:472:MET:HB2	1.80	0.64
1:A:242:LYS:H	1:A:242:LYS:CE	2.11	0.63
1:A:136:GLN:HG3	1:A:140:GLN:HE21	1.64	0.63
1:A:87:ASP:OD1	1:A:95:LYS:NZ	2.32	0.62
1:A:515:ASP:HA	1:A:522:ARG:CD	2.21	0.62
1:A:396:MET:HE1	1:A:477:GLU:HG2	1.81	0.62
1:B:159:ILE:HD11	1:B:176:PHE:CD2	2.34	0.62
1:B:159:ILE:HD11	1:B:176:PHE:CG	2.35	0.62
1:A:515:ASP:CA	1:A:522:ARG:HD3	2.20	0.61
1:B:96:GLU:OE2	1:B:109:ARG:NH1	2.34	0.61
1:B:501:LEU:HB3	1:B:513:MET:CE	2.30	0.61
1:B:152:LYS:O	1:B:152:LYS:CG	2.48	0.60
1:B:186:ILE:O	1:B:190:VAL:HG23	2.01	0.60
1:B:136:GLN:OE1	1:B:136:GLN:N	2.35	0.60
1:B:362:LYS:O	1:B:366:LYS:HG2	2.01	0.59
1:A:322:ILE:HD12	1:A:471:LEU:HG	1.85	0.59
1:A:323:LEU:HD23	1:A:497:SER:OG	2.03	0.59
1:B:178:GLU:H	1:B:178:GLU:CD	2.06	0.58
1:B:454:GLU:H	1:B:454:GLU:CD	2.07	0.58
1:B:159:ILE:HD12	1:B:176:PHE:CB	2.34	0.58
1:B:210:GLU:OE1	4:B:702:HOH:O	2.17	0.57
1:B:350:LYS:HG2	1:B:354:GLU:HG3	1.87	0.56
1:A:253:GLY:HA3	1:A:273:ILE:HG21	1.87	0.56
1:B:494:VAL:O	1:B:498:VAL:HG22	2.05	0.56
1:B:107:ILE:HD12	1:B:302:PHE:CE1	2.40	0.56
1:A:137:GLY:HA2	1:A:199:LEU:HD12	1.89	0.55
1:A:105:GLU:OE2	4:A:702:HOH:O	2.18	0.55
1:B:357:THR:HG21	1:B:505:MET:HB3	1.89	0.55
1:B:563:VAL:O	1:B:567:ILE:HG13	2.06	0.55
1:B:87:ASP:OD1	1:B:106:TYR:HE2	1.90	0.54
1:B:382:LYS:HE2	1:B:382:LYS:HA	1.90	0.54
1:A:345:GLU:HG2	1:A:440:ARG:HH21	1.72	0.54
1:A:123:LYS:HE3	1:A:124:GLY:H	1.72	0.54
1:A:242:LYS:CE	4:A:712:HOH:O	2.57	0.53
1:B:138:PRO:O	1:B:142:GLN:HG3	2.09	0.53
1:B:454:GLU:OE1	1:B:454:GLU:N	2.34	0.53
1:A:347:MET:HA	1:A:347:MET:HE2	1.91	0.53
1:A:133:TRP:CE2	1:A:138:PRO:HG3	2.44	0.53
1:B:158:LYS:HD2	1:B:181:GLY:O	2.09	0.52
1:B:87:ASP:OD1	1:B:106:TYR:CE2	2.63	0.52
1:A:326:ALA:O	1:A:330:ILE:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:LEU:HD23	4:A:704:HOH:O	2.09	0.52
1:A:374:ASN:ND2	4:A:703:HOH:O	2.18	0.51
1:A:529:ALA:HB3	1:A:530:PRO:HD3	1.92	0.51
1:B:136:GLN:O	1:B:140:GLN:HG3	2.10	0.51
1:B:242[B]:LYS:NZ	1:B:281:GLN:HE22	2.09	0.51
1:A:187:TRP:CE2	1:A:211:LYS:HD3	2.45	0.51
1:B:118:LEU:N	1:B:119:PRO:HD2	2.26	0.51
1:B:242[A]:LYS:HZ1	1:B:281:GLN:HE22	1.58	0.51
1:B:187:TRP:CZ2	1:B:211:LYS:HE2	2.45	0.51
1:B:99:SER:O	1:B:100:LEU:HD23	2.11	0.50
1:A:261:LEU:HD13	1:A:576:THR:HG23	1.94	0.50
1:A:515:ASP:OD1	1:A:522:ARG:HD2	2.11	0.50
1:B:136:GLN:HB3	1:B:140:GLN:HE21	1.75	0.50
1:B:347:MET:HA	1:B:347:MET:HE2	1.94	0.50
1:A:330:ILE:HG13	1:A:331:VAL:N	2.27	0.50
1:A:486:TYR:O	1:A:490:ILE:HD12	2.12	0.50
1:A:345:GLU:OE2	1:A:440:ARG:NE	2.45	0.49
1:A:123:LYS:HE3	1:A:124:GLY:N	2.28	0.49
1:B:449:ARG:HG2	1:B:452:ARG:NH1	2.27	0.49
1:B:347:MET:HE2	1:B:347:MET:CA	2.43	0.49
1:A:309:GLU:OE2	1:A:313:LYS:NZ	2.42	0.49
1:B:106:TYR:N	1:B:106:TYR:CD1	2.79	0.49
1:B:159:ILE:CD1	1:B:176:PHE:CG	2.96	0.49
1:A:396:MET:CE	1:A:477:GLU:HG2	2.42	0.49
1:B:561:ASP:OD1	1:B:563:VAL:HG12	2.13	0.49
1:A:319:GLU:HA	1:A:323:LEU:HB2	1.94	0.48
1:A:212:ILE:O	1:A:216:MET:HG3	2.14	0.48
1:A:367:LYS:HE2	1:A:371:GLU:OE2	2.13	0.48
1:B:252:LYS:HD2	1:B:252:LYS:HA	1.43	0.48
1:A:126:LYS:HB3	1:A:126:LYS:HE3	1.56	0.48
1:B:242[A]:LYS:NZ	1:B:281:GLN:HE22	2.11	0.48
1:A:221:ILE:HD13	1:A:290:VAL:HG21	1.96	0.48
1:B:115:PHE:N	1:B:116:PRO:HD2	2.28	0.48
1:B:490:ILE:HG22	1:B:495:ILE:HD12	1.95	0.48
1:B:496:GLU:O	1:B:500:SER:HB2	2.13	0.48
1:A:516:ASN:HB3	3:A:603:A1AKJ:C17	2.44	0.47
1:A:136:GLN:HG3	1:A:140:GLN:NE2	2.29	0.47
1:B:362:LYS:HA	1:B:362:LYS:HD3	1.58	0.47
1:A:183:LEU:HD12	1:A:184:GLY:H	1.79	0.47
1:A:322:ILE:CD1	1:A:472:MET:HB2	2.44	0.47
1:A:287:ALA:O	1:A:290:VAL:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:LYS:HD3	1:B:104:GLU:CD	2.34	0.47
1:B:357:THR:OG1	1:B:506:HIS:HB2	2.14	0.47
1:A:123:LYS:HD2	1:A:123:LYS:HA	1.78	0.46
1:B:294:TRP:O	1:B:298:LEU:HG	2.15	0.46
1:B:461:HIS:HD2	1:B:463:PHE:H	1.62	0.46
1:A:183:LEU:HD12	1:A:184:GLY:N	2.31	0.46
1:B:350:LYS:HA	1:B:354:GLU:HB2	1.97	0.46
1:B:107:ILE:HD12	1:B:302:PHE:CD1	2.51	0.46
1:A:224:LEU:O	1:A:248:ALA:HA	2.16	0.46
1:B:357:THR:HB	1:B:506:HIS:HB2	1.98	0.46
1:A:517:CYS:HA	3:A:603:A1AKJ:N09	2.31	0.46
1:A:226:HIS:CD2	1:A:228:PHE:HB2	2.51	0.46
1:A:242:LYS:NZ	4:A:712:HOH:O	2.46	0.46
1:B:367:LYS:HD3	1:B:371:GLU:HG2	1.97	0.45
1:B:357:THR:CB	1:B:506:HIS:HB2	2.45	0.45
1:B:224:LEU:O	1:B:248:ALA:HA	2.16	0.45
1:A:396:MET:HE2	1:A:477:GLU:HB3	1.99	0.45
1:B:490:ILE:HG22	1:B:495:ILE:CD1	2.47	0.45
1:B:529:ALA:HB3	1:B:530:PRO:HD3	1.98	0.45
1:A:442:TRP:CH2	1:A:510:VAL:HB	2.52	0.45
1:B:558:PHE:O	1:B:564:HIS:NE2	2.47	0.45
1:B:373:TYR:CE2	1:B:559:MET:HE2	2.52	0.44
1:A:166:LYS:HE2	1:A:166:LYS:HB2	1.82	0.44
1:A:319:GLU:O	1:A:324:LEU:HB2	2.17	0.44
1:A:262:TYR:HD1	1:A:299:GLY:HA3	1.83	0.44
1:A:270:GLY:C	1:A:576:THR:H	2.21	0.44
1:A:87:ASP:OD1	1:A:88:PHE:N	2.50	0.44
1:A:159:ILE:HD13	1:A:176:PHE:CD1	2.52	0.44
1:B:373:TYR:CD2	1:B:559:MET:HE1	2.53	0.44
1:A:95:LYS:CD	1:A:106:TYR:CD1	3.00	0.44
1:B:135[B]:SER:OG	1:B:136:GLN:NE2	2.52	0.43
1:B:154:ASP:OD1	1:B:154:ASP:N	2.45	0.43
1:A:242:LYS:HE2	4:A:712:HOH:O	2.15	0.43
1:A:367:LYS:HD3	1:A:371:GLU:OE2	2.18	0.43
1:A:534:TYR:CG	1:B:530:PRO:HG3	2.53	0.43
1:B:287:ALA:HA	1:B:290:VAL:CG1	2.49	0.43
1:B:252:LYS:CB	1:B:252:LYS:HZ2	2.30	0.43
1:B:449:ARG:HG2	1:B:452:ARG:CZ	2.47	0.43
1:A:343:MET:SD	1:A:348:ALA:HA	2.58	0.43
1:A:133:TRP:HB3	1:A:134:GLY:H	1.55	0.43
1:B:487:SER:O	1:B:491:ASN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:LEU:O	1:B:513:MET:HE3	2.18	0.43
1:A:320:ARG:HG2	1:A:528:TRP:CD1	2.54	0.42
1:B:323:LEU:HD23	1:B:501:LEU:HD11	1.99	0.42
1:A:313:LYS:O	1:A:317:PHE:HB3	2.19	0.42
1:B:159:ILE:CD1	1:B:176:PHE:CB	2.97	0.42
1:B:183:LEU:HD12	1:B:184:GLY:H	1.84	0.42
1:A:369:MET:HB2	4:A:714:HOH:O	2.19	0.42
1:A:261:LEU:CB	1:A:272:GLY:H	2.24	0.41
1:B:356:ILE:HA	1:B:360:ILE:HD12	2.02	0.41
1:A:451:THR:HG22	1:A:451:THR:O	2.20	0.41
1:B:457:LEU:HD23	1:B:457:LEU:N	2.35	0.41
1:B:456:ASP:O	1:B:457:LEU:HD23	2.20	0.41
1:A:115:PHE:N	1:A:116:PRO:CD	2.84	0.41
1:A:247:ILE:HD13	1:A:290:VAL:HG23	2.01	0.41
1:B:112:ARG:HE	1:B:112:ARG:H	1.68	0.41
1:B:309:GLU:CD	1:B:309:GLU:H	2.24	0.41
1:A:244:ILE:O	1:A:244:ILE:HD12	2.22	0.40
1:A:392:PHE:CD2	1:A:554:LEU:HD21	2.56	0.40
1:A:272:GLY:O	1:A:273:ILE:HD13	2.21	0.40
1:A:286:ARG:O	1:A:290:VAL:HG13	2.22	0.40
1:A:388:TYR:HE1	1:A:554:LEU:HD22	1.86	0.40
1:B:98:VAL:HG13	1:B:107:ILE:HG12	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LYS:O	1:B:109:ARG:NH2[4_546]	1.99	0.21

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	479/525 (91%)	467 (98%)	12 (2%)	0	100	100
1	B	478/525 (91%)	465 (97%)	13 (3%)	0	100	100
All	All	957/1050 (91%)	932 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	398/432 (92%)	389 (98%)	9 (2%)	45	39
1	B	397/432 (92%)	386 (97%)	11 (3%)	38	29
All	All	795/864 (92%)	775 (98%)	20 (2%)	44	34

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	LYS
1	A	136	GLN
1	A	166	LYS
1	A	179	GLU
1	A	242	LYS
1	A	261	LEU
1	A	312	TYR
1	A	347	MET
1	A	556	SER
1	B	95	LYS
1	B	112	ARG
1	B	123	LYS
1	B	152	LYS
1	B	242[A]	LYS
1	B	242[B]	LYS
1	B	252	LYS
1	B	317	PHE
1	B	331	VAL

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Mol	Chain	Res	Type
1	B	375	SER
1	B	383	GLU

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

Mol	Chain	Res	Type
1	A	435	ASN
1	B	281	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
3	A1AKJ	A	603	2	16,20,20	2.15	7 (43%)	13,29,29	2.35	5 (38%)
3	A1AKJ	B	603	2	16,20,20	2.32	6 (37%)	13,29,29	2.36	5 (38%)

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
3	A1AKJ	A	603	2	-	0/4/4/4	0/3/3/3
3	A1AKJ	B	603	2	-	0/4/4/4	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	A1AKJ	C04-N05	-5.84	1.34	1.38
3	A	603	A1AKJ	C04-N05	-4.92	1.35	1.38
3	B	603	A1AKJ	C01-C06	-3.91	1.38	1.47
3	A	603	A1AKJ	C01-C06	-3.67	1.39	1.47
3	A	603	A1AKJ	C04-N03	-2.96	1.32	1.36
3	B	603	A1AKJ	C08-S07	-2.90	1.69	1.73
3	B	603	A1AKJ	C04-N03	-2.66	1.33	1.36
3	B	603	A1AKJ	C01-S07	-2.42	1.71	1.75
3	B	603	A1AKJ	O11-C04	-2.32	1.19	1.23
3	A	603	A1AKJ	C08-S07	-2.30	1.70	1.73
3	A	603	A1AKJ	C02-N03	-2.28	1.35	1.38
3	A	603	A1AKJ	C01-S07	-2.26	1.72	1.75
3	A	603	A1AKJ	O11-C04	-2.23	1.19	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	603	A1AKJ	O12-N05-C04	4.58	119.71	116.38
3	A	603	A1AKJ	C01-C06-N05	4.38	120.13	114.84
3	B	603	A1AKJ	C01-C06-N05	4.30	120.03	114.84
3	B	603	A1AKJ	O12-N05-C04	3.89	119.20	116.38
3	B	603	A1AKJ	N03-C04-N05	3.61	120.43	115.65
3	A	603	A1AKJ	N03-C04-N05	3.50	120.28	115.65
3	B	603	A1AKJ	O11-C04-N05	-3.49	119.35	123.45
3	A	603	A1AKJ	O11-C04-N05	-2.71	120.26	123.45
3	B	603	A1AKJ	O10-C06-C01	-2.58	119.92	124.16
3	A	603	A1AKJ	O10-C06-C01	-2.46	120.11	124.16

There are no chirality outliers.

There are no torsion outliers.

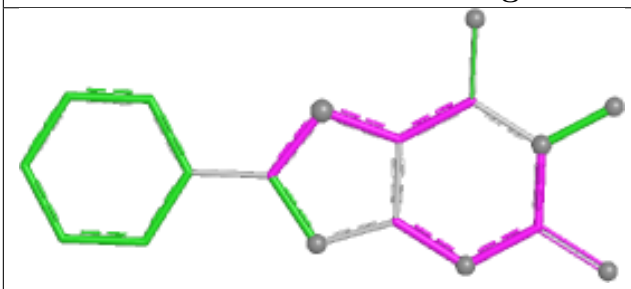
There are no ring outliers.

1 monomer is involved in 2 short contacts:

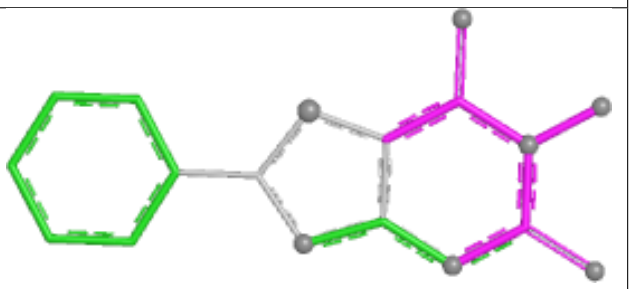
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	A1AKJ	2	0

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.

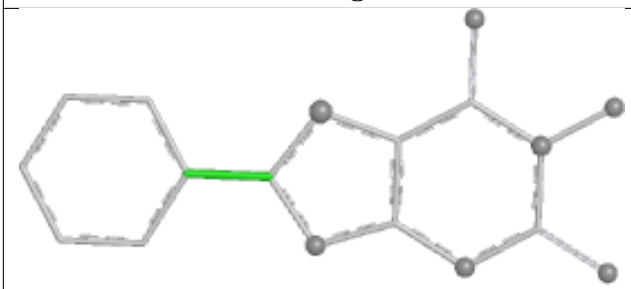
Ligand A1AKJ A 603



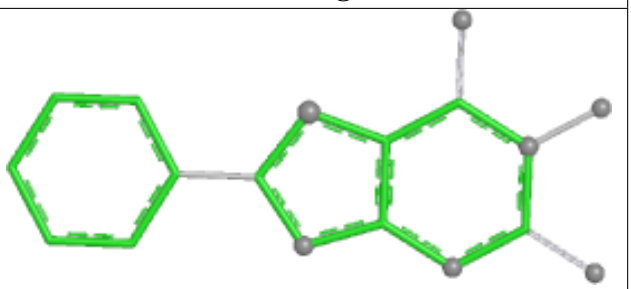
Bond lengths



Bond angles

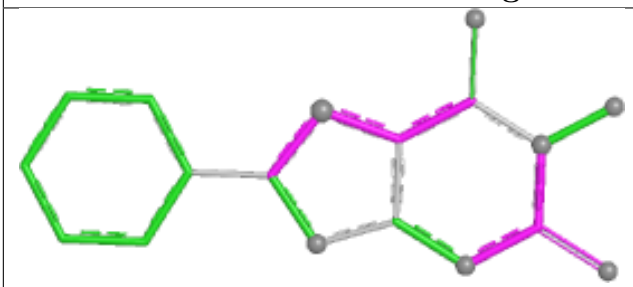


Torsions

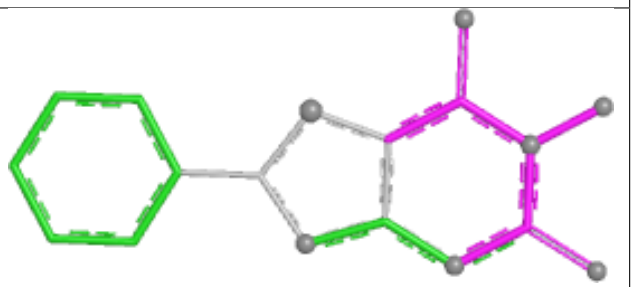


Rings

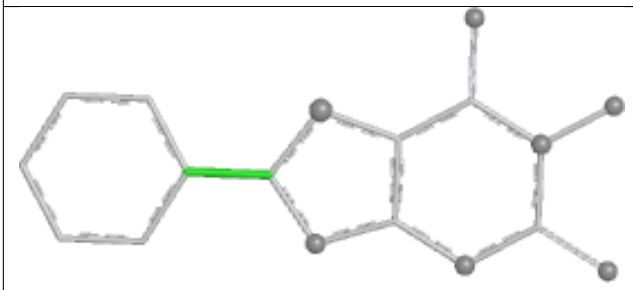
Ligand A1AKJ B 603



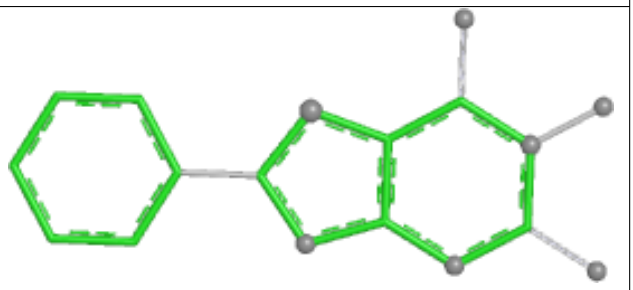
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	480/525 (91%)	0.56	24 (5%)	35	42	20, 41, 60, 88	5 (1%)
1	B	476/525 (90%)	0.84	35 (7%)	22	27	21, 47, 68, 96	6 (1%)
All	All	956/1050 (91%)	0.70	59 (6%)	28	33	20, 43, 65, 96	11 (1%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	268	ILE	7.1
1	A	270	GLY	6.9
1	A	577	VAL	5.3
1	A	262	TYR	5.3
1	B	271	ALA	5.1
1	B	272	GLY	5.0
1	A	261	LEU	5.0
1	A	253	GLY	5.0
1	A	271	ALA	4.8
1	B	302	PHE	4.7
1	A	576	THR	4.7
1	B	253	GLY	4.6
1	A	263	VAL	4.4
1	B	270	GLY	4.0
1	B	133	TRP	3.6
1	B	106	TYR	3.2
1	B	134	GLY	3.1
1	B	107	ILE	2.9
1	B	114	LEU	2.8
1	B	159	ILE	2.8
1	B	168	PHE	2.7
1	B	252	LYS	2.7
1	B	242[A]	LYS	2.7
1	A	454	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	376	LEU	2.6
1	B	183	LEU	2.5
1	B	161	LEU	2.5
1	A	578	ASP	2.5
1	A	87	ASP	2.5
1	B	111	GLY	2.5
1	B	499	ASP	2.4
1	A	207	ASP	2.4
1	B	181	GLY	2.4
1	A	86	LEU	2.4
1	A	272	GLY	2.4
1	B	175	GLY	2.4
1	B	269	ASN	2.3
1	A	186	ILE	2.3
1	B	125	ILE	2.3
1	B	371	GLU	2.3
1	B	455	ASN	2.2
1	A	575	PRO	2.2
1	A	133	TRP	2.2
1	B	457	LEU	2.2
1	A	199	LEU	2.1
1	A	372	VAL	2.1
1	A	542	VAL	2.1
1	B	176	PHE	2.1
1	B	305	ALA	2.1
1	A	89	ASP	2.1
1	B	491	ASN	2.1
1	A	98	VAL	2.1
1	B	92	VAL	2.1
1	B	440	ARG	2.1
1	B	89	ASP	2.0
1	A	550	ILE	2.0
1	B	113	ASN	2.0
1	B	173	ALA	2.0
1	B	148	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

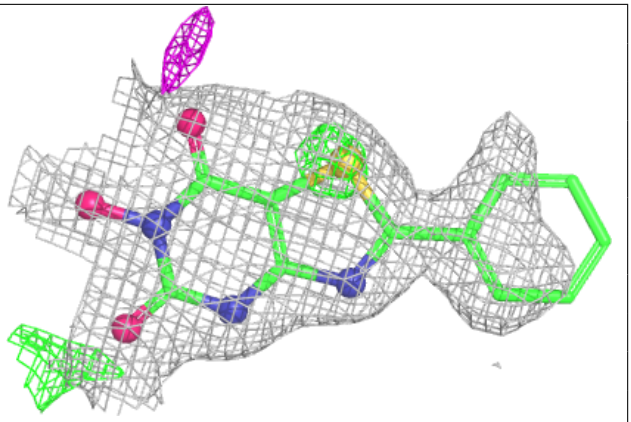
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

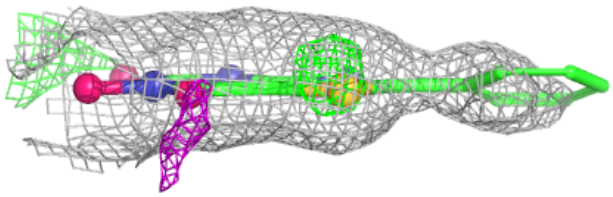
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	B	601	1/1	0.84	0.07	44,44,44,44	0
2	MG	B	602	1/1	0.84	0.11	60,60,60,60	0
3	A1AKJ	B	603	18/18	0.86	0.13	51,66,75,120	0
3	A1AKJ	A	603	18/18	0.92	0.10	37,45,61,62	0
2	MG	A	602	1/1	0.95	0.06	37,37,37,37	0
2	MG	A	601	1/1	0.98	0.06	39,39,39,39	0

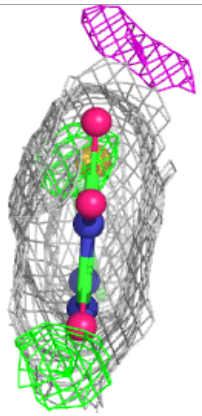
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1AKJ B 603:

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

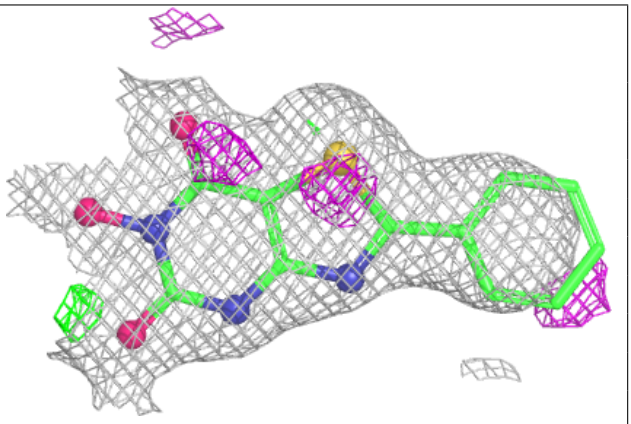


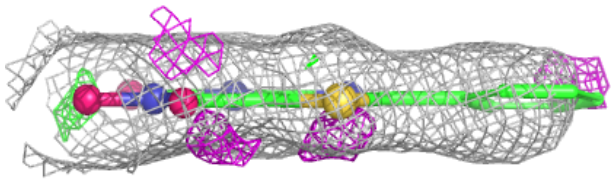


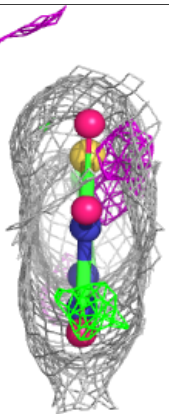


Electron density around A1AKJ A 603:

$2mF_o$-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.