Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 09:07 PM EDT

PDB ID	:	6BKY
Title	:	Novel Binding Modes of Inhibition of Wild-Type IDH1: Allosteric Inhibition with Cmpd2
Authors	:	Jakob, C.G.; Qiu, W.
Deposited on	:	2017-11-09
Resolution	:	2.17 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:

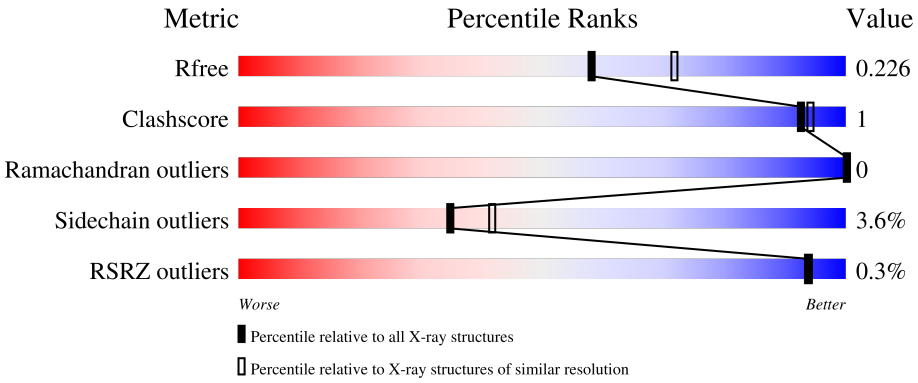
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.17 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	425	90% 8% ·
1	B	425	% 92% 5% ·
1	C	425	91% 6% ·
1	D	425	91% 7% ·
1	E	425	91% 6% ·

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Mol	Chain	Length	Quality of chain
1	F	425	90% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LMR	A	503	-	X	-	-
2	LMR	F	501	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 21135 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 Isocitrate dehydrogenase [NADP] cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	416	Total	C	N	O	S	0	0	0
			3287	2090	557	622	18			
1	C	414	Total	C	N	O	S	0	0	0
			3268	2079	553	618	18			
1	F	413	Total	C	N	O	S	0	0	0
			3265	2076	554	617	18			
1	A	416	Total	C	N	O	S	0	0	0
			3288	2090	558	622	18			
1	E	416	Total	C	N	O	S	0	0	0
			3292	2093	559	622	18			
1	B	413	Total	C	N	O	S	0	0	0
			3261	2073	553	617	18			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	415	SER	-	expression tag	UNP O75874
D	416	LEU	-	expression tag	UNP O75874
D	417	GLU	-	expression tag	UNP O75874
D	418	HIS	-	expression tag	UNP O75874
D	419	HIS	-	expression tag	UNP O75874
D	420	HIS	-	expression tag	UNP O75874
D	421	HIS	-	expression tag	UNP O75874
D	422	HIS	-	expression tag	UNP O75874
D	423	HIS	-	expression tag	UNP O75874
D	424	HIS	-	expression tag	UNP O75874
D	425	HIS	-	expression tag	UNP O75874
C	415	SER	-	expression tag	UNP O75874
C	416	LEU	-	expression tag	UNP O75874
C	417	GLU	-	expression tag	UNP O75874
C	418	HIS	-	expression tag	UNP O75874
C	419	HIS	-	expression tag	UNP O75874
C	420	HIS	-	expression tag	UNP O75874

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Chain	Residue	Modelled	Actual	Comment	Reference
C	421	HIS	-	expression tag	UNP O75874
C	422	HIS	-	expression tag	UNP O75874
C	423	HIS	-	expression tag	UNP O75874
C	424	HIS	-	expression tag	UNP O75874
C	425	HIS	-	expression tag	UNP O75874
F	415	SER	-	expression tag	UNP O75874
F	416	LEU	-	expression tag	UNP O75874
F	417	GLU	-	expression tag	UNP O75874
F	418	HIS	-	expression tag	UNP O75874
F	419	HIS	-	expression tag	UNP O75874
F	420	HIS	-	expression tag	UNP O75874
F	421	HIS	-	expression tag	UNP O75874
F	422	HIS	-	expression tag	UNP O75874
F	423	HIS	-	expression tag	UNP O75874
F	424	HIS	-	expression tag	UNP O75874
F	425	HIS	-	expression tag	UNP O75874
A	415	SER	-	expression tag	UNP O75874
A	416	LEU	-	expression tag	UNP O75874
A	417	GLU	-	expression tag	UNP O75874
A	418	HIS	-	expression tag	UNP O75874
A	419	HIS	-	expression tag	UNP O75874
A	420	HIS	-	expression tag	UNP O75874
A	421	HIS	-	expression tag	UNP O75874
A	422	HIS	-	expression tag	UNP O75874
A	423	HIS	-	expression tag	UNP O75874
A	424	HIS	-	expression tag	UNP O75874
A	425	HIS	-	expression tag	UNP O75874
E	415	SER	-	expression tag	UNP O75874
E	416	LEU	-	expression tag	UNP O75874
E	417	GLU	-	expression tag	UNP O75874
E	418	HIS	-	expression tag	UNP O75874
E	419	HIS	-	expression tag	UNP O75874
E	420	HIS	-	expression tag	UNP O75874
E	421	HIS	-	expression tag	UNP O75874
E	422	HIS	-	expression tag	UNP O75874
E	423	HIS	-	expression tag	UNP O75874
E	424	HIS	-	expression tag	UNP O75874
E	425	HIS	-	expression tag	UNP O75874
B	415	SER	-	expression tag	UNP O75874
B	416	LEU	-	expression tag	UNP O75874
B	417	GLU	-	expression tag	UNP O75874
B	418	HIS	-	expression tag	UNP O75874

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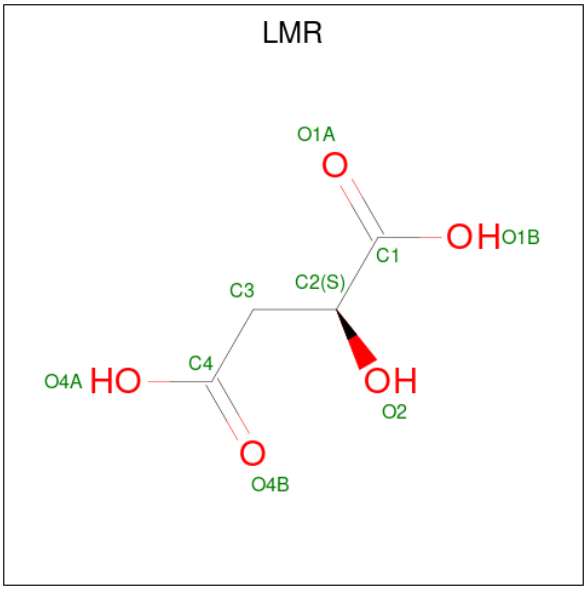
Chain	Residue	Modelled	Actual	Comment	Reference
B	419	HIS	-	expression tag	UNP O75874
B	420	HIS	-	expression tag	UNP O75874
B	421	HIS	-	expression tag	UNP O75874
B	422	HIS	-	expression tag	UNP O75874
B	423	HIS	-	expression tag	UNP O75874
B	424	HIS	-	expression tag	UNP O75874
B	425	HIS	-	expression tag	UNP O75874

- Molecule 2 is (2S)-2-hydroxybutanedioic acid (three-letter code: LMR) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 9 4 5	0	0
2	F	1	Total C O 9 4 5	0	0
2	A	1	Total C O 9 4 5	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	2	Total Mg 2 2	0	0
3	F	1	Total Mg 1 1	0	0

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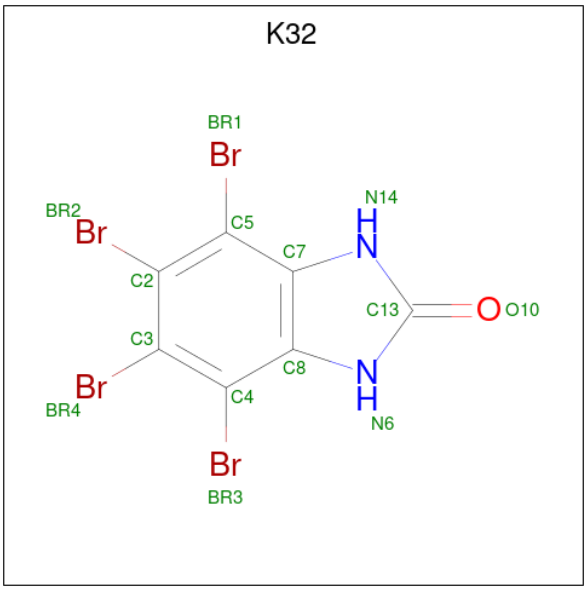
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is 4,5,6,7-TETRABROMO-1H,3H-BENZIMIDAZOL-2-ONE (three-letter code: K32) (formula: $C_7H_2Br_4N_2O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Br C N O 14 4 7 2 1	0	0
4	A	1	Total Br C N O 14 4 7 2 1	0	0
4	E	1	Total Br C N O 14 4 7 2 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	322	Total O 322 322	0	0
5	C	310	Total O 310 310	0	0
5	F	174	Total O 174 174	0	0
5	A	178	Total O 178 178	0	0
5	E	215	Total O 215 215	0	0

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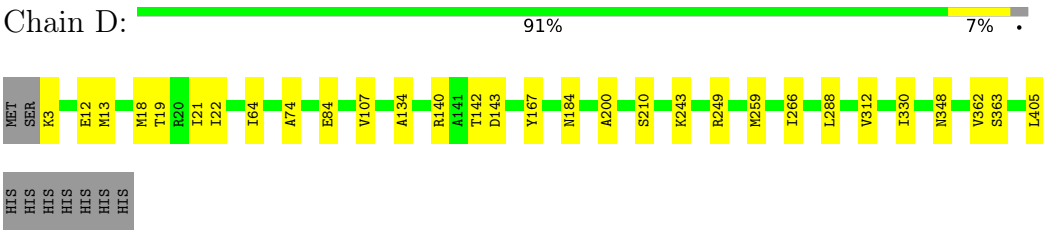
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	202	Total 202	O 202	0	0

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.

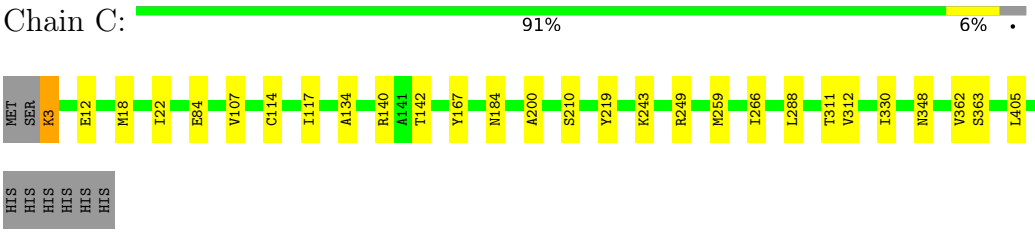
• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain D:



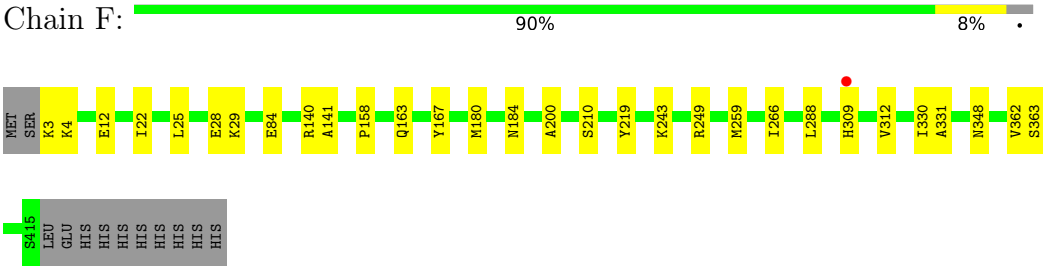
• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain C:



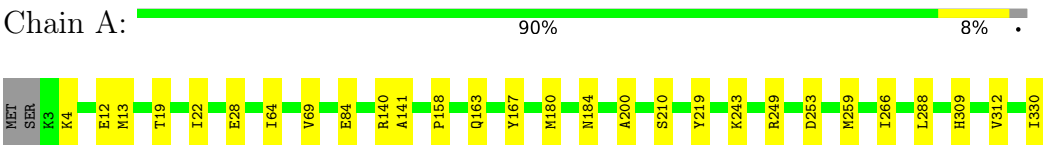
• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

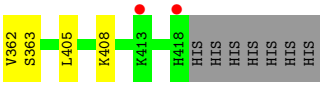
Chain F:



• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

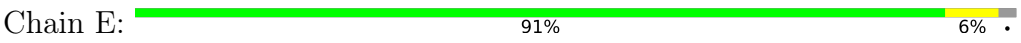
Chain A:

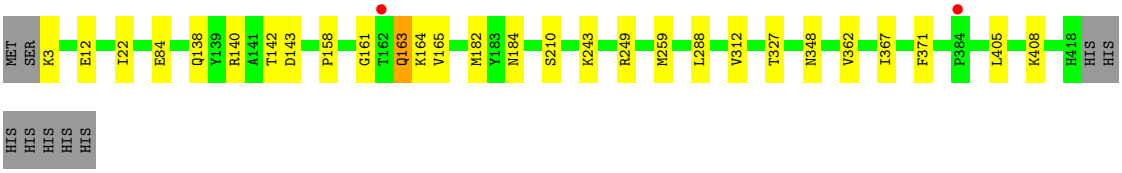




• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

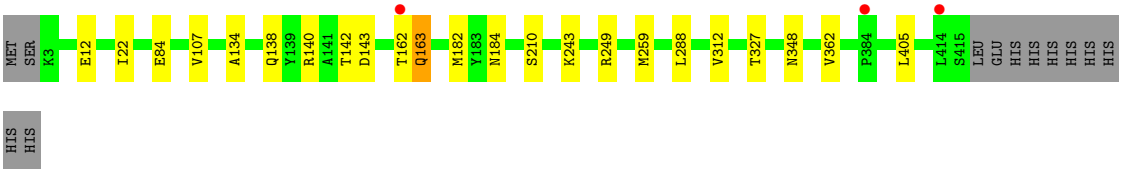
Chain E:





• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

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	98.67Å 274.89Å 116.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	137.44 – 2.17 137.44 – 2.17	Depositor EDS
% Data completeness (in resolution range)	97.8 (137.44-2.17) 97.9 (137.44-2.17)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.16Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.185 , 0.221 0.192 , 0.226	Depositor DCC
R_{free} test set	7727 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	38.1	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.479 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	21135	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: MG, LMR, K32

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	0.48	0/3357	0.64	0/4529
1	B	0.48	0/3329	0.65	0/4491
1	C	0.51	0/3335	0.64	0/4498
1	D	0.51	0/3355	0.65	0/4525
1	E	0.49	0/3361	0.65	0/4533
1	F	0.48	0/3333	0.64	0/4495
All	All	0.49	0/20070	0.65	0/27071

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3288	0	3244	11	0
1	B	3261	0	3220	10	0
1	C	3268	0	3237	13	0
1	D	3287	0	3250	13	0
1	E	3292	0	3255	9	0
1	F	3265	0	3231	12	0
2	A	9	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	9	0	4	0	0
2	F	9	0	4	0	0
3	A	1	0	0	0	0
3	D	2	0	0	0	0
3	F	1	0	0	0	0
4	A	14	0	2	2	0
4	D	14	0	2	2	0
4	E	14	0	2	2	0
5	A	178	0	0	0	0
5	B	202	0	0	0	0
5	C	310	0	0	1	0
5	D	322	0	0	1	0
5	E	215	0	0	0	0
5	F	174	0	0	0	0
All	All	21135	0	19456	58	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 1.

All (58) 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:D:3:LYS:HB2	1:E:163:GLN:HB3	1.54	0.88
1:C:3:LYS:HG3	1:B:163:GLN:HB2	1.79	0.63
1:A:167:TYR:HB3	1:B:142:THR:HG21	1.88	0.55
1:D:19:THR:HG21	1:D:74:ALA:HB3	1.88	0.55
1:F:167:TYR:HB3	1:E:142:THR:HG21	1.89	0.55
1:E:259:MET:HG2	4:E:501:K32:BR4	2.66	0.51
1:C:3:LYS:HB2	1:B:163:GLN:HG3	1.93	0.51
1:D:167:TYR:HB3	1:C:142:THR:HG21	1.93	0.50
4:A:502:K32:BR2	1:B:259:MET:HG2	2.67	0.50
1:A:330:ILE:HD12	1:A:363:SER:HB3	1.94	0.50
4:D:503:K32:BR4	1:C:259:MET:HG2	2.68	0.49
1:D:259:MET:HG2	4:D:503:K32:BR2	2.68	0.49
1:F:259:MET:HG2	4:E:501:K32:BR2	2.67	0.49
1:D:142:THR:HG21	1:C:167:TYR:HB3	1.96	0.48
1:C:200:ALA:HA	1:C:266:ILE:HG13	1.96	0.48
1:C:18:MET:HE2	5:C:603:HOH:O	2.13	0.48
1:F:330:ILE:HD12	1:F:363:SER:HB3	1.95	0.47
1:D:330:ILE:HD12	1:D:363:SER:HB3	1.97	0.47
1:D:200:ALA:HA	1:D:266:ILE:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:MET:CE	1:A:64:ILE:HD11	2.46	0.46
1:C:107:VAL:HG23	1:C:134:ALA:HB2	1.97	0.46
1:A:158:PRO:HD2	1:A:163:GLN:O	2.15	0.46
1:C:362:VAL:HG21	1:C:405:LEU:HA	1.97	0.45
1:F:362:VAL:HG21	1:F:405:LEU:HA	1.97	0.45
1:D:13:MET:CE	1:D:64:ILE:HD11	2.47	0.45
1:F:25:LEU:HD22	1:F:29:LYS:HD2	1.99	0.45
1:F:309:HIS:NE2	1:F:331:ALA:HB3	2.32	0.44
1:D:362:VAL:HG21	1:D:405:LEU:HA	1.98	0.44
1:D:210:SER:HA	1:D:249:ARG:O	2.17	0.44
1:C:210:SER:HA	1:C:249:ARG:O	2.17	0.44
1:F:219:TYR:HB2	1:E:143:ASP:HB2	1.99	0.44
1:A:362:VAL:HG21	1:A:405:LEU:HA	1.98	0.44
1:D:107:VAL:HG23	1:D:134:ALA:HB2	2.01	0.43
1:A:219:TYR:HB2	1:B:143:ASP:HB2	2.00	0.43
1:C:330:ILE:HD12	1:C:363:SER:HB3	2.00	0.43
1:B:107:VAL:HG23	1:B:134:ALA:HB2	2.01	0.43
1:A:259:MET:HG2	4:A:502:K32:BR4	2.74	0.43
1:B:163:GLN:O	1:B:163:GLN:HG2	2.18	0.43
1:E:210:SER:HA	1:E:249:ARG:O	2.19	0.42
1:B:362:VAL:HG21	1:B:405:LEU:HA	2.02	0.42
1:A:210:SER:HA	1:A:249:ARG:O	2.20	0.42
1:E:362:VAL:HG21	1:E:405:LEU:HA	2.02	0.42
1:B:210:SER:HA	1:B:249:ARG:O	2.19	0.42
1:F:141:ALA:HB1	1:F:180:MET:HE3	2.02	0.42
1:A:141:ALA:HB1	1:A:180:MET:HE3	2.02	0.42
1:F:210:SER:HA	1:F:249:ARG:O	2.20	0.42
1:A:309:HIS:NE2	1:A:331:ALA:HB3	2.34	0.41
1:D:18:MET:HE2	5:D:604:HOH:O	2.20	0.41
1:A:200:ALA:HA	1:A:266:ILE:HG13	2.02	0.41
1:B:138:GLN:HG3	1:B:182:MET:HE1	2.02	0.41
1:D:143:ASP:HB2	1:C:219:TYR:HB2	2.01	0.41
1:F:362:VAL:HG12	1:F:401:LEU:HD23	2.01	0.41
1:E:158:PRO:HB2	1:E:161:GLY:H	1.86	0.40
1:F:200:ALA:HA	1:F:266:ILE:HG13	2.03	0.40
1:E:367:ILE:HA	1:E:371:PHE:O	2.21	0.40
1:C:114:CYS:HB2	1:C:117:ILE:HG12	2.04	0.40
1:F:158:PRO:HD2	1:F:163:GLN:O	2.22	0.40
1:E:138:GLN:HG3	1:E:182:MET:HE1	2.03	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	414/425 (97%)	400 (97%)	14 (3%)	0	100	100
1	B	411/425 (97%)	395 (96%)	16 (4%)	0	100	100
1	C	412/425 (97%)	397 (96%)	15 (4%)	0	100	100
1	D	414/425 (97%)	400 (97%)	14 (3%)	0	100	100
1	E	414/425 (97%)	398 (96%)	16 (4%)	0	100	100
1	F	411/425 (97%)	398 (97%)	13 (3%)	0	100	100
All	All	2476/2550 (97%)	2388 (96%)	88 (4%)	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	349/361 (97%)	334 (96%)	15 (4%)	29	34
1	B	346/361 (96%)	334 (96%)	12 (4%)	36	43
1	C	347/361 (96%)	336 (97%)	11 (3%)	39	47
1	D	349/361 (97%)	338 (97%)	11 (3%)	39	47
1	E	350/361 (97%)	335 (96%)	15 (4%)	29	34
1	F	347/361 (96%)	335 (96%)	12 (4%)	36	43
All	All	2088/2166 (96%)	2012 (96%)	76 (4%)	35	42

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	12	GLU
1	D	21	ILE
1	D	22	ILE
1	D	84	GLU
1	D	140	ARG
1	D	184	ASN
1	D	243	LYS
1	D	288	LEU
1	D	312	VAL
1	D	348	ASN
1	D	416	LEU
1	C	3	LYS
1	C	12	GLU
1	C	22	ILE
1	C	84	GLU
1	C	140	ARG
1	C	184	ASN
1	C	243	LYS
1	C	288	LEU
1	C	311	THR
1	C	312	VAL
1	C	348	ASN
1	F	3	LYS
1	F	4	LYS
1	F	12	GLU
1	F	22	ILE
1	F	28	GLU
1	F	84	GLU
1	F	140	ARG
1	F	184	ASN
1	F	243	LYS
1	F	288	LEU
1	F	312	VAL
1	F	348	ASN
1	A	4	LYS
1	A	12	GLU
1	A	19	THR
1	A	22	ILE
1	A	28	GLU
1	A	69	VAL
1	A	84	GLU
1	A	140	ARG

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Mol	Chain	Res	Type
1	A	184	ASN
1	A	243	LYS
1	A	253	ASP
1	A	288	LEU
1	A	312	VAL
1	A	348	ASN
1	A	408	LYS
1	E	3	LYS
1	E	12	GLU
1	E	22	ILE
1	E	84	GLU
1	E	140	ARG
1	E	163	GLN
1	E	164	LYS
1	E	165	VAL
1	E	184	ASN
1	E	243	LYS
1	E	288	LEU
1	E	312	VAL
1	E	327	THR
1	E	348	ASN
1	E	408	LYS
1	B	12	GLU
1	B	22	ILE
1	B	84	GLU
1	B	140	ARG
1	B	162	THR
1	B	163	GLN
1	B	184	ASN
1	B	243	LYS
1	B	288	LEU
1	B	312	VAL
1	B	327	THR
1	B	348	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	101	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 10 ligands modelled in this entry, 4 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	K32	A	502	-	13,15,15	2.00	3 (23%)	19,23,23	2.52	6 (31%)
4	K32	E	501	-	13,15,15	1.93	3 (23%)	19,23,23	2.40	5 (26%)
2	LMR	F	501	3	8,8,8	2.56	4 (50%)	10,10,10	3.31	6 (60%)
2	LMR	A	503	3	8,8,8	0.95	0	10,10,10	1.54	3 (30%)
4	K32	D	503	-	13,15,15	2.10	4 (30%)	19,23,23	2.72	5 (26%)
2	LMR	D	501	-	8,8,8	1.96	2 (25%)	10,10,10	2.86	2 (20%)

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	K32	A	502	-	-	-	0/2/2/2
4	K32	E	501	-	-	-	0/2/2/2
2	LMR	F	501	3	-	6/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMR	A	503	3	-	8/8/8/8	-
4	K32	D	503	-	-	-	0/2/2/2
2	LMR	D	501	-	-	6/8/8/8	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	K32	BR1-C5	5.05	1.99	1.89
2	F	501	LMR	O1A-C1	4.93	1.37	1.22
2	D	501	LMR	O1A-C1	4.84	1.36	1.22
4	E	501	K32	BR3-C4	4.69	1.99	1.89
4	D	503	K32	BR1-C5	4.49	1.98	1.89
4	D	503	K32	BR3-C4	4.46	1.98	1.89
2	F	501	LMR	O4B-C4	4.15	1.35	1.22
4	A	502	K32	BR3-C4	3.26	1.96	1.89
4	E	501	K32	BR2-C2	3.18	1.96	1.89
4	A	502	K32	BR4-C3	2.83	1.95	1.89
4	E	501	K32	BR1-C5	2.70	1.95	1.89
4	D	503	K32	BR4-C3	2.66	1.94	1.89
2	F	501	LMR	O4A-C4	-2.26	1.23	1.30
2	F	501	LMR	O1B-C1	-2.26	1.23	1.30
2	D	501	LMR	O1B-C1	-2.22	1.23	1.30
4	D	503	K32	BR2-C2	2.07	1.93	1.89

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	502	K32	BR1-C5-C2	7.01	131.15	120.60
4	E	501	K32	BR3-C4-C3	6.90	130.98	120.60
4	D	503	K32	BR1-C5-C2	6.88	130.95	120.60
4	D	503	K32	BR3-C4-C3	6.51	130.39	120.60
2	D	501	LMR	O1B-C1-C2	6.24	126.42	112.72
2	F	501	LMR	O1B-C1-C2	6.23	126.40	112.72
2	D	501	LMR	O1A-C1-C2	-6.03	110.75	122.54
2	F	501	LMR	O1A-C1-C2	-5.89	111.02	122.54
4	A	502	K32	BR3-C4-C3	4.64	127.59	120.60
4	E	501	K32	BR1-C5-C2	4.32	127.10	120.60
4	D	503	K32	BR2-C2-C5	-4.27	114.18	120.60
4	E	501	K32	BR2-C2-C5	-3.79	114.90	120.60
4	A	502	K32	BR4-C3-C4	-3.60	115.19	120.60
4	D	503	K32	BR4-C3-C4	-3.54	115.28	120.60
2	F	501	LMR	O4A-C4-C3	3.45	125.12	114.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	502	K32	C3-C2-C5	3.42	124.47	119.96
4	E	501	K32	C4-C3-C2	3.04	123.97	119.96
4	D	503	K32	C3-C2-C5	2.86	123.73	119.96
4	A	502	K32	BR2-C2-C3	-2.82	116.37	120.60
2	F	501	LMR	O4B-C4-C3	-2.72	114.06	122.80
2	A	503	LMR	O2-C2-C1	-2.68	103.22	110.36
4	E	501	K32	BR2-C2-C3	2.63	124.55	120.60
2	F	501	LMR	O2-C2-C1	-2.49	103.72	110.36
2	A	503	LMR	C2-C3-C4	2.28	117.77	112.13
2	F	501	LMR	C2-C3-C4	2.24	117.68	112.13
2	A	503	LMR	O1A-C1-C2	2.17	126.78	122.54
4	A	502	K32	C8-C7-N14	-2.06	106.25	106.89

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	LMR	O1A-C1-C2-O2
2	D	501	LMR	O1B-C1-C2-O2
2	D	501	LMR	C1-C2-C3-C4
2	D	501	LMR	O2-C2-C3-C4
2	F	501	LMR	O1A-C1-C2-O2
2	F	501	LMR	O1B-C1-C2-O2
2	F	501	LMR	C1-C2-C3-C4
2	F	501	LMR	O2-C2-C3-C4
2	A	503	LMR	O1A-C1-C2-O2
2	A	503	LMR	O1B-C1-C2-O2
2	A	503	LMR	C1-C2-C3-C4
2	A	503	LMR	O2-C2-C3-C4
2	A	503	LMR	O1B-C1-C2-C3
2	F	501	LMR	O1A-C1-C2-C3
2	A	503	LMR	O1A-C1-C2-C3
2	A	503	LMR	C2-C3-C4-O4A
2	A	503	LMR	C2-C3-C4-O4B
2	D	501	LMR	O1A-C1-C2-C3
2	D	501	LMR	O1B-C1-C2-C3
2	F	501	LMR	O1B-C1-C2-C3

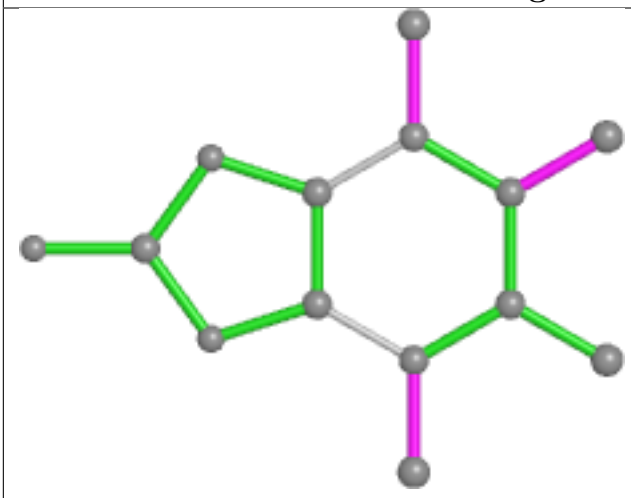
There are no ring outliers.

3 monomers are involved in 6 short contacts:

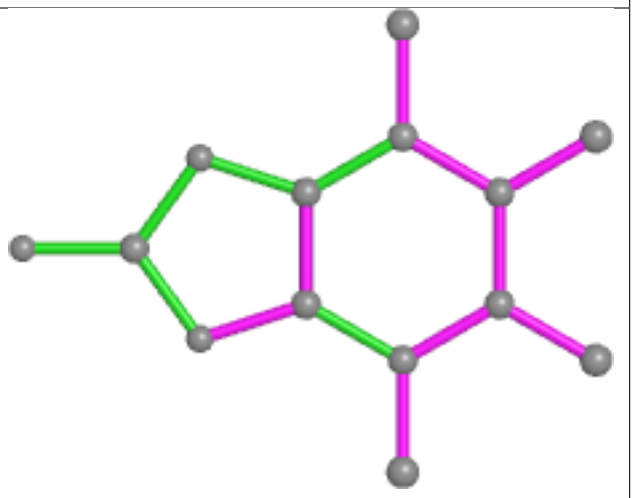
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	K32	2	0
4	E	501	K32	2	0
4	D	503	K32	2	0

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.

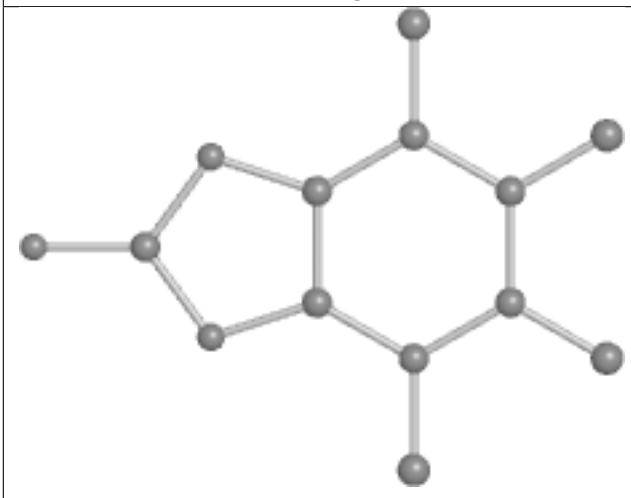
Ligand K32 A 502



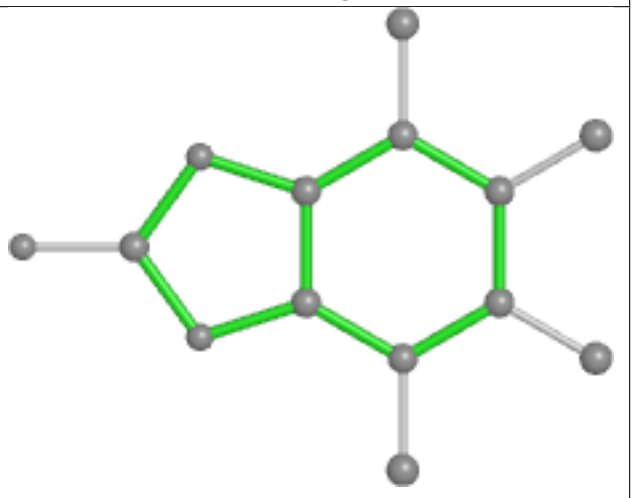
Bond lengths



Bond angles

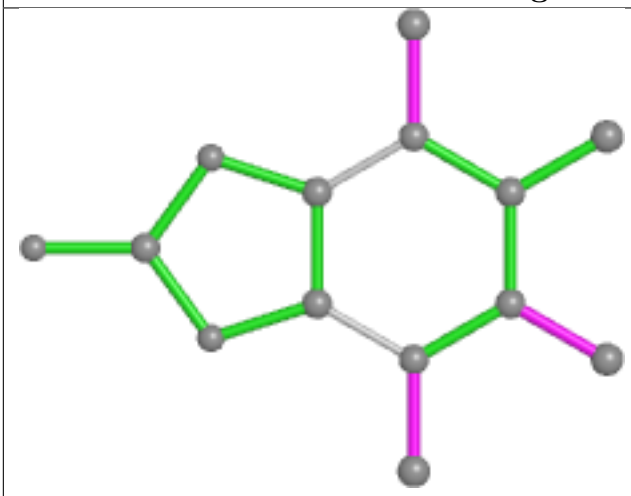


Torsions

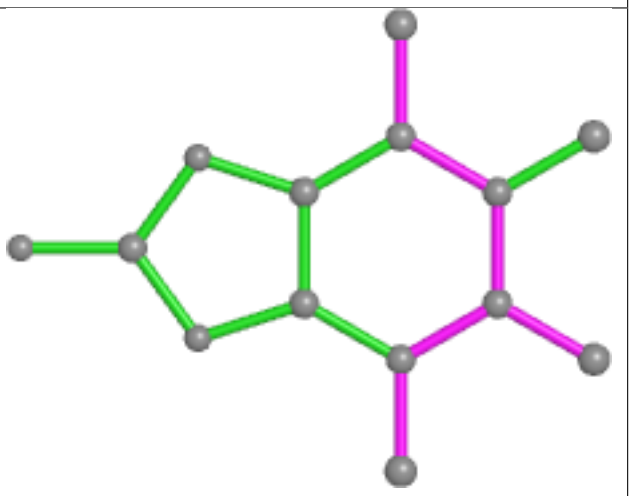


Rings

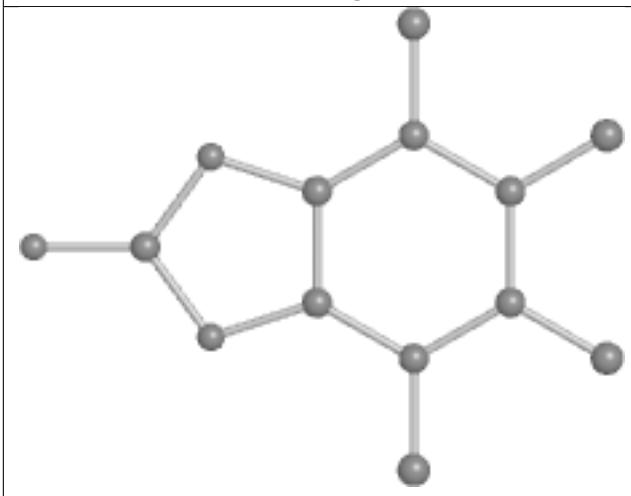
Ligand K32 E 501



Bond lengths



Bond angles



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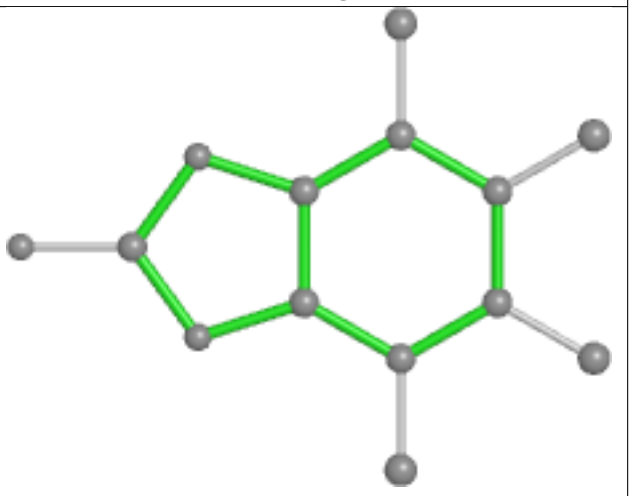
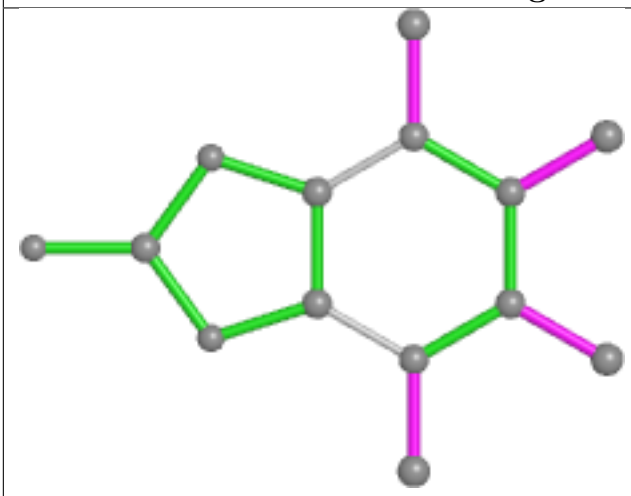
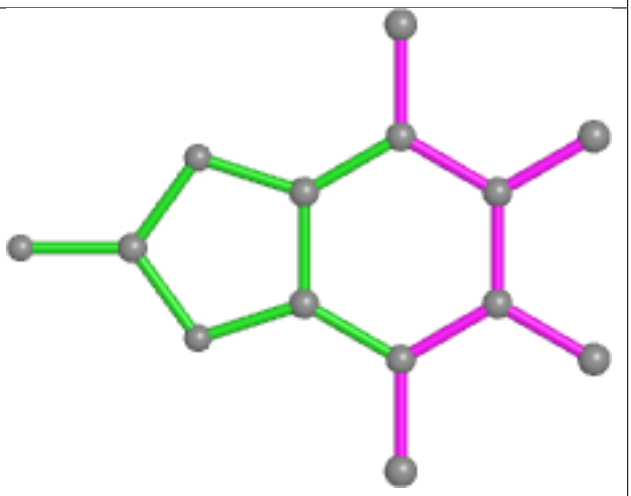


Rings

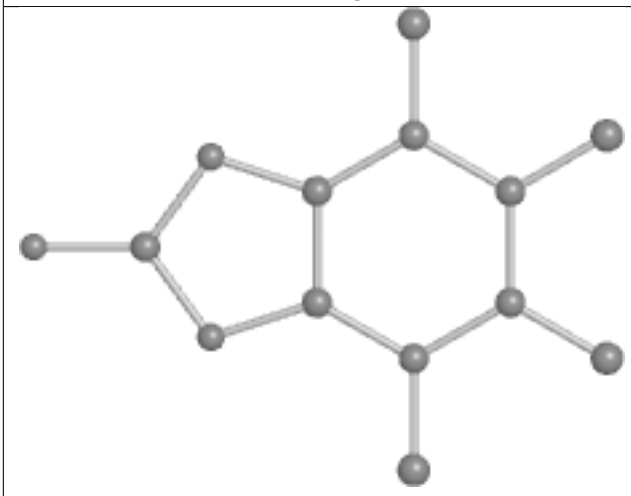
Ligand K32 D 503



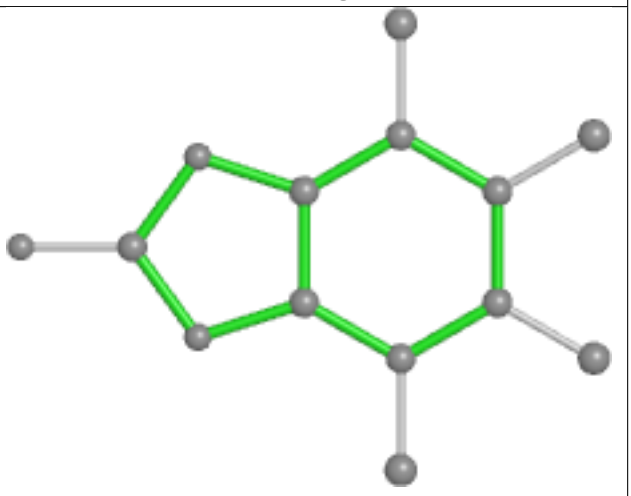
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	416/425 (97%)	-0.16	2 (0%)	91	91	28, 45, 70, 145	0
1	B	413/425 (97%)	-0.18	3 (0%)	87	88	27, 44, 75, 110	0
1	C	414/425 (97%)	-0.25	0	100	100	21, 36, 64, 90	0
1	D	416/425 (97%)	-0.25	0	100	100	21, 36, 65, 107	0
1	E	416/425 (97%)	-0.15	2 (0%)	91	91	28, 45, 76, 158	0
1	F	413/425 (97%)	-0.18	1 (0%)	95	95	29, 45, 69, 87	0
All	All	2488/2550 (97%)	-0.19	8 (0%)	94	94	21, 43, 70, 158	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	418	HIS	4.9
1	E	162	THR	4.9
1	B	162	THR	2.5
1	E	384	PRO	2.5
1	B	414	LEU	2.3
1	B	384	PRO	2.3
1	F	309	HIS	2.0
1	A	413	LYS	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

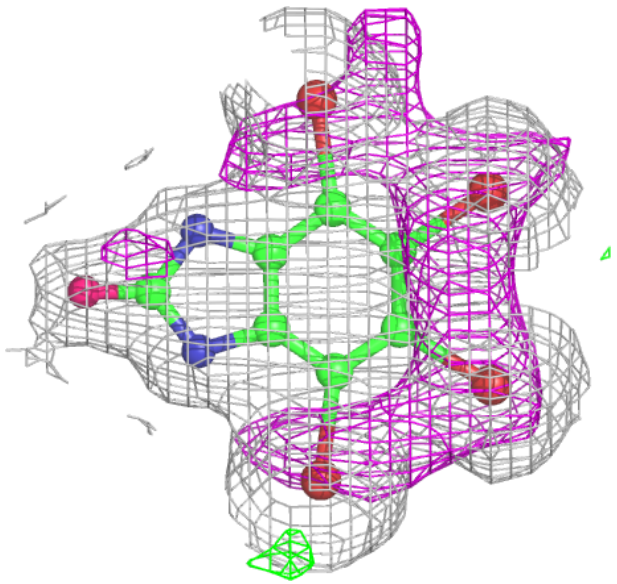
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

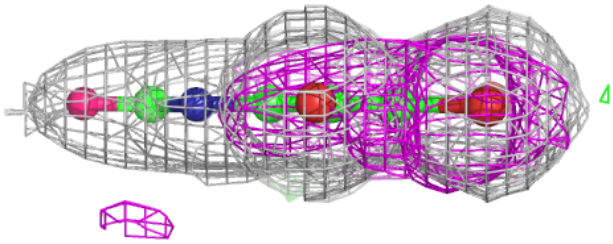
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LMR	F	501	9/9	0.67	0.21	56,63,65,65	0
2	LMR	D	501	9/9	0.84	0.12	73,78,81,82	0
2	LMR	A	503	9/9	0.84	0.16	51,58,62,63	0
3	MG	D	502	1/1	0.86	0.12	54,54,54,54	0
3	MG	F	502	1/1	0.94	0.06	46,46,46,46	0
3	MG	D	504	1/1	0.95	0.11	52,52,52,52	0
3	MG	A	501	1/1	0.95	0.13	49,49,49,49	0
4	K32	D	503	14/14	0.96	0.09	40,50,64,64	0
4	K32	A	502	14/14	0.96	0.07	37,48,62,65	0
4	K32	E	501	14/14	0.96	0.08	43,52,63,65	0

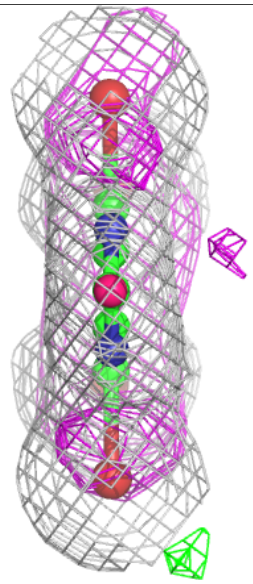
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around K32 D 503:

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

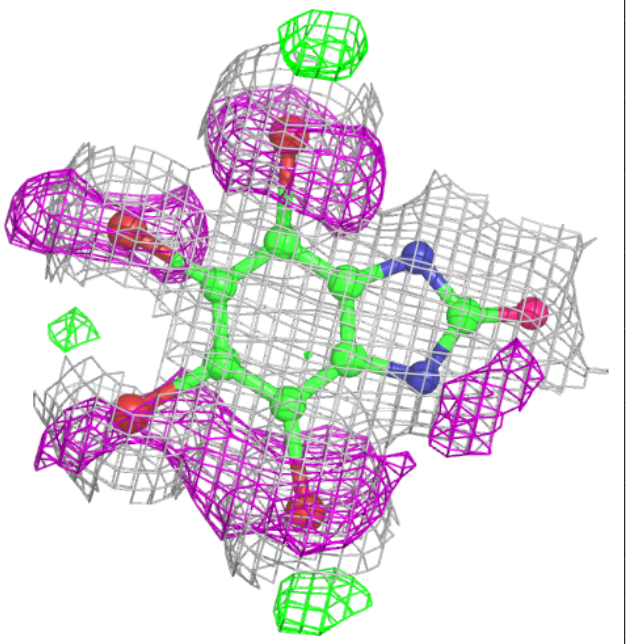


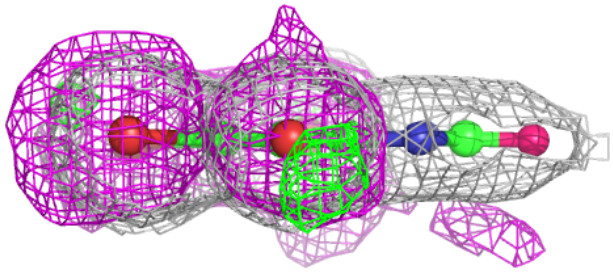


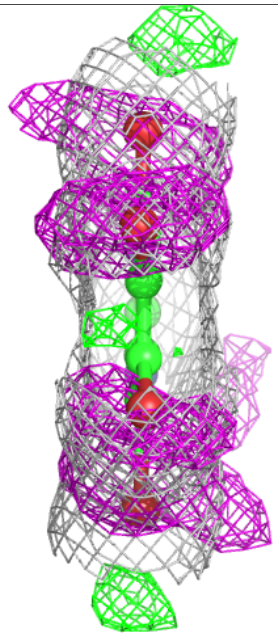


Electron density around K32 A 502:

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

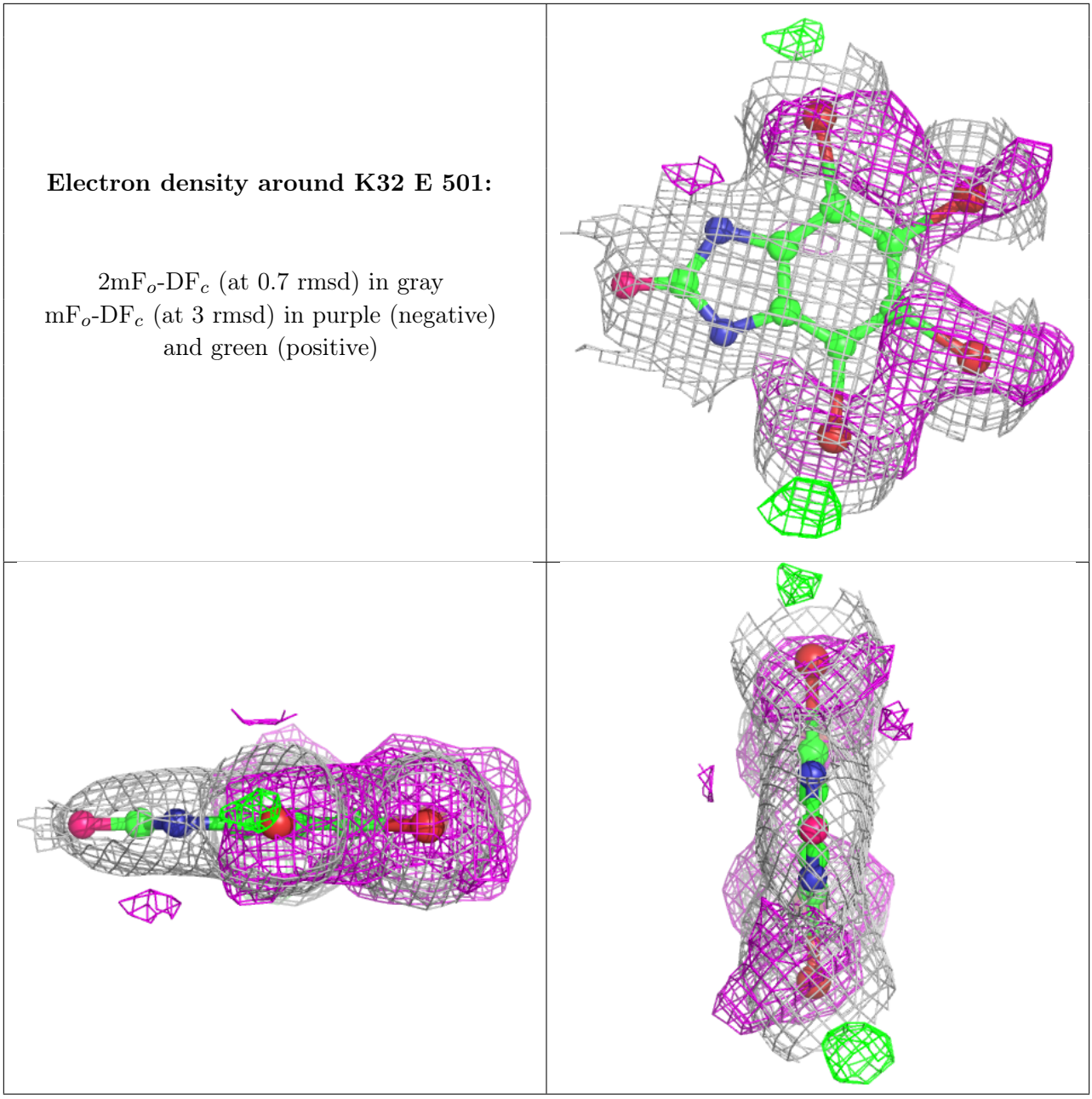






Electron density around K32 E 501:

$2mF_o$-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.