Full wwPDB X-ray Structure Validation Report ⓘ

Aug 2, 2021 – 04:10 pm BST

PDB ID	:	6S1I
Title	:	Crystal Structure of DYRK1A with small molecule inhibitor
Authors	:	Sorrell, F.J.; Henderson, S.H.; Redondo, C.; Burgess-Brown, N.A.; von Delft, F.; Arrowsmith, C.H.; Bountra, C.; Edwards, A.M.; Elkins, J.M.
Deposited on	:	2019-06-18
Resolution	:	2.38 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 following versions of software and data (see references ⓘ) were used in the production of this report:

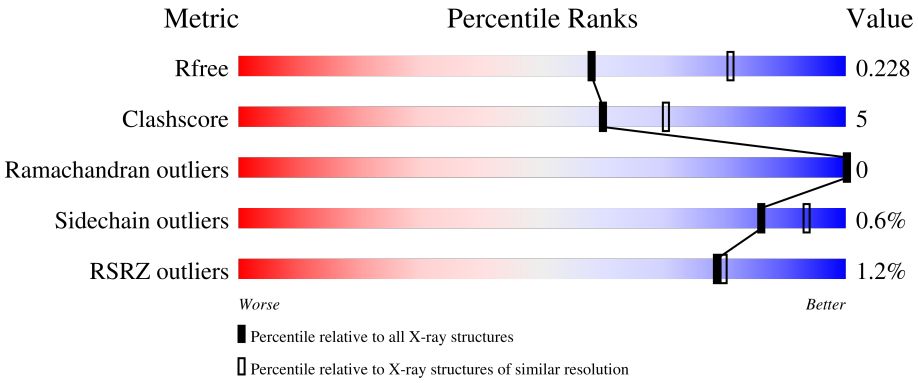
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	361	85% 10%
1	B	361	87% 8%
1	C	361	88% 7%
1	D	361	85% 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12084 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.

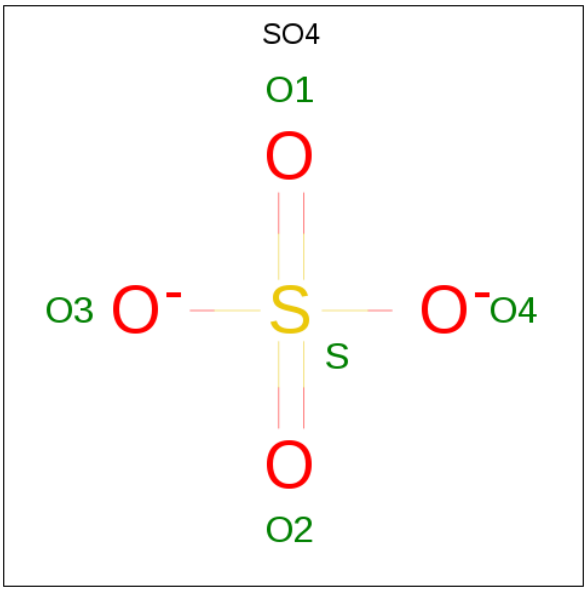
- Molecule 1 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	P	S	0	3	0
			2848	1829	493	508	1	17			
1	B	346	Total	C	N	O	P	S	0	2	0
			2810	1805	487	500	1	17			
1	C	345	Total	C	N	O	S		5	2	0
			2788	1794	487	490	17				
1	D	346	Total	C	N	O	P	S	0	2	0
			2799	1798	474	508	2	17			

There are 8 discrepancies between the modelled and reference sequences:

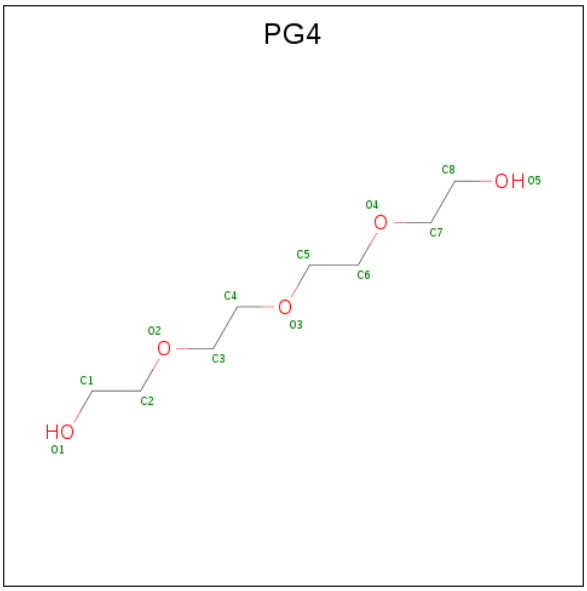
Chain	Residue	Modelled	Actual	Comment	Reference
A	125	SER	-	expression tag	UNP Q13627
A	126	MET	-	expression tag	UNP Q13627
B	125	SER	-	expression tag	UNP Q13627
B	126	MET	-	expression tag	UNP Q13627
C	125	SER	-	expression tag	UNP Q13627
C	126	MET	-	expression tag	UNP Q13627
D	125	SER	-	expression tag	UNP Q13627
D	126	MET	-	expression tag	UNP Q13627

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



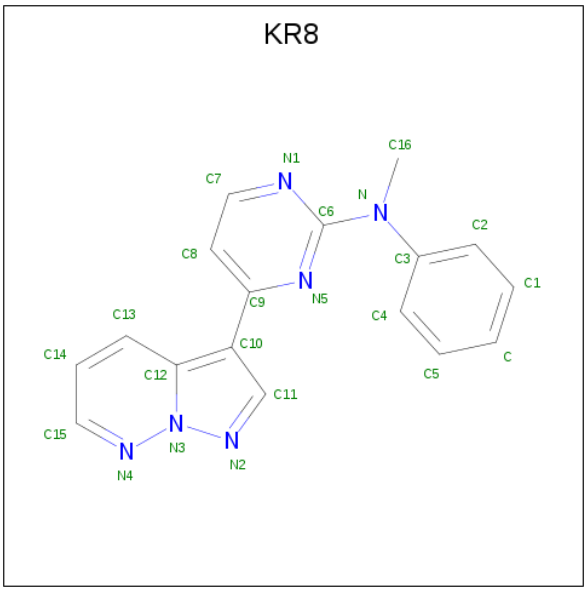
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 8 5	0	0
3	B	1	Total C O 13 8 5	0	0
3	B	1	Total C O 13 8 5	0	0
3	C	1	Total C O 13 8 5	0	0
3	C	1	Total C O 13 8 5	0	0

- Molecule 4 is {N}-methyl- {N}-phenyl-4-pyrazolo[1,5-b]pyridazin-3-yl-pyrimidin-2-amine (three-letter code: KR8) (formula: $C_{17}H_{14}N_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 23 17 6	0	0
4	B	1	Total C N 23 17 6	0	0
4	C	1	Total C N 23 17 6	0	0
4	D	1	Total C N 23 17 6	0	0

- Molecule 5 is water.

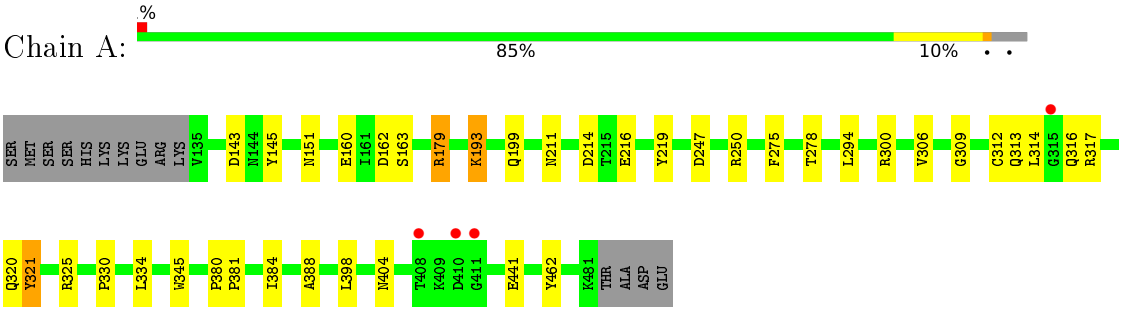
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	233	Total O 233 233	0	0
5	B	191	Total O 191 191	0	0
5	C	89	Total O 89 89	0	0
5	D	134	Total O 134 134	0	0

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.

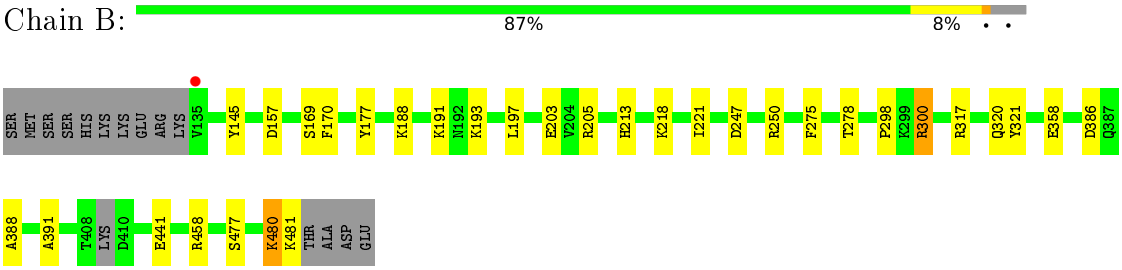
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

Chain A:



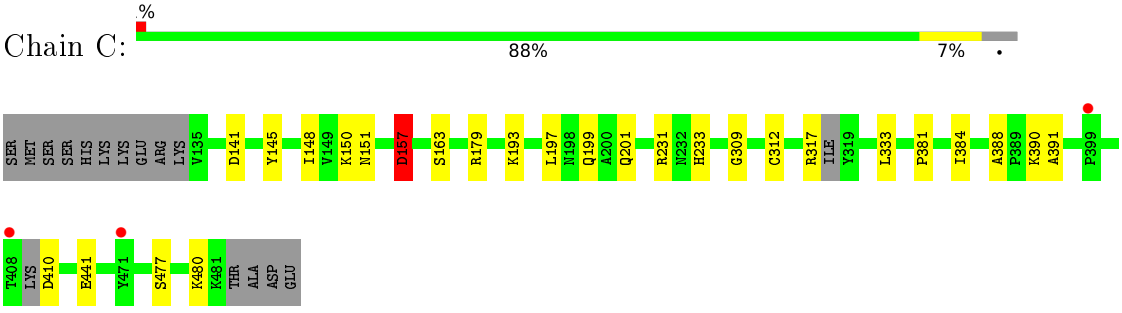
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

Chain B:



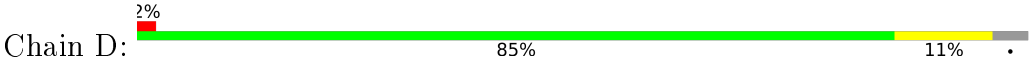
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

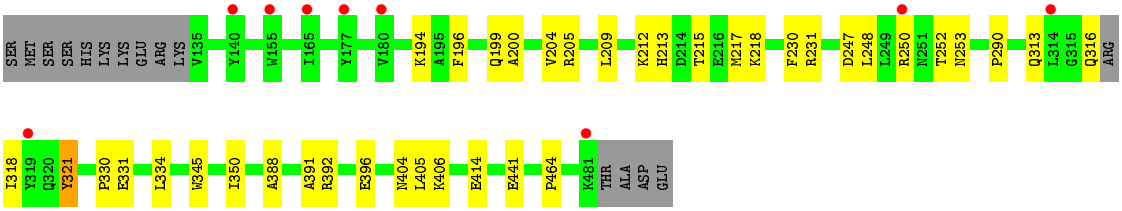
Chain C:



- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

Chain D:




SER MET SER SER HIS LYS LYS GLU ARG LYS V135 Y140 W155 I165 Y177 V180 K194 A195 F196 Q199 A200 V204 R205 L209 K212 H213 D214 T215 E216 M217 K218 F230 R231 D247 L248 L249 R250 N251 T252 N253 P290 Q313 L314 G315 Q316 ARG
I318 Y319 Q320 Y321 P330 E331 L334 W345 I350 A388 A391 R392 E396 N404 L405 K406 E414 E441 P464 K481 THR ALA ASP GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	244.32Å 64.50Å 147.59Å 90.00° 115.74° 90.00°	Depositor
Resolution (Å)	70.97 – 2.38 70.97 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.2 (70.97-2.38) 98.2 (70.97-2.38)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.37Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.201 , 0.228 0.201 , 0.228	Depositor DCC
R_{free} test set	4184 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	39.9	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.9	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	0.95	EDS
Total number of atoms	12084	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: SO4, PTR, KR8, PG4

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	0.30	0/2903	0.52	0/3914
1	B	0.31	0/2863	0.53	1/3862 (0.0%)
1	C	0.29	0/2851	0.69	2/3841 (0.1%)
1	D	0.30	0/2834	0.56	3/3827 (0.1%)
All	All	0.30	0/11451	0.58	6/15444 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	157	ASP	CB-CG-OD2	-22.65	97.92	118.30
1	C	157	ASP	CB-CG-OD1	17.69	134.22	118.30
1	D	392	ARG	NE-CZ-NH2	-11.94	114.33	120.30
1	B	480	LYS	CD-CE-NZ	8.91	132.19	111.70
1	D	392	ARG	CD-NE-CZ	6.31	132.43	123.60
1	D	392	ARG	NE-CZ-NH1	5.39	122.99	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	157	ASP	Sidechain

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	2848	0	2838	33	0
1	B	2810	0	2786	30	0
1	C	2788	0	2778	16	0
1	D	2799	0	2726	26	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	13	0	18	0	0
3	B	26	0	36	2	0
3	C	26	0	36	0	0
4	A	23	0	0	0	0
4	B	23	0	0	0	0
4	C	23	0	0	0	0
4	D	23	0	0	0	0
5	A	233	0	0	11	4
5	B	191	0	0	13	4
5	C	89	0	0	2	1
5	D	134	0	0	5	1
All	All	12084	0	11218	103	6

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 5.

All (103) 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:194:LYS:NZ	5:D:601:HOH:O	1.83	1.11
1:D:215:THR:HG22	1:D:217:MET:H	1.26	1.00
1:A:441:GLU:O	5:A:601:HOH:O	1.80	0.99
1:B:358:GLU:OE2	5:B:601:HOH:O	1.87	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:GLU:OE2	5:A:602:HOH:O	1.89	0.90
1:B:203:GLU:OE1	5:B:602:HOH:O	1.88	0.89
1:B:481:LYS:O	5:B:604:HOH:O	1.97	0.81
1:A:320:GLN:HB3	5:A:606:HOH:O	1.81	0.81
1:D:318:ILE:N	5:D:604:HOH:O	2.16	0.79
3:B:504:PG4:O1	5:B:605:HOH:O	2.01	0.77
1:A:314:LEU:O	5:A:604:HOH:O	2.03	0.75
1:C:441:GLU:O	5:C:601:HOH:O	2.07	0.73
1:D:414:GLU:OE2	5:D:602:HOH:O	2.06	0.72
1:B:221:ILE:HD13	1:B:275:PHE:CE2	2.25	0.71
1:C:410:ASP:N	5:C:603:HOH:O	2.23	0.70
1:B:317:ARG:HA	5:B:644:HOH:O	1.93	0.69
1:B:298:PRO:O	5:B:606:HOH:O	2.11	0.68
1:D:316:GLN:OE1	5:D:603:HOH:O	2.11	0.68
1:B:169:SER:O	1:B:191:LYS:NZ	2.20	0.67
1:B:247:ASP:OD1	1:B:250[B]:ARG:NH1	2.27	0.67
1:A:250[B]:ARG:NH1	5:A:603:HOH:O	2.03	0.66
1:A:145:TYR:CZ	1:A:193:LYS:HE3	2.30	0.66
1:B:441:GLU:O	5:B:608:HOH:O	2.14	0.66
1:D:404:ASN:OD1	1:D:405:LEU:N	2.29	0.65
1:B:386:ASP:OD2	5:B:607:HOH:O	2.14	0.65
1:A:151:ASN:ND2	1:A:163:SER:HA	2.11	0.64
1:D:396:GLU:HG3	1:D:406:LYS:HG3	1.79	0.64
1:A:151:ASN:ND2	1:A:162:ASP:O	2.29	0.62
1:B:221:ILE:CD1	1:B:275:PHE:CD2	2.82	0.62
1:A:250[B]:ARG:NE	5:A:603:HOH:O	2.32	0.61
1:C:312:CYS:SG	1:C:317:ARG:HB3	2.41	0.60
1:B:221:ILE:HD13	1:B:275:PHE:CD2	2.36	0.60
1:D:215:THR:HG22	1:D:217:MET:N	2.10	0.59
1:D:200:ALA:O	1:D:204:VAL:HG13	2.02	0.59
1:A:398:LEU:HD11	1:A:404:ASN:ND2	2.17	0.58
1:B:205:ARG:NH2	5:B:603:HOH:O	2.36	0.58
1:B:205:ARG:NE	5:B:603:HOH:O	1.96	0.58
1:A:300:ARG:HD3	1:B:177:TYR:CZ	2.39	0.58
1:A:247:ASP:OD1	1:A:250[B]:ARG:NH1	2.37	0.57
1:C:477:SER:HA	1:C:480:LYS:HG2	1.86	0.57
1:A:151:ASN:HD21	1:A:163:SER:HA	1.70	0.57
1:A:199:GLN:HG3	1:A:309:GLY:O	2.04	0.57
1:A:381:PRO:HG2	1:A:384:ILE:HD12	1.86	0.55
1:A:250[B]:ARG:CZ	5:A:603:HOH:O	2.51	0.54
1:B:275:PHE:O	1:B:278:THR:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:PHE:O	1:A:278:THR:HG23	2.08	0.53
1:D:205:ARG:NH2	1:D:313:GLN:OE1	2.42	0.53
1:D:441:GLU:OE2	5:D:605:HOH:O	2.19	0.52
1:B:221:ILE:HD11	1:B:275:PHE:HD2	1.75	0.52
1:A:313:GLN:HB2	1:A:316:GLN:HE21	1.74	0.52
1:B:458[B]:ARG:HA	5:B:632:HOH:O	2.11	0.51
1:D:334:LEU:HB3	1:D:388:ALA:HB1	1.92	0.51
1:B:388:ALA:HB3	1:B:391:ALA:HB2	1.90	0.51
1:D:230:PHE:CE2	1:D:231:ARG:HG3	2.46	0.51
1:B:477:SER:HA	1:B:480:LYS:HZ3	1.76	0.51
1:D:247:ASP:OD1	1:D:250[B]:ARG:NH1	2.44	0.51
1:A:294:LEU:HD22	1:A:306:VAL:HG11	1.93	0.50
1:A:334:LEU:HB3	1:A:388:ALA:HB1	1.94	0.50
1:B:477:SER:CA	1:B:480:LYS:HZ3	2.24	0.50
1:C:148:ILE:HD13	1:C:150:LYS:HE2	1.93	0.50
1:B:458[A]:ARG:HA	5:B:632:HOH:O	2.12	0.50
1:A:398:LEU:HD11	1:A:404:ASN:HD21	1.76	0.49
1:A:313:GLN:OE1	1:A:316:GLN:NE2	2.45	0.49
1:A:160:GLU:OE2	1:A:179:ARG:NE	2.42	0.49
1:B:170:PHE:CD1	1:B:188:LYS:HE3	2.48	0.49
1:B:218:LYS:NZ	5:B:621:HOH:O	2.46	0.49
1:A:214:ASP:CG	1:B:300:ARG:HH22	2.17	0.48
1:B:477:SER:HA	1:B:480:LYS:HG2	1.96	0.48
1:B:145:TYR:CZ	1:B:193:LYS:HD2	2.48	0.48
1:A:320:GLN:OE1	5:A:606:HOH:O	2.20	0.48
1:A:316:GLN:NE2	5:A:626:HOH:O	2.47	0.47
1:A:312:CYS:SG	1:A:317:ARG:HG2	2.54	0.47
1:A:321:PTR:O1P	1:A:325:ARG:HD3	2.13	0.47
1:C:151:ASN:OD1	1:C:163:SER:HA	2.15	0.47
1:C:381:PRO:HG2	1:C:384:ILE:HD12	1.97	0.47
1:C:179:ARG:HH21	1:D:253:ASN:HB3	1.79	0.46
1:B:221:ILE:HD11	1:B:275:PHE:CD2	2.50	0.46
1:A:219:TYR:OH	5:A:605:HOH:O	2.18	0.46
1:C:145:TYR:CE2	1:C:193:LYS:HD2	2.51	0.45
1:C:231:ARG:O	1:C:233:HIS:HD2	2.00	0.45
1:D:396:GLU:HG3	1:D:406:LYS:CG	2.44	0.45
1:C:199:GLN:HG3	1:C:309:GLY:O	2.17	0.45
1:D:290:PRO:HD3	1:D:350:ILE:HG12	1.97	0.45
1:D:209:LEU:HA	1:D:212:LYS:HE3	1.98	0.44
1:D:248:LEU:O	1:D:252:THR:HG23	2.18	0.44
1:B:213:HIS:O	1:B:218:LYS:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:LEU:O	1:C:201:GLN:HG3	2.18	0.43
1:D:388:ALA:HB3	1:D:391:ALA:HB2	2.01	0.43
1:D:213:HIS:O	1:D:218:LYS:HD3	2.18	0.43
1:D:331:GLU:HG2	1:D:464:PRO:HG3	2.00	0.42
1:D:330:PRO:HD3	1:D:345:TRP:CE2	2.54	0.42
1:C:333:LEU:O	1:C:390:LYS:HE3	2.19	0.42
1:A:380:PRO:HG3	1:A:462:TYR:CE1	2.55	0.42
1:C:388:ALA:HB3	1:C:391:ALA:HB2	2.01	0.41
1:D:321[A]:PTR:O1P	1:D:321[A]:PTR:HE2	2.20	0.41
1:B:197:LEU:HD11	3:B:503:PG4:H52	2.03	0.41
1:C:141:ASP:OD1	1:C:233:HIS:NE2	2.51	0.41
1:D:321[B]:PTR:O1P	1:D:321[B]:PTR:HE2	2.21	0.40
1:A:211:ASN:ND2	5:A:632:HOH:O	2.53	0.40
1:C:480:LYS:HA	1:C:480:LYS:HD3	1.81	0.40
1:A:330:PRO:HD3	1:A:345:TRP:CE2	2.57	0.40
1:D:196:PHE:O	1:D:199:GLN:HB2	2.22	0.40
1:A:312:CYS:HB2	1:A:316:GLN:O	2.20	0.40

All (6) 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)
5:C:675:HOH:O	5:D:710:HOH:O[4_447]	1.92	0.28
5:B:784:HOH:O	5:B:786:HOH:O[2_558]	2.02	0.18
5:A:700:HOH:O	5:B:767:HOH:O[1_565]	2.08	0.12
5:A:823:HOH:O	5:B:783:HOH:O[1_565]	2.11	0.09
5:A:624:HOH:O	5:A:624:HOH:O[2_557]	2.18	0.02
5:A:783:HOH:O	5:B:748:HOH:O[1_565]	2.18	0.02

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	347/361 (96%)	330 (95%)	17 (5%)	0	100	100
1	B	343/361 (95%)	329 (96%)	14 (4%)	0	100	100
1	C	340/361 (94%)	326 (96%)	14 (4%)	0	100	100
1	D	342/361 (95%)	328 (96%)	14 (4%)	0	100	100
All	All	1372/1444 (95%)	1313 (96%)	59 (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	304/320 (95%)	301 (99%)	3 (1%)	76	87
1	B	297/320 (93%)	294 (99%)	3 (1%)	76	87
1	C	295/320 (92%)	294 (100%)	1 (0%)	92	97
1	D	292/320 (91%)	292 (100%)	0	100	100
All	All	1188/1280 (93%)	1181 (99%)	7 (1%)	86	93

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	ASP
1	A	179	ARG
1	A	193	LYS
1	B	157	ASP
1	B	300	ARG
1	B	320	GLN
1	C	157	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	GLN

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Mol	Chain	Res	Type
1	A	404	ASN
1	C	404	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)

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PTR	B	321	1	15,16,17	1.26	2 (13%)	19,22,24	0.86	1 (5%)
1	PTR	D	321[B]	1	15,16,17	1.28	2 (13%)	19,22,24	0.74	0
1	PTR	A	321	1	15,16,17	1.32	1 (6%)	19,22,24	0.77	1 (5%)
1	PTR	D	321[A]	1	15,16,17	1.28	1 (6%)	19,22,24	0.91	2 (10%)
1	PTR	C	321	1	3,4,17	0.65	0	2,4,24	0.80	0

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
1	PTR	B	321	1	-	2/10/11/13	0/1/1/1
1	PTR	D	321[B]	1	-	2/10/11/13	0/1/1/1
1	PTR	A	321	1	-	1/10/11/13	0/1/1/1
1	PTR	D	321[A]	1	-	2/10/11/13	0/1/1/1
1	PTR	C	321	1	-	0/0/2/13	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	321[A]	PTR	OH-CZ	-4.42	1.30	1.40
1	A	321	PTR	OH-CZ	-4.33	1.30	1.40
1	D	321[B]	PTR	OH-CZ	-3.78	1.32	1.40
1	B	321	PTR	OH-CZ	-3.70	1.32	1.40
1	D	321[B]	PTR	P-OH	2.62	1.63	1.59
1	B	321	PTR	P-OH	2.61	1.63	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	321	PTR	O2P-P-OH	2.33	112.54	105.24
1	D	321[A]	PTR	P-OH-CZ	-2.26	116.52	123.75
1	B	321	PTR	O2P-P-OH	2.21	112.16	105.24
1	D	321[A]	PTR	O3P-P-OH	2.19	112.09	105.24

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	321	PTR	N-CA-CB-CG
1	B	321	PTR	C-CA-CB-CG
1	D	321[A]	PTR	N-CA-CB-CG
1	D	321[A]	PTR	C-CA-CB-CG
1	D	321[B]	PTR	C-CA-CB-CG
1	A	321	PTR	CZ-OH-P-O1P
1	D	321[B]	PTR	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	321[B]	PTR	1	0
1	A	321	PTR	1	0
1	D	321[A]	PTR	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	KR8	B	505	-	22,26,26	0.54	0	25,36,36	0.83	1 (4%)
3	PG4	C	503	-	12,12,12	0.52	0	11,11,11	0.44	0
4	KR8	C	505	-	22,26,26	0.53	0	25,36,36	0.85	1 (4%)
3	PG4	C	504	-	12,12,12	0.54	0	11,11,11	0.25	0
2	SO4	C	502	-	4,4,4	0.15	0	6,6,6	0.08	0
2	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.08	0
3	PG4	A	502	-	12,12,12	0.54	0	11,11,11	0.41	0
2	SO4	C	501	-	4,4,4	0.12	0	6,6,6	0.16	0
3	PG4	B	503	-	12,12,12	0.51	0	11,11,11	0.23	0
2	SO4	D	502	-	4,4,4	0.13	0	6,6,6	0.09	0
3	PG4	B	504	-	12,12,12	0.52	0	11,11,11	0.23	0
2	SO4	B	501	-	4,4,4	0.14	0	6,6,6	0.21	0
2	SO4	B	502	-	4,4,4	0.15	0	6,6,6	0.10	0
4	KR8	D	503	-	22,26,26	0.51	0	25,36,36	0.76	1 (4%)
2	SO4	D	501	-	4,4,4	0.15	0	6,6,6	0.09	0
4	KR8	A	503	-	22,26,26	0.50	0	25,36,36	0.88	1 (4%)

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	KR8	B	505	-	-	0/8/12/12	0/4/4/4
3	PG4	C	503	-	-	4/10/10/10	-
4	KR8	C	505	-	-	2/8/12/12	0/4/4/4
3	PG4	C	504	-	-	5/10/10/10	-
3	PG4	B	504	-	-	1/10/10/10	-
3	PG4	A	502	-	-	2/10/10/10	-
3	PG4	B	503	-	-	1/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	KR8	D	503	-	-	0/8/12/12	0/4/4/4
4	KR8	A	503	-	-	0/8/12/12	0/4/4/4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	505	KR8	C13-C14-C15	-2.71	115.44	118.93
4	D	503	KR8	C13-C14-C15	-2.65	115.52	118.93
4	C	505	KR8	C13-C14-C15	-2.62	115.56	118.93
4	A	503	KR8	C13-C14-C15	-2.49	115.72	118.93

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	505	KR8	N1-C6-N-C3
4	C	505	KR8	N5-C6-N-C3
3	C	504	PG4	O2-C3-C4-O3
3	C	503	PG4	O3-C5-C6-O4
3	C	503	PG4	O2-C3-C4-O3
3	B	504	PG4	O1-C1-C2-O2
3	C	504	PG4	O1-C1-C2-O2
3	A	502	PG4	O3-C5-C6-O4
3	C	503	PG4	O4-C7-C8-O5
3	C	503	PG4	C3-C4-O3-C5
3	A	502	PG4	C8-C7-O4-C6
3	C	504	PG4	C6-C5-O3-C4
3	C	504	PG4	C4-C3-O2-C2
3	C	504	PG4	C1-C2-O2-C3
3	B	503	PG4	O1-C1-C2-O2

There are no ring outliers.

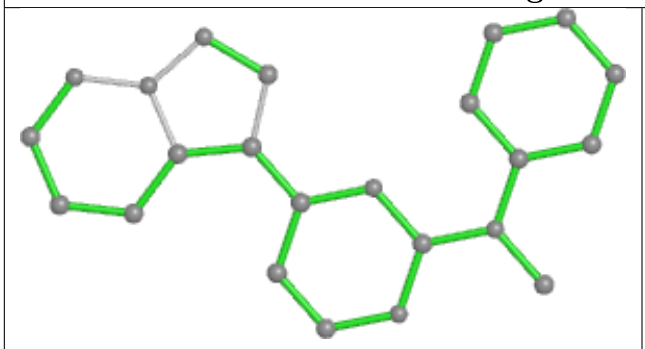
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	503	PG4	1	0
3	B	504	PG4	1	0

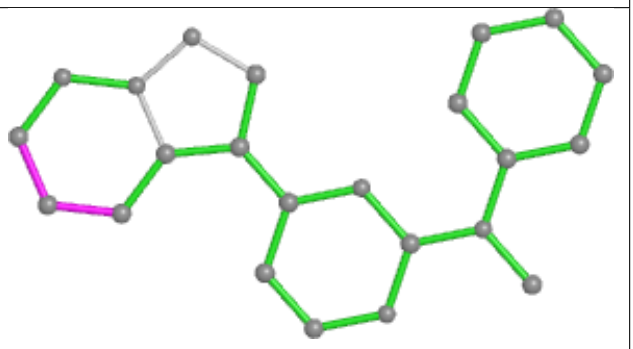
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

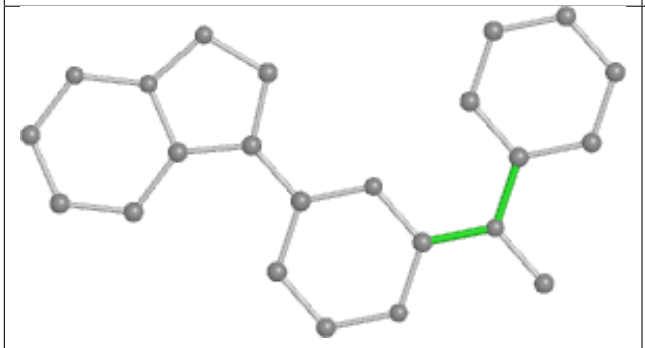
Ligand KR8 B 505



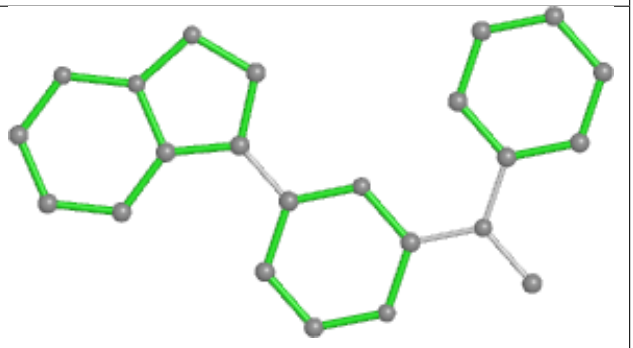
Bond lengths



Bond angles

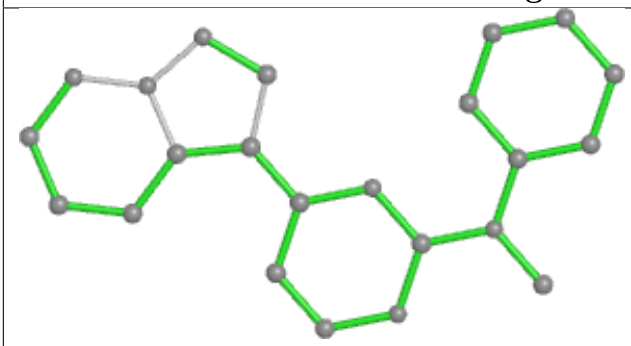


Torsions

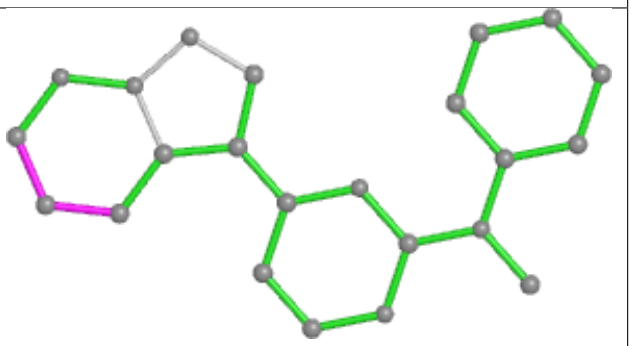


Rings

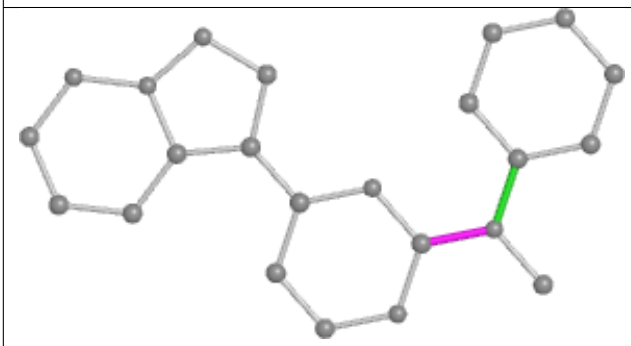
Ligand KR8 C 505



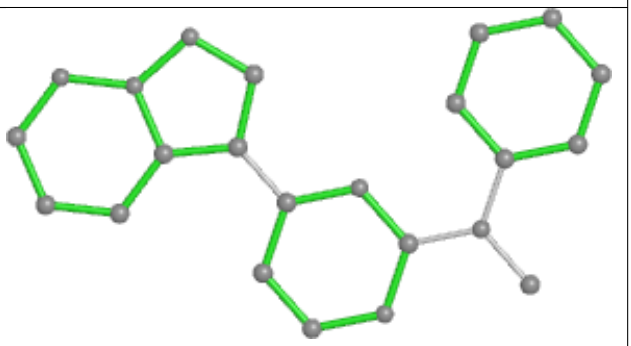
Bond lengths



Bond angles

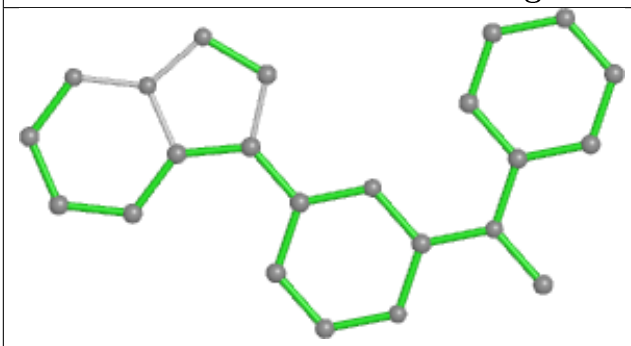


Torsions

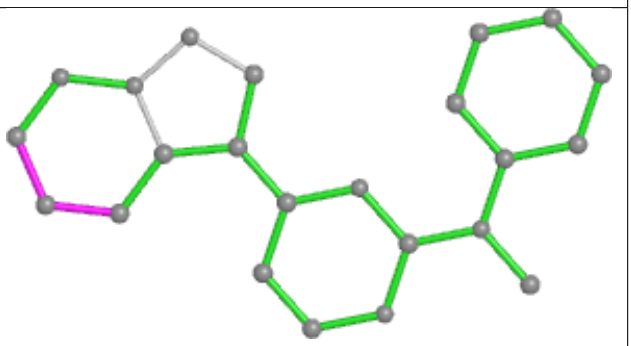


Rings

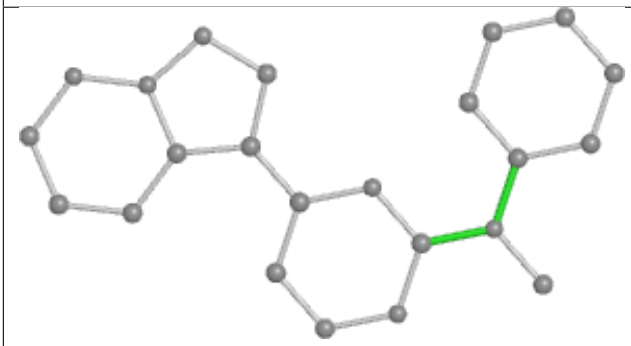
Ligand KR8 D 503



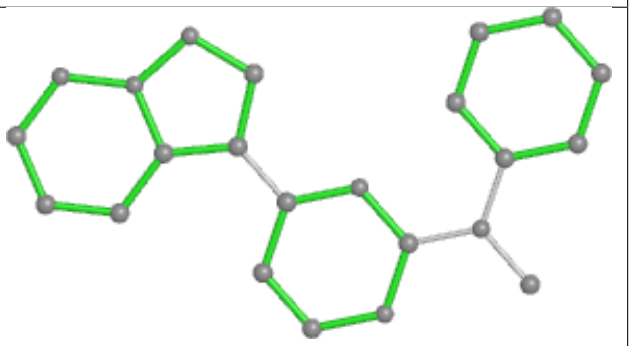
Bond lengths



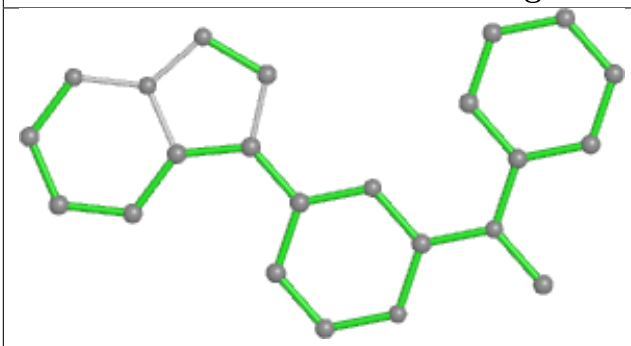
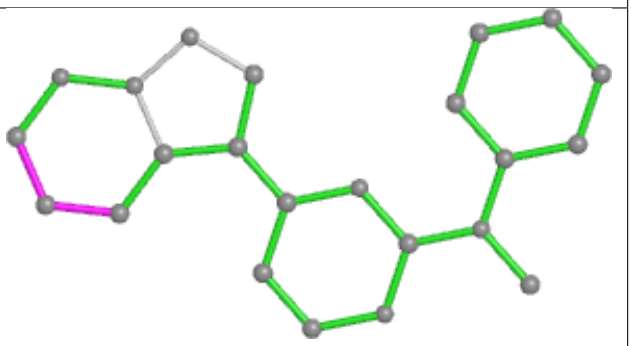
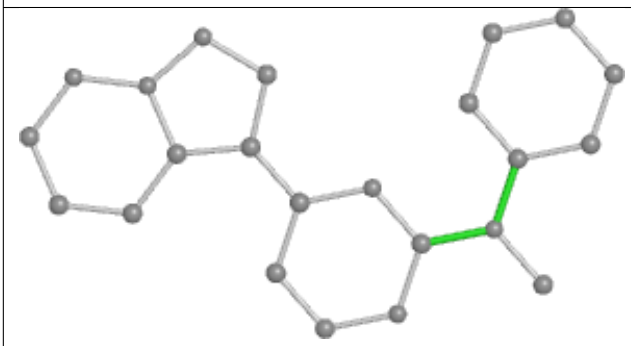
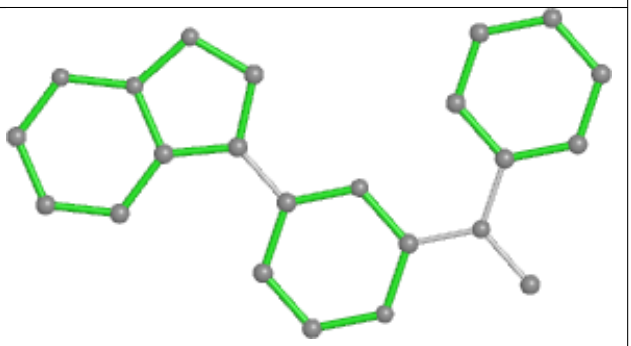
Bond angles



Torsions



Rings

Ligand KR8 A 503	
 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	346/361 (95%)	-0.01	4 (1%)	79	80	27, 38, 77, 115	0
1	B	345/361 (95%)	-0.07	1 (0%)	94	94	30, 41, 74, 98	0
1	C	344/361 (95%)	-0.02	3 (0%)	84	84	40, 58, 88, 117	0
1	D	345/361 (95%)	0.07	9 (2%)	56	57	32, 53, 93, 111	0
All	All	1380/1444 (95%)	-0.01	17 (1%)	79	80	27, 48, 87, 117	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	408	THR	4.7
1	D	481	LYS	4.4
1	B	135	VAL	4.1
1	A	408	THR	3.1
1	C	399	PRO	3.0
1	A	411	GLY	2.7
1	A	410	ASP	2.6
1	A	315	GLY	2.6
1	D	177	TYR	2.5
1	D	165	ILE	2.4
1	D	155	TRP	2.3
1	D	140	TYR	2.2
1	C	471	TYR	2.1
1	D	250[A]	ARG	2.1
1	D	314	LEU	2.1
1	D	319	TYR	2.0
1	D	180	VAL	2.0

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

MODRES-RSR INFOmissingINFO

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
3	PG4	C	504	13/13	0.64	0.25	75,80,81,82	0
2	SO4	A	501	5/5	0.79	0.28	118,118,119,122	0
3	PG4	B	504	13/13	0.86	0.15	59,67,69,70	0
2	SO4	D	502	5/5	0.88	0.11	117,118,119,120	0
3	PG4	A	502	13/13	0.88	0.18	69,70,74,75	0
2	SO4	C	502	5/5	0.91	0.14	79,85,85,86	0
2	SO4	B	502	5/5	0.93	0.14	77,81,82,83	0
3	PG4	C	503	13/13	0.95	0.12	40,48,54,55	0
3	PG4	B	503	13/13	0.95	0.16	40,45,54,59	0
4	KR8	C	505	23/23	0.95	0.13	65,67,70,70	0
4	KR8	D	503	23/23	0.96	0.15	39,49,62,64	0
2	SO4	D	501	5/5	0.97	0.13	70,73,73,73	0
4	KR8	B	505	23/23	0.97	0.14	32,40,45,46	0
2	SO4	B	501	5/5	0.98	0.13	62,64,65,65	0
2	SO4	C	501	5/5	0.98	0.15	38,49,50,53	0
4	KR8	A	503	23/23	0.98	0.18	36,42,46,47	0

6.5 Other polymers (i)

There are no such residues in this entry.