Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 05:50 PM EST

PDB ID	:	4K4F
Title	:	Co-crystal structure of TNKS1 with compound 18 [4-[(4S)-5,5-dimethyl-2-oxo-4-phenyl-1,3-oxazolidin-3-yl]-N-(quinolin-8-yl)benzamide]
Authors	:	Huang, X.; Bregman, H.; Wilson, C.; DiMauro, E.; Gunaydin, H.
Deposited on	:	2013-04-12
Resolution	:	2.90 Å(reported)

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

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

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

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

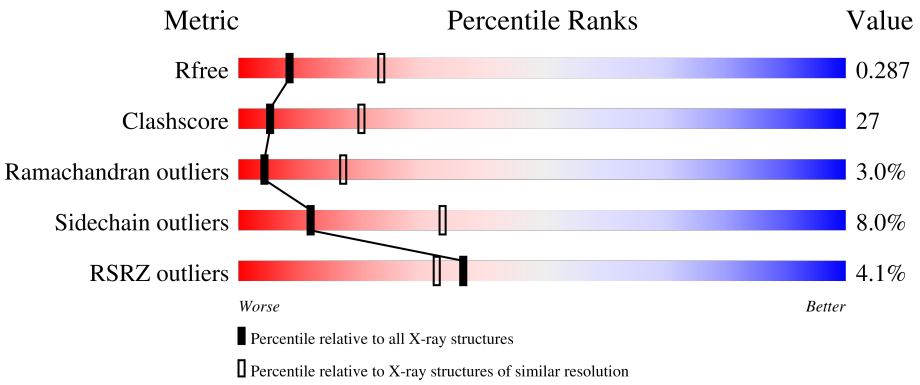
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	217	3% 61% 28% 6% • •
1	B	217	5% 56% 32% 5% • 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3360 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 Tankyrase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	210	1685	1058	311	305	11	0	0	0
1	B	203	1607	1005	299	293	10	0	0	0

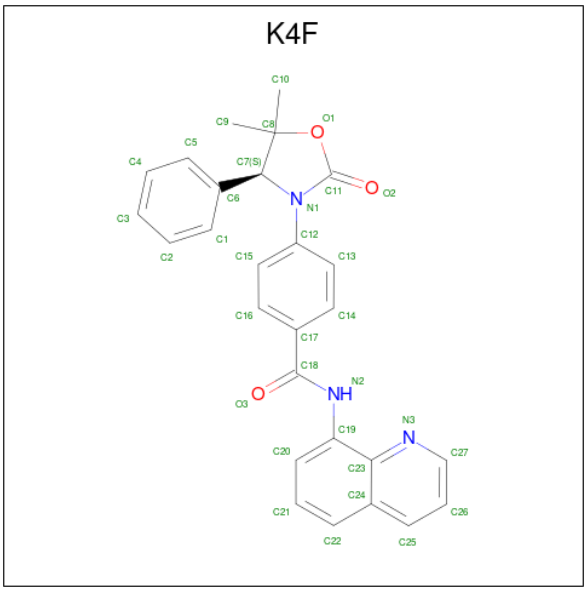
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1315	HIS	-	expression tag	UNP O95271
A	1316	HIS	-	expression tag	UNP O95271
A	1317	HIS	-	expression tag	UNP O95271
A	1318	HIS	-	expression tag	UNP O95271
A	1319	HIS	-	expression tag	UNP O95271
A	1320	HIS	-	expression tag	UNP O95271
B	1315	HIS	-	expression tag	UNP O95271
B	1316	HIS	-	expression tag	UNP O95271
B	1317	HIS	-	expression tag	UNP O95271
B	1318	HIS	-	expression tag	UNP O95271
B	1319	HIS	-	expression tag	UNP O95271
B	1320	HIS	-	expression tag	UNP O95271

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- Molecule 3 is 4-[(4S)-5,5-dimethyl-2-oxo-4-phenyl-1,3-oxazolidin-3-yl]-N-(quinolin-8-yl)benzamide (three-letter code: K4F) (formula: $C_{27}H_{23}N_3O_3$).



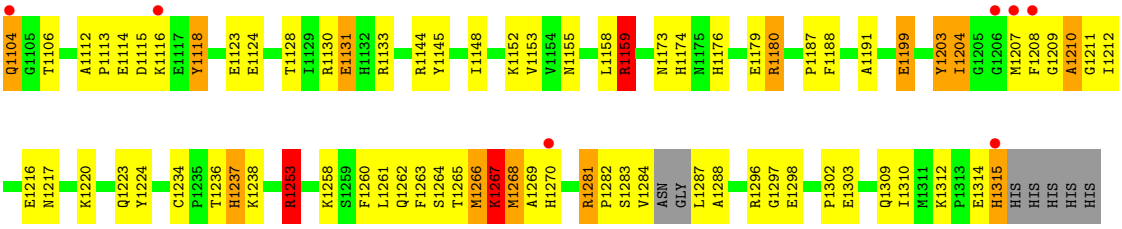
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	33	27	3	3	0	0
			Total	C	N	O		
3	B	1	33	27	3	3	0	0

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.

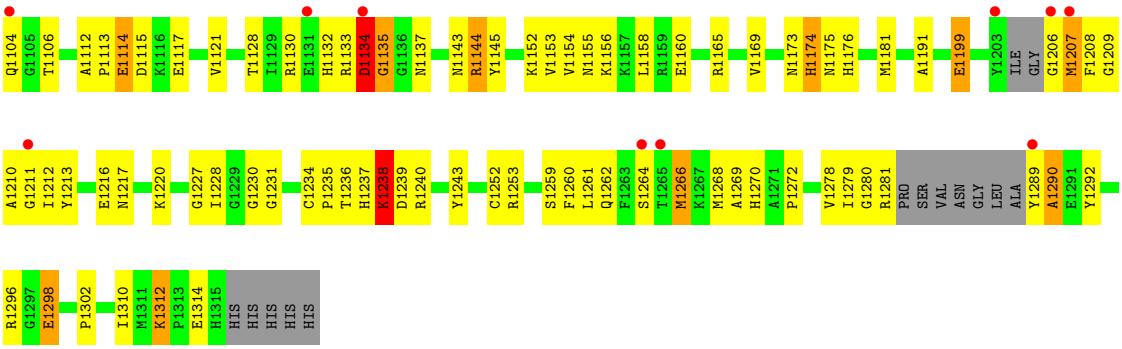
- Molecule 1: Tankyrase-1

Chain A:



- Molecule 1: Tankyrase-1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	41.69Å 78.12Å 146.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 41.44 – 2.72	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.90) 96.6 (41.44-2.72)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.73Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.280 , 0.290 0.273 , 0.287	Depositor DCC
R_{free} test set	637 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	43.7	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 30.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	3360	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, K4F

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.67	0/1727	1.01	10/2321 (0.4%)
1	B	0.58	0/1645	0.96	9/2213 (0.4%)
All	All	0.63	0/3372	0.99	19/4534 (0.4%)

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	A	0	4

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1135	GLY	N-CA-C	-9.42	89.56	113.10
1	A	1159	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	B	1266	MET	N-CA-C	8.21	133.17	111.00
1	A	1253	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	B	1314	GLU	C-N-CA	7.70	140.96	121.70
1	A	1268	MET	N-CA-C	7.62	131.58	111.00
1	B	1290	ALA	N-CA-C	7.36	130.87	111.00
1	A	1159	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	B	1134	ASP	N-CA-C	-6.77	92.73	111.00
1	B	1210	ALA	N-CA-C	-6.66	93.02	111.00
1	B	1314	GLU	CA-C-N	-6.29	103.37	117.20
1	B	1314	GLU	N-CA-C	6.15	127.62	111.00
1	A	1282	PRO	N-CA-C	6.15	128.08	112.10
1	A	1131	GLU	CB-CA-C	6.10	122.59	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1281	ARG	NE-CZ-NH1	-6.09	117.26	120.30
1	B	1314	GLU	O-C-N	6.05	132.38	122.70
1	A	1159	ARG	CG-CD-NE	6.05	124.51	111.80
1	A	1159	ARG	CD-NE-CZ	-5.99	115.21	123.60
1	A	1268	MET	N-CA-CB	-5.87	100.03	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1159	ARG	Sidechain
1	A	1224	TYR	Sidechain
1	A	1253	ARG	Sidechain
1	A	1266	MET	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1685	0	1608	93	1
1	B	1607	0	1499	85	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	33	0	22	3	0
3	B	33	0	22	5	0
All	All	3360	0	3151	174	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 27.

All (174) 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:1267:LYS:HB3	1:A:1268:MET:CE	1.55	1.34
1:A:1267:LYS:HG2	1:A:1268:MET:CE	1.67	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1267:LYS:CB	1:A:1268:MET:CE	2.16	1.22
1:A:1210:ALA:CB	1:A:1269:ALA:HA	1.70	1.21
1:A:1267:LYS:CG	1:A:1268:MET:CE	2.22	1.16
1:A:1267:LYS:CB	1:A:1268:MET:HE2	1.74	1.15
1:A:1253:ARG:HD2	1:A:1303:GLU:CG	1.81	1.10
1:A:1210:ALA:HB3	1:A:1269:ALA:HA	1.31	1.08
1:A:1267:LYS:CB	1:A:1268:MET:HE3	1.85	1.05
1:A:1253:ARG:HD2	1:A:1303:GLU:HG3	1.41	1.01
1:A:1253:ARG:HG2	1:A:1253:ARG:HH11	1.25	1.00
1:A:1267:LYS:CG	1:A:1268:MET:HE3	1.88	1.00
1:A:1260:PHE:HE2	1:A:1262:GLN:NE2	1.59	0.99
1:A:1267:LYS:HG2	1:A:1268:MET:HE3	1.40	0.99
1:A:1267:LYS:HG2	1:A:1268:MET:HE1	1.44	0.99
1:A:1253:ARG:HH11	1:A:1253:ARG:CG	1.79	0.95
1:B:1112:ALA:O	1:B:1115:ASP:HB3	1.68	0.94
1:B:1253:ARG:HH11	1:B:1253:ARG:HG2	1.34	0.92
1:A:1267:LYS:HB3	1:A:1268:MET:HE2	0.92	0.91
1:B:1253:ARG:HG2	1:B:1253:ARG:NH1	1.86	0.91
1:A:1260:PHE:HE2	1:A:1262:GLN:HE21	0.91	0.87
1:A:1133:ARG:CZ	1:A:1288:ALA:HB2	2.04	0.86
1:A:1298:GLU:H	1:A:1298:GLU:CD	1.79	0.84
1:A:1253:ARG:HD2	1:A:1303:GLU:HG2	1.59	0.84
1:A:1180:ARG:NH2	1:A:1216:GLU:OE1	2.10	0.83
1:A:1210:ALA:CB	1:A:1269:ALA:CA	2.56	0.83
1:A:1281:ARG:NH1	1:B:1259:SER:O	2.12	0.82
1:A:1263:PHE:CZ	1:B:1261:LEU:HG	2.15	0.81
1:A:1260:PHE:CE2	1:A:1262:GLN:NE2	2.46	0.80
1:B:1279:ILE:HG12	1:B:1292:TYR:CD1	2.17	0.80
1:B:1268:MET:HE1	1:B:1272:PRO:HD3	1.61	0.80
1:A:1159:ARG:O	1:A:1159:ARG:HG3	1.83	0.79
1:A:1261:LEU:CD2	1:A:1281:ARG:NH1	2.46	0.78
1:B:1212:ILE:HG23	3:B:1402:K4F:H15	1.65	0.78
1:A:1253:ARG:HG2	1:A:1253:ARG:NH1	1.94	0.77
1:B:1281:ARG:CB	1:B:1281:ARG:HH11	1.99	0.75
1:A:1261:LEU:HD23	1:A:1281:ARG:NH1	2.01	0.75
1:B:1234:CYS:SG	1:B:1237:HIS:HB2	2.28	0.74
1:A:1115:ASP:OD1	1:A:1116:LYS:N	2.21	0.73
1:A:1173:ASN:HD21	1:A:1258:LYS:HB2	1.56	0.71
1:B:1206:GLY:O	1:B:1207:MET:CB	2.38	0.70
1:B:1128:THR:HB	1:B:1217:ASN:HA	1.74	0.69
1:B:1211:GLY:O	3:B:1402:K4F:H12	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1179:GLU:OE2	1:A:1253:ARG:NH1	2.26	0.68
1:B:1207:MET:CB	1:B:1213:TYR:CE2	2.76	0.68
1:A:1253:ARG:CD	1:A:1303:GLU:CG	2.69	0.68
1:B:1117:GLU:OE2	1:B:1152:LYS:NZ	2.26	0.67
1:B:1227:GLY:HA2	3:B:1402:K4F:H3	1.76	0.67
1:A:1207:MET:HA	1:A:1266:MET:HE2	1.78	0.65
1:A:1130:ARG:HH11	1:A:1217:ASN:ND2	1.95	0.65
1:A:1210:ALA:HB2	1:A:1269:ALA:HA	1.72	0.65
1:A:1173:ASN:ND2	1:A:1258:LYS:HB2	2.12	0.64
1:B:1279:ILE:CD1	1:B:1292:TYR:HE1	2.11	0.64
1:B:1269:ALA:O	1:B:1270:HIS:CD2	2.51	0.64
1:B:1216:GLU:OE2	1:B:1290:ALA:HB3	1.99	0.63
1:B:1207:MET:CB	1:B:1213:TYR:HE2	2.12	0.61
1:B:1235:PRO:O	1:B:1238:LYS:NZ	2.34	0.61
1:A:1268:MET:HE2	1:A:1268:MET:N	2.15	0.60
1:A:1104:GLN:O	1:A:1104:GLN:HG3	2.00	0.60
1:B:1113:PRO:HD2	1:B:1114:GLU:OE2	2.01	0.60
1:B:1260:PHE:HE2	1:B:1262:GLN:HB3	1.66	0.60
1:A:1253:ARG:CD	1:A:1303:GLU:HG2	2.31	0.60
1:A:1130:ARG:HH11	1:A:1217:ASN:HD21	1.49	0.60
1:A:1211:GLY:O	3:A:1402:K4F:H12	2.02	0.59
1:B:1174:HIS:O	1:B:1175:ASN:HB2	2.02	0.59
1:A:1253:ARG:CG	1:A:1253:ARG:NH1	2.49	0.59
1:A:1173:ASN:O	1:A:1174:HIS:HB2	2.02	0.58
1:B:1112:ALA:HB1	1:B:1114:GLU:OE2	2.02	0.58
1:B:1106:THR:HA	1:B:1154:VAL:O	2.03	0.58
1:B:1155:ASN:HB3	1:B:1158:LEU:HB2	1.84	0.58
1:B:1281:ARG:HH11	1:B:1281:ARG:HB3	1.67	0.58
1:B:1281:ARG:HB2	1:B:1281:ARG:NH1	2.17	0.58
1:A:1144:ARG:CG	1:A:1145:TYR:N	2.67	0.58
1:B:1279:ILE:HG12	1:B:1292:TYR:CE1	2.39	0.58
1:A:1187:PRO:HD2	1:A:1188:PHE:CE2	2.39	0.57
1:B:1213:TYR:CD1	1:B:1213:TYR:N	2.73	0.57
1:B:1117:GLU:CD	1:B:1152:LYS:HZ1	2.06	0.57
1:A:1261:LEU:HD23	1:A:1281:ARG:HH11	1.66	0.56
1:B:1213:TYR:N	1:B:1213:TYR:HD1	2.03	0.56
1:B:1281:ARG:CB	1:B:1281:ARG:NH1	2.69	0.56
1:A:1180:ARG:NH1	1:A:1180:ARG:CG	2.69	0.55
1:A:1180:ARG:CG	1:A:1180:ARG:HH11	2.20	0.55
1:B:1117:GLU:OE1	1:B:1152:LYS:NZ	2.40	0.54
1:A:1261:LEU:HD21	1:A:1281:ARG:NH1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1279:ILE:CD1	1:B:1292:TYR:CE1	2.91	0.53
1:A:1283:SER:HG	1:A:1287:LEU:N	2.07	0.53
1:B:1117:GLU:CD	1:B:1152:LYS:NZ	2.63	0.53
1:A:1191:ALA:HB1	3:A:1402:K4F:C22	2.39	0.53
1:B:1279:ILE:HG22	1:B:1280:GLY:N	2.24	0.53
1:B:1239:ASP:OD1	1:B:1240:ARG:N	2.41	0.52
1:B:1268:MET:HE3	1:B:1270:HIS:O	2.09	0.52
1:A:1297:GLY:N	1:A:1298:GLU:OE2	2.43	0.52
1:B:1268:MET:CE	1:B:1270:HIS:O	2.57	0.52
1:B:1134:ASP:HB3	1:B:1137:ASN:H	1.74	0.52
1:B:1253:ARG:NH1	1:B:1253:ARG:CG	2.63	0.51
1:B:1144:ARG:HD2	1:B:1145:TYR:O	2.11	0.51
1:B:1114:GLU:H	1:B:1114:GLU:CD	2.13	0.51
1:B:1191:ALA:HB1	3:B:1402:K4F:C22	2.41	0.51
1:A:1133:ARG:NH2	1:A:1288:ALA:HB2	2.24	0.50
1:A:1298:GLU:CD	1:A:1298:GLU:N	2.57	0.50
1:B:1217:ASN:OD1	1:B:1289:TYR:CB	2.59	0.50
1:B:1228:ILE:HG22	1:B:1228:ILE:O	2.10	0.50
1:B:1279:ILE:HD13	1:B:1292:TYR:HE1	1.75	0.50
1:A:1263:PHE:CE2	1:B:1261:LEU:HG	2.47	0.50
1:A:1268:MET:HE2	1:A:1268:MET:H	1.77	0.49
1:B:1243:TYR:HD1	1:B:1310:ILE:O	1.95	0.49
1:A:1265:THR:O	1:A:1266:MET:C	2.50	0.49
1:A:1180:ARG:HH11	1:A:1180:ARG:HG3	1.78	0.49
1:B:1130:ARG:O	1:B:1132:HIS:CD2	2.66	0.49
1:A:1212:ILE:HG23	3:A:1402:K4F:H15	1.94	0.49
1:B:1206:GLY:N	1:B:1228:ILE:CD1	2.76	0.48
1:B:1279:ILE:HG12	1:B:1292:TYR:HD1	1.77	0.48
1:A:1112:ALA:HB1	1:A:1114:GLU:OE2	2.14	0.48
1:A:1118:TYR:CD2	1:A:1118:TYR:C	2.87	0.48
1:A:1155:ASN:HB3	1:A:1158:LEU:HB2	1.96	0.47
1:B:1133:ARG:C	1:B:1134:ASP:O	2.50	0.47
1:B:1209:GLY:O	1:B:1213:TYR:OH	2.29	0.47
1:B:1260:PHE:CG	1:B:1272:PRO:HG2	2.49	0.47
1:A:1113:PRO:HA	1:A:1118:TYR:CD2	2.50	0.47
1:A:1210:ALA:HB2	1:A:1269:ALA:CA	2.37	0.47
1:A:1267:LYS:HB3	1:A:1268:MET:H	1.35	0.47
1:A:1266:MET:HG2	1:A:1267:LYS:H	1.80	0.47
1:A:1220:LYS:HD2	1:A:1223:GLN:OE1	2.14	0.47
1:A:1314:GLU:O	1:A:1315:HIS:HB2	2.14	0.47
1:B:1310:ILE:O	1:B:1310:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1260:PHE:HB3	1:B:1278:VAL:HG22	1.96	0.47
1:A:1153:VAL:HB	1:A:1302:PRO:O	2.15	0.47
1:A:1199:GLU:HG2	1:A:1296:ARG:HA	1.96	0.47
1:A:1261:LEU:HD21	1:A:1281:ARG:CZ	2.45	0.47
1:A:1266:MET:CG	1:A:1267:LYS:N	2.77	0.47
1:B:1112:ALA:O	1:B:1115:ASP:CB	2.53	0.47
1:B:1137:ASN:OD1	1:B:1240:ARG:NH2	2.39	0.47
1:B:1212:ILE:HG23	3:B:1402:K4F:C15	2.42	0.47
1:B:1268:MET:CE	1:B:1272:PRO:HD3	2.41	0.46
1:A:1209:GLY:O	1:A:1211:GLY:N	2.42	0.46
1:A:1310:ILE:HG13	1:A:1310:ILE:O	2.14	0.46
1:A:1144:ARG:HG3	1:A:1145:TYR:N	2.31	0.46
1:A:1210:ALA:HB2	1:A:1269:ALA:CB	2.46	0.46
1:B:1260:PHE:CE2	1:B:1262:GLN:HB3	2.48	0.46
1:B:1312:LYS:HB2	1:B:1312:LYS:HE3	1.59	0.46
1:A:1263:PHE:CZ	1:B:1261:LEU:CG	2.94	0.46
1:B:1181:MET:HA	1:B:1252:CYS:O	2.16	0.46
1:B:1207:MET:CB	1:B:1213:TYR:OH	2.64	0.45
1:A:1253:ARG:HH11	1:A:1253:ARG:HG3	1.76	0.45
1:B:1298:GLU:H	1:B:1298:GLU:CD	2.20	0.45
1:A:1113:PRO:HA	1:A:1118:TYR:CG	2.51	0.45
1:A:1173:ASN:HB3	1:A:1176:HIS:O	2.17	0.45
1:B:1234:CYS:O	1:B:1238:LYS:HA	2.17	0.45
1:B:1279:ILE:HD13	1:B:1292:TYR:CE1	2.52	0.45
1:B:1156:LYS:O	1:B:1160:GLU:HG3	2.17	0.45
1:A:1112:ALA:HA	1:A:1113:PRO:HD2	1.77	0.44
1:A:1267:LYS:CG	1:A:1268:MET:HE1	2.20	0.44
1:B:1173:ASN:ND2	1:B:1176:HIS:O	2.46	0.44
1:B:1173:ASN:O	1:B:1175:ASN:N	2.50	0.44
1:B:1206:GLY:N	1:B:1228:ILE:HD13	2.32	0.43
1:B:1165:ARG:O	1:B:1169:VAL:HG23	2.18	0.43
1:B:1181:MET:SD	1:B:1253:ARG:NH1	2.92	0.43
1:B:1153:VAL:HB	1:B:1302:PRO:O	2.20	0.42
1:A:1128:THR:HB	1:A:1217:ASN:HA	2.02	0.42
1:A:1234:CYS:SG	1:A:1237:HIS:N	2.88	0.42
1:A:1106:THR:CG2	1:A:1153:VAL:HG13	2.50	0.42
1:A:1208:PHE:CD1	1:A:1208:PHE:N	2.87	0.42
1:B:1230:GLY:O	1:B:1231:GLY:C	2.58	0.42
1:B:1268:MET:HB2	1:B:1268:MET:HE2	1.77	0.42
1:A:1237:HIS:O	1:A:1238:LYS:C	2.58	0.42
1:A:1148:ILE:HD11	1:A:1309:GLN:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1199:GLU:H	1:A:1199:GLU:HG3	1.25	0.41
1:A:1203:TYR:O	1:A:1204:ILE:CB	2.68	0.41
1:B:1199:GLU:H	1:B:1199:GLU:HG3	1.54	0.41
1:B:1281:ARG:HH11	1:B:1281:ARG:HB2	1.72	0.41
1:B:1117:GLU:O	1:B:1121:VAL:HG23	2.19	0.41
1:B:1207:MET:CB	1:B:1213:TYR:CZ	3.03	0.41
1:B:1279:ILE:CG2	1:B:1280:GLY:N	2.83	0.41
1:A:1266:MET:CG	1:A:1267:LYS:H	2.34	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:1199:GLU:OE2	1:B:1296:ARG:NH2[1_455]	2.16	0.04

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	206/217 (95%)	193 (94%)	9 (4%)	4 (2%)	8 28
1	B	197/217 (91%)	176 (89%)	13 (7%)	8 (4%)	3 11
All	All	403/434 (93%)	369 (92%)	22 (6%)	12 (3%)	4 17

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1203	TYR
1	A	1204	ILE
1	A	1210	ALA
1	A	1267	LYS
1	B	1174	HIS

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Mol	Chain	Res	Type
1	B	1207	MET
1	B	1264	SER
1	B	1266	MET
1	B	1208	PHE
1	B	1134	ASP
1	B	1238	LYS
1	B	1135	GLY

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	176/185 (95%)	159 (90%)	17 (10%)	8 25
1	B	163/185 (88%)	153 (94%)	10 (6%)	18 48
All	All	339/370 (92%)	312 (92%)	27 (8%)	12 33

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1104	GLN
1	A	1118	TYR
1	A	1123	GLU
1	A	1124	GLU
1	A	1131	GLU
1	A	1152	LYS
1	A	1180	ARG
1	A	1199	GLU
1	A	1236	THR
1	A	1237	HIS
1	A	1253	ARG
1	A	1264	SER
1	A	1267	LYS
1	A	1270	HIS
1	A	1284	VAL
1	A	1312	LYS

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Mol	Chain	Res	Type
1	A	1315	HIS
1	B	1104	GLN
1	B	1114	GLU
1	B	1143	ASN
1	B	1144	ARG
1	B	1199	GLU
1	B	1220	LYS
1	B	1236	THR
1	B	1238	LYS
1	B	1298	GLU
1	B	1312	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1166	GLN
1	A	1173	ASN
1	A	1217	ASN
1	A	1270	HIS
1	B	1223	GLN
1	B	1270	HIS

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 4 ligands modelled in this entry, 2 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	K4F	A	1402	-	37,37,37	2.82	15 (40%)	54,54,54	2.74	18 (33%)
3	K4F	B	1402	-	37,37,37	2.60	14 (37%)	54,54,54	2.70	16 (29%)

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	K4F	A	1402	-	-	0/16/35/35	0/5/5/5
3	K4F	B	1402	-	-	0/16/35/35	0/5/5/5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1402	K4F	C6-C7	-10.75	1.36	1.51
3	A	1402	K4F	C6-C7	-10.68	1.36	1.51
3	A	1402	K4F	O1-C11	5.80	1.44	1.35
3	A	1402	K4F	C5-C6	5.23	1.47	1.39
3	B	1402	K4F	C5-C6	4.72	1.46	1.39
3	A	1402	K4F	C12-N1	-4.11	1.35	1.43
3	A	1402	K4F	C24-C23	3.74	1.47	1.42
3	B	1402	K4F	C24-C23	3.34	1.47	1.42
3	B	1402	K4F	C12-N1	-3.33	1.37	1.43
3	B	1402	K4F	O1-C8	3.24	1.53	1.48
3	A	1402	K4F	C4-C5	2.70	1.44	1.38
3	B	1402	K4F	C4-C5	2.55	1.44	1.38
3	A	1402	K4F	C13-C12	2.46	1.44	1.39
3	A	1402	K4F	C16-C15	2.42	1.43	1.38
3	B	1402	K4F	C21-C22	2.40	1.42	1.36
3	B	1402	K4F	C26-C25	2.40	1.42	1.36
3	A	1402	K4F	C27-N3	2.37	1.37	1.32
3	A	1402	K4F	C21-C22	2.34	1.42	1.36
3	A	1402	K4F	C20-C19	2.33	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1402	K4F	C9-C8	2.31	1.56	1.52
3	A	1402	K4F	C26-C25	2.25	1.41	1.36
3	B	1402	K4F	C13-C12	2.24	1.43	1.39
3	B	1402	K4F	C27-N3	2.18	1.36	1.32
3	B	1402	K4F	C26-C27	2.15	1.44	1.37
3	B	1402	K4F	C11-N1	2.14	1.39	1.36
3	B	1402	K4F	C20-C19	2.14	1.42	1.38
3	A	1402	K4F	C10-C8	-2.11	1.48	1.52
3	A	1402	K4F	C26-C27	2.02	1.43	1.37
3	A	1402	K4F	C21-C20	2.00	1.43	1.38

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1402	K4F	O1-C8-C7	-9.96	94.03	102.66
3	A	1402	K4F	O1-C8-C7	-9.10	94.78	102.66
3	A	1402	K4F	C6-C7-N1	8.42	122.10	113.06
3	B	1402	K4F	C6-C7-N1	8.24	121.90	113.06
3	B	1402	K4F	C8-C7-C6	6.93	122.80	115.55
3	A	1402	K4F	C7-N1-C11	-6.90	105.29	111.25
3	A	1402	K4F	C8-C7-C6	6.85	122.70	115.55
3	B	1402	K4F	C7-N1-C11	-6.42	105.71	111.25
3	B	1402	K4F	C27-N3-C23	3.98	122.26	117.30
3	A	1402	K4F	C27-N3-C23	3.97	122.25	117.30
3	A	1402	K4F	C8-C7-N1	3.89	103.97	100.52
3	A	1402	K4F	O1-C8-C10	3.83	111.04	106.77
3	A	1402	K4F	C5-C6-C7	-3.43	113.48	120.70
3	A	1402	K4F	C24-C23-N3	-3.38	118.92	122.62
3	B	1402	K4F	C24-C23-N3	-3.36	118.94	122.62
3	B	1402	K4F	C8-C7-N1	3.36	103.50	100.52
3	B	1402	K4F	C8-O1-C11	3.32	113.56	110.04
3	B	1402	K4F	C5-C6-C7	-3.29	113.78	120.70
3	A	1402	K4F	C19-C23-N3	3.22	120.22	117.48
3	A	1402	K4F	C1-C6-C7	3.19	127.42	120.70
3	B	1402	K4F	C19-C23-N3	3.18	120.19	117.48
3	B	1402	K4F	C1-C6-C7	2.93	126.88	120.70
3	A	1402	K4F	C26-C27-N3	-2.85	119.57	123.94
3	A	1402	K4F	O1-C8-C9	-2.85	103.60	106.77
3	B	1402	K4F	C26-C27-N3	-2.77	119.69	123.94
3	A	1402	K4F	C12-N1-C11	2.53	127.65	123.67
3	B	1402	K4F	O1-C8-C10	2.51	109.57	106.77
3	B	1402	K4F	C12-N1-C11	2.39	127.42	123.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1402	K4F	C10-C8-C7	2.29	118.72	113.42
3	A	1402	K4F	O1-C11-N1	-2.27	106.91	108.76
3	B	1402	K4F	C19-C23-C24	2.23	120.87	119.42
3	B	1402	K4F	C10-C8-C7	2.23	118.58	113.42
3	A	1402	K4F	C19-C23-C24	2.22	120.86	119.42
3	A	1402	K4F	C12-N1-C7	2.02	126.49	121.81

There are no chirality outliers.

There are no torsion outliers.

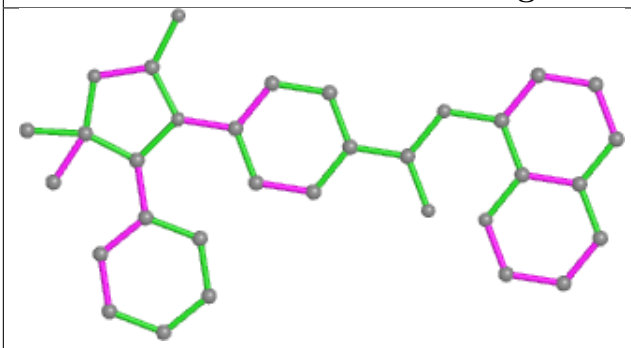
There are no ring outliers.

2 monomers are involved in 8 short contacts:

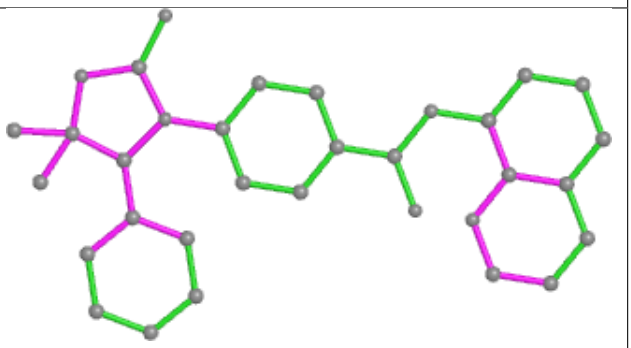
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1402	K4F	3	0
3	B	1402	K4F	5	0

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.

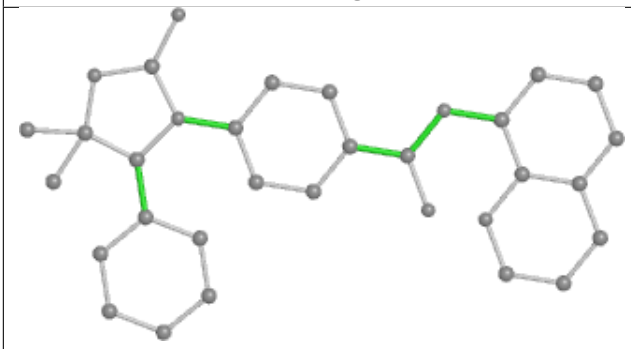
Ligand K4F A 1402



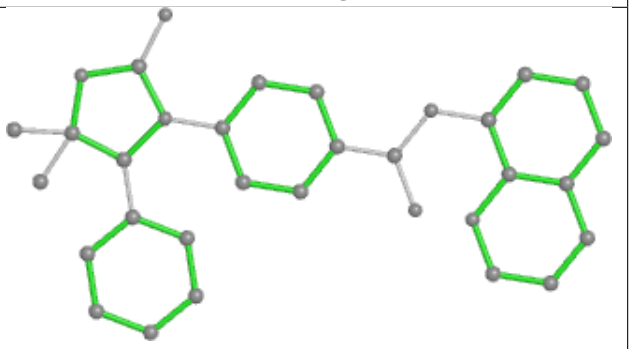
Bond lengths



Bond angles

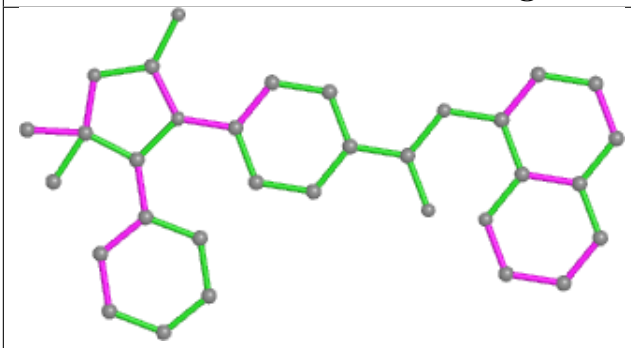


Torsions

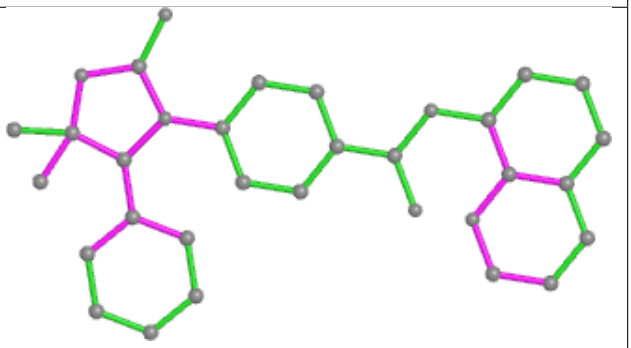


Rings

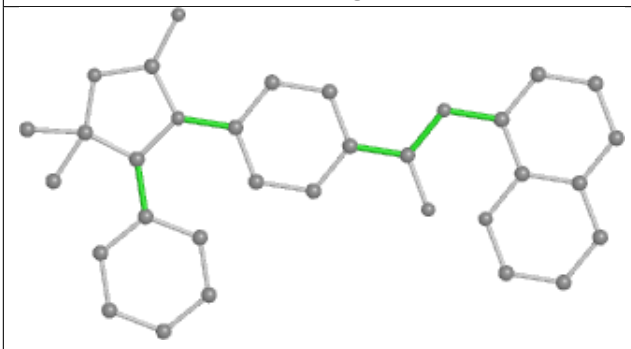
Ligand K4F B 1402



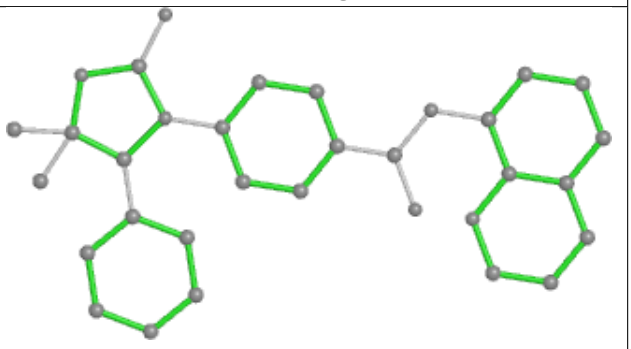
Bond lengths



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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	210/217 (96%)	0.14	7 (3%)	46	41	7, 26, 41, 50	0
1	B	203/217 (93%)	0.25	10 (4%)	29	26	14, 31, 51, 59	0
All	All	413/434 (95%)	0.20	17 (4%)	37	32	7, 29, 44, 59	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1206	GLY	10.1
1	B	1207	MET	4.3
1	B	1265	THR	4.1
1	A	1104	GLN	4.0
1	A	1207	MET	3.9
1	B	1264	SER	3.5
1	B	1134	ASP	3.4
1	B	1104	GLN	3.2
1	A	1270	HIS	2.7
1	A	1208	PHE	2.5
1	B	1203	TYR	2.5
1	A	1315	HIS	2.4
1	B	1289	TYR	2.2
1	A	1206	GLY	2.1
1	A	1116	LYS	2.1
1	B	1131	GLU	2.1
1	B	1211	GLY	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

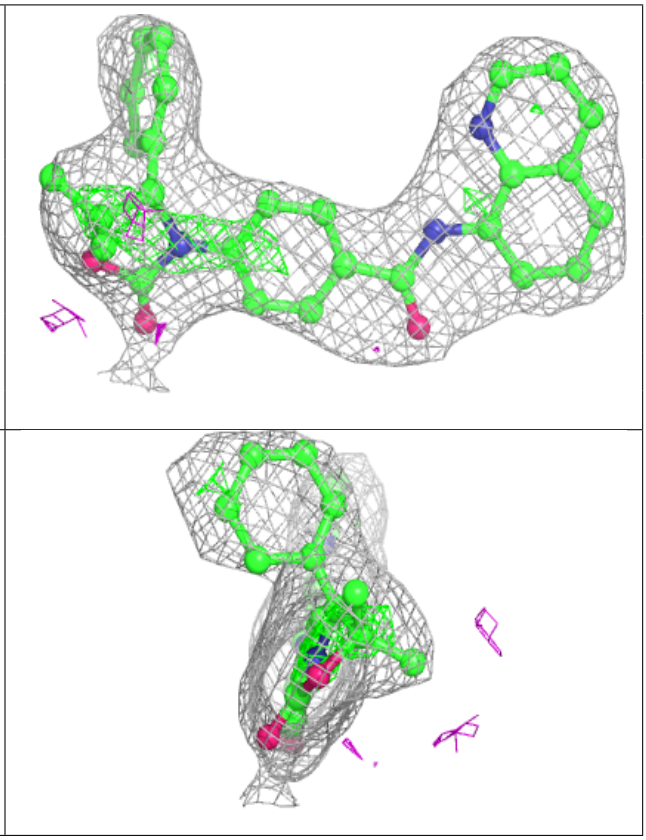
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	K4F	A	1402	33/33	0.90	0.32	40,68,90,93	0
3	K4F	B	1402	33/33	0.90	0.29	44,66,86,90	0
2	ZN	B	1401	1/1	0.96	0.06	38,38,38,38	0
2	ZN	A	1401	1/1	0.99	0.06	24,24,24,24	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.

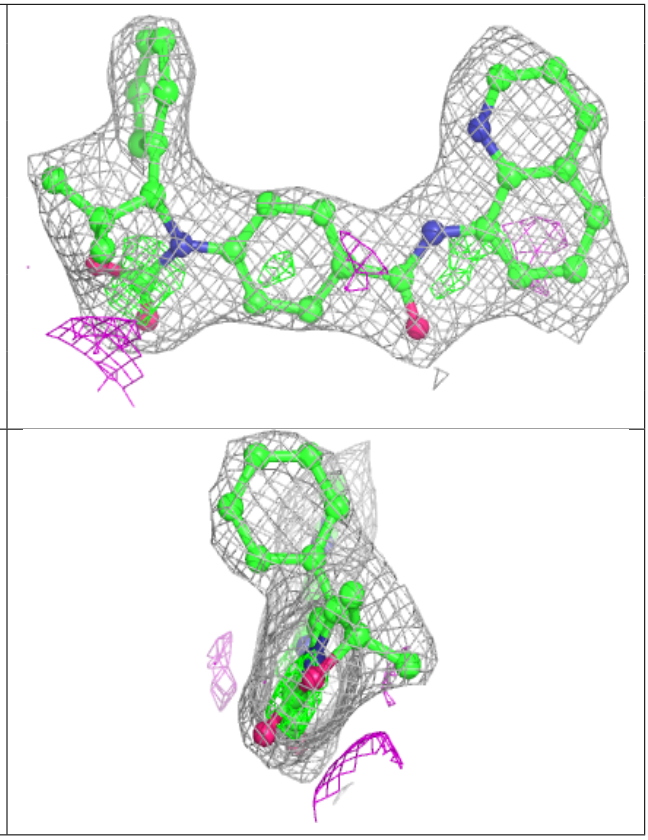
Electron density around K4F A 1402:

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 K4F B 1402:

$2mF_o$-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.