



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 11:03 AM BST

PDB ID : 6Q3W  
Title : Structure of human galactokinase 1 bound with Ethyl 1-(2-pyrazinyl)-4-piperidinecarboxylate  
Authors : Mackinnon, S.R.; Bezerra, G.A.; Zhang, M.; Foster, W.; Krojer, T.; Brandao-Neto, J.; Douangamath, A.; Arrowsmith, C.; Edwards, A.; Bountra, C.; Brennan, P.; Lai, K.; Yue, W.W.  
Deposited on : 2018-12-04  
Resolution : 1.96 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : 2.13.1  
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) : 2.13.1

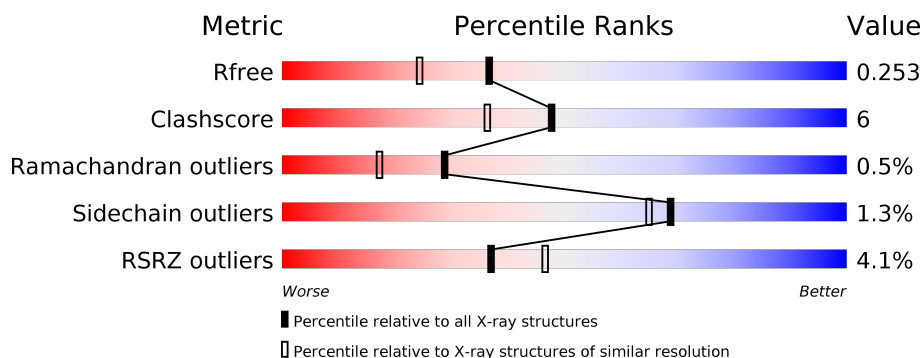
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.96 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	391	<div> <div>0%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
1	B	391	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>••</div> </div> </div>
1	C	391	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div>•</div> </div> </div>
1	D	391	<div> <div>8%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>•</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11460 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.

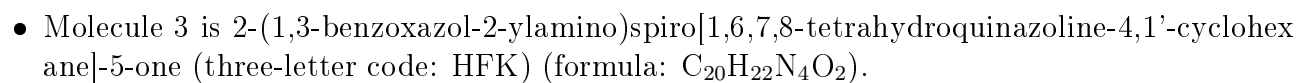
- Molecule 1 is a protein called Galactokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			2798	1755	495	532	16			
1	B	385	Total	C	N	O	S	0	0	0
			2722	1711	473	523	15			
1	C	390	Total	C	N	O	S	0	0	0
			2710	1694	477	524	15			
1	D	357	Total	C	N	O	S	0	0	0
			2458	1539	433	472	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	252	ALA	LYS	conflict	UNP P51570
A	253	ALA	GLU	conflict	UNP P51570
B	252	ALA	LYS	conflict	UNP P51570
B	253	ALA	GLU	conflict	UNP P51570
C	252	ALA	LYS	conflict	UNP P51570
C	253	ALA	GLU	conflict	UNP P51570
D	252	ALA	LYS	conflict	UNP P51570
D	253	ALA	GLU	conflict	UNP P51570

- Molecule 2 is beta-D-galactopyranose (three-letter code: GAL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



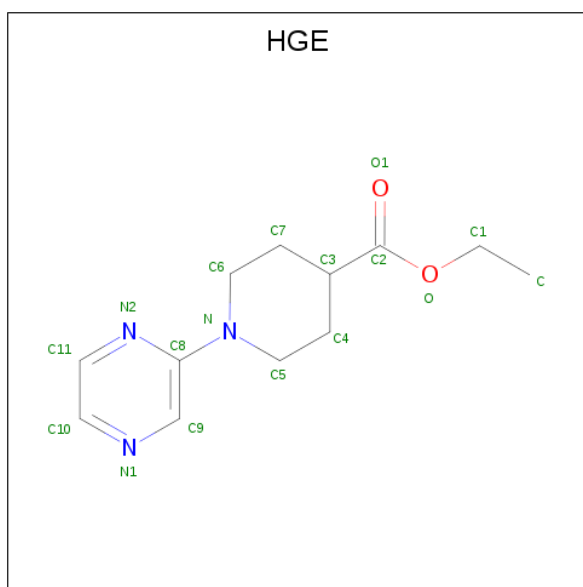
- Molecule 3 is 2-(1,3-benzoxazol-2-ylamino)spiro[1,6,7,8-tetrahydroquinazoline-4,1'-cyclohexane]-5-one (three-letter code: HFK) (formula: C<sub>20</sub>H<sub>22</sub>N<sub>4</sub>O<sub>2</sub>).

- Molecule 3 is 2-(1,3-benzoxazol-2-ylamino)spiro[1,6,7,8-tetrahydroquinazoline-4,1'-cyclohexane]-5-one (three-letter code: HFK) (formula: C<sub>20</sub>H<sub>22</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			26	20	4	2		
3	B	1	Total	C	N	O	0	0
			26	20	4	2		
3	C	1	Total	C	N	O	0	0
			26	20	4	2		

- Molecule 4 is ethyl 1-pyrazin-2-ylpiperidine-4-carboxylate (three-letter code: HGE) (formula:  $C_{12}H_{17}N_3O_2$ ).

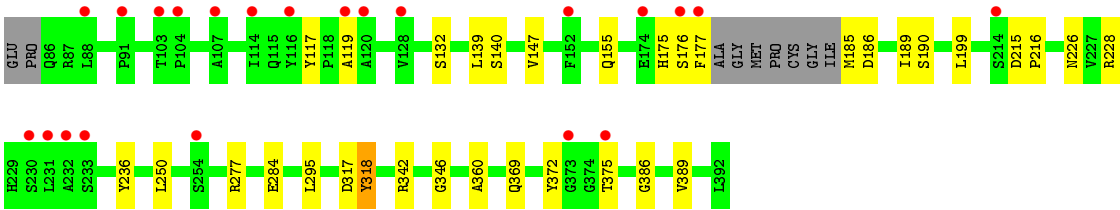


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			17	12	3	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	206	Total	O	0	0
			206	206		
5	B	154	Total	O	0	0
			154	154		
5	C	157	Total	O	0	0
			157	157		
5	D	124	Total	O	0	0
			124	124		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.26Å 114.81Å 120.82Å 90.00° 100.49° 90.00°	Depositor
Resolution (Å)	82.56 – 1.96 82.56 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.3 (82.56-1.96) 99.4 (82.56-1.96)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 1.97Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.232 , 0.255 0.233 , 0.253	Depositor DCC
$R_{free}$ test set	7036 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 49.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11460	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: HFK, HGE, GAL

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	0.26	0/2851	0.45	0/3889
1	B	0.25	0/2772	0.44	0/3786
1	C	0.26	0/2761	0.47	1/3775 (0.0%)
1	D	0.26	0/2499	0.49	0/3414
All	All	0.26	0/10883	0.46	1/14864 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	231	LEU	C-N-CA	5.21	134.73	121.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2798	0	2683	29	0
1	B	2722	0	2567	25	0
1	C	2710	0	2500	37	0
1	D	2458	0	2245	36	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	12	0	12	0	0
3	A	26	0	0	0	0
3	B	26	0	0	0	0
3	C	26	0	0	0	0
4	C	17	0	0	0	0
5	A	206	0	0	9	0
5	B	154	0	0	6	0
5	C	157	0	0	12	0
5	D	124	0	0	14	0
All	All	11460	0	10031	127	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 6.

All (127) 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:392:LEU:O	5:A:501:HOH:O	1.83	0.96
1:B:27:GLU:OE1	5:B:501:HOH:O	1.89	0.90
1:D:250:LEU:O	5:D:401:HOH:O	1.91	0.87
1:A:37:ARG:CZ	5:A:504:HOH:O	2.23	0.85
1:A:37:ARG:NH2	5:A:504:HOH:O	2.07	0.85
1:C:243:CYS:SG	5:C:528:HOH:O	2.34	0.84
1:C:379:TYR:OH	5:C:501:HOH:O	1.87	0.84
1:C:380:LEU:N	5:C:503:HOH:O	2.01	0.83
1:C:289:ALA:O	5:C:502:HOH:O	1.98	0.81
1:D:228:ARG:NH2	5:D:404:HOH:O	2.14	0.80
1:C:2:ALA:N	5:C:505:HOH:O	2.14	0.80
1:A:122:LEU:O	5:A:502:HOH:O	1.98	0.79
1:A:37:ARG:HH12	1:A:186:ASP:CG	1.86	0.79
1:D:226:ASN:OD1	5:D:402:HOH:O	2.01	0.78
1:D:185:MET:N	5:D:406:HOH:O	2.17	0.77
1:A:174:GLU:OE2	5:A:503:HOH:O	2.03	0.75
1:A:37:ARG:NH1	1:A:186:ASP:OD1	2.21	0.74
1:D:43:GLU:HG3	1:D:44:HIS:CE1	2.22	0.74
1:B:297:ARG:NH2	5:B:505:HOH:O	2.20	0.73
1:A:264:GLU:OE2	5:A:505:HOH:O	2.08	0.72
1:B:257:GLU:OE2	5:B:502:HOH:O	2.08	0.72
1:D:155:GLN:OE1	1:D:389:VAL:HG11	1.89	0.71
1:D:375:THR:O	5:D:402:HOH:O	2.10	0.69
1:B:309:GLU:OE1	5:B:503:HOH:O	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLU:OE2	5:A:506:HOH:O	2.14	0.66
1:C:84:GLU:OE1	5:C:504:HOH:O	2.13	0.66
1:C:37:ARG:HH21	1:C:37:ARG:HG2	1.61	0.66
1:B:7:PRO:HG3	1:B:59:LEU:HD23	1.81	0.63
1:C:37:ARG:NH2	1:C:140:SER:OG	2.31	0.63
1:D:277:ARG:HA	5:D:418:HOH:O	1.99	0.62
1:D:236:TYR:OH	1:D:346:GLY:O	2.12	0.62
1:C:307:MET:SD	5:C:509:HOH:O	2.56	0.61
1:D:43:GLU:HG3	1:D:44:HIS:ND1	2.16	0.61
1:C:339:TYR:OH	1:C:357:GLU:OE2	2.11	0.61
1:A:37:ARG:HA	1:A:57:LEU:HG	1.83	0.60
1:A:37:ARG:HD3	1:A:189:ILE:HG21	1.83	0.59
1:D:185:MET:N	5:D:414:HOH:O	2.35	0.59
1:D:369:GLN:O	5:D:405:HOH:O	2.16	0.59
1:D:37:ARG:HD3	1:D:189:ILE:HG21	1.84	0.59
1:B:43:GLU:HB2	1:B:342:ARG:NH2	2.19	0.58
1:B:37:ARG:HH22	1:B:345:GLY:HA2	1.69	0.58
1:D:54:PRO:HD2	1:D:199:LEU:O	2.04	0.57
1:D:27:GLU:O	5:D:407:HOH:O	2.17	0.57
1:C:218:LEU:O	5:C:507:HOH:O	2.18	0.57
1:B:262:GLU:OE1	5:B:504:HOH:O	2.18	0.56
1:C:207:GLU:OE1	5:C:508:HOH:O	2.18	0.55
1:A:23:GLU:OE1	1:A:87:ARG:NH2	2.39	0.55
1:C:43:GLU:HB3	1:C:314:LEU:HD21	1.88	0.54
1:D:44:HIS:ND1	1:D:44:HIS:N	2.56	0.54
1:C:140:SER:HB3	1:C:143:ALA:HB3	1.89	0.54
1:A:379:TYR:OH	5:A:507:HOH:O	2.14	0.53
1:C:43:GLU:HB2	1:C:342:ARG:NH2	2.23	0.53
1:A:37:ARG:NH1	1:A:186:ASP:HA	2.24	0.52
1:B:43:GLU:HB2	1:B:342:ARG:HH22	1.75	0.51
1:D:37:ARG:NE	1:D:186:ASP:OD1	2.43	0.51
1:D:32:VAL:HG12	1:D:389:VAL:HG22	1.93	0.51
1:B:46:ASP:HB3	1:B:52:VAL:HG11	1.93	0.50
1:B:267:ARG:NH1	5:B:513:HOH:O	2.42	0.50
1:B:32:VAL:HG12	1:B:389:VAL:HG22	1.94	0.50
1:D:147:VAL:HG21	1:D:190:SER:HB3	1.93	0.49
1:C:188:PHE:CE2	1:C:208:THR:HG21	2.48	0.49
1:A:43:GLU:HB2	1:A:342:ARG:NH2	2.28	0.49
1:C:49:GLN:O	1:C:256:ARG:HD2	2.13	0.49
1:D:12:LEU:HD21	1:D:132:SER:HB3	1.95	0.49
1:B:39:ASN:HA	1:B:54:PRO:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:TYR:O	5:D:405:HOH:O	2.20	0.48
1:C:340:GLY:O	5:C:509:HOH:O	2.20	0.48
1:A:17:ARG:HH21	1:A:27:GLU:HG3	1.79	0.47
1:D:35:PRO:HG3	1:D:386:GLY:HA2	1.97	0.47
1:B:8:GLN:O	1:B:9:VAL:HG12	2.14	0.47
1:C:366:ARG:O	1:C:370:GLU:N	2.36	0.46
1:A:37:ARG:NE	5:A:504:HOH:O	2.44	0.46
1:A:356:LEU:HD11	1:A:361:ALA:HA	1.97	0.46
1:C:54:PRO:HD2	1:C:199:LEU:O	2.15	0.46
1:B:20:PHE:CE2	1:B:65:GLY:HA2	2.50	0.46
1:C:37:ARG:NH2	1:C:37:ARG:HG2	2.27	0.46
1:B:30:LEU:HD21	1:B:155:GLN:CB	2.46	0.45
1:A:218:LEU:HD11	1:A:355:LEU:HG	1.97	0.45
1:D:317:ASP:C	5:D:418:HOH:O	2.54	0.45
1:A:273:GLU:O	1:A:277:ARG:HG2	2.17	0.45
1:A:109:TYR:CE1	1:A:142:SER:HB2	2.51	0.45
1:A:17:ARG:HH21	1:A:27:GLU:CG	2.29	0.45
1:C:272:LYS:C	1:C:275:PHE:H	2.19	0.45
1:D:318:TYR:HA	5:D:418:HOH:O	2.16	0.45
1:D:386:GLY:HA3	5:D:413:HOH:O	2.17	0.45
1:B:54:PRO:HD2	1:B:199:LEU:O	2.17	0.44
1:D:117:TYR:CE2	1:D:119:ALA:HB3	2.53	0.44
1:C:222:ILE:HB	1:C:379:TYR:HB2	1.99	0.44
1:B:199:LEU:HD23	1:B:201:ILE:HD11	2.00	0.44
1:B:85:PRO:HD2	1:B:104:PRO:HD3	1.99	0.44
1:C:231:LEU:N	1:C:232:ALA:HB2	2.33	0.44
1:C:174:GLU:HG2	1:C:182:CYS:SG	2.58	0.44
1:B:51:LEU:HD23	1:B:202:ASP:HA	1.99	0.43
1:D:215:ASP:HA	1:D:216:PRO:HD3	1.84	0.43
1:D:360:ALA:HA	5:D:423:HOH:O	2.18	0.43
1:A:292:ALA:O	1:A:296:ARG:HG3	2.18	0.43
1:D:176:SER:O	1:D:177:PHE:HB2	2.17	0.43
1:B:37:ARG:HD3	1:B:189:ILE:HG21	2.00	0.43
1:A:88:LEU:HD22	1:A:104:PRO:HD2	2.00	0.42
1:D:28:PRO:HG3	1:D:64:VAL:HG13	2.01	0.42
1:A:37:ARG:HG2	1:A:37:ARG:HH11	1.84	0.42
1:C:47:TYR:CE1	1:C:240:ARG:HG2	2.54	0.42
1:D:40:LEU:O	1:D:342:ARG:HD3	2.20	0.42
1:C:236:TYR:HB3	1:C:237:PRO:HD3	2.00	0.42
1:B:147:VAL:HG21	1:B:190:SER:HB3	2.02	0.42
1:B:259:GLN:OE1	1:B:261:GLU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:LEU:HD12	1:B:295:LEU:HA	1.91	0.42
1:D:295:LEU:HD23	1:D:295:LEU:HA	1.85	0.42
1:A:147:VAL:HG21	1:A:190:SER:HB3	2.00	0.41
1:C:228:ARG:HG2	1:C:228:ARG:NH1	2.35	0.41
1:A:54:PRO:HD2	1:A:199:LEU:O	2.20	0.41
1:C:255:LEU:HA	1:C:255:LEU:HD23	1.89	0.41
1:C:314:LEU:HD11	1:C:342:ARG:HH21	1.86	0.41
1:D:37:ARG:HH11	1:D:37:ARG:HG2	1.86	0.41
1:C:228:ARG:HG2	1:C:228:ARG:HH11	1.85	0.41
1:C:292:ALA:N	5:C:502:HOH:O	2.53	0.41
1:D:42:GLY:HA2	1:D:284:GLU:HG3	2.01	0.41
1:A:311:HIS:CE1	1:A:329:VAL:HG21	2.55	0.41
1:C:109:TYR:CE1	1:C:142:SER:HB2	2.55	0.41
1:A:27:GLU:HG3	1:A:28:PRO:HD2	2.03	0.41
1:D:140:SER:OG	1:D:186:ASP:HB3	2.21	0.41
1:C:175:HIS:CD2	1:C:181:PRO:HA	2.56	0.41
1:C:43:GLU:HB2	1:C:342:ARG:HH22	1.86	0.41
1:D:139:LEU:HD23	1:D:139:LEU:HA	1.84	0.41
1:B:273:GLU:O	1:B:277:ARG:HG2	2.22	0.40
1:C:119:ALA:HB2	1:C:159:ASP:HA	2.02	0.40
1:C:347:GLY:N	5:C:520:HOH:O	2.40	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	389/391 (100%)	382 (98%)	6 (2%)	1 (0%)	41	30
1	B	379/391 (97%)	367 (97%)	8 (2%)	4 (1%)	14	5
1	C	388/391 (99%)	375 (97%)	12 (3%)	1 (0%)	41	30
1	D	347/391 (89%)	329 (95%)	17 (5%)	1 (0%)	41	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1503/1564 (96%)	1453 (97%)	43 (3%)	7 (0%)	29	17

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	9	VAL
1	C	232	ALA
1	D	175	HIS
1	A	217	LYS
1	B	8	GLN
1	B	80	GLU
1	B	7	PRO

### 5.3.2 Protein sidechains ⓘ

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	273/308 (89%)	271 (99%)	2 (1%)	84	82
1	B	260/308 (84%)	257 (99%)	3 (1%)	71	68
1	C	249/308 (81%)	246 (99%)	3 (1%)	71	68
1	D	221/308 (72%)	216 (98%)	5 (2%)	50	42
All	All	1003/1232 (81%)	990 (99%)	13 (1%)	69	65

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

Mol	Chain	Res	Type
1	A	37	ARG
1	A	188	PHE
1	B	9	VAL
1	B	37	ARG
1	B	55	MET
1	C	64	VAL
1	C	233	SER
1	C	382	GLN

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Mol	Chain	Res	Type
1	D	43	GLU
1	D	44	HIS
1	D	55	MET
1	D	64	VAL
1	D	318	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

7 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	$\# Z  > 2$
2	GAL	A	401	-	12,12,12	0.75	0	17,17,17	1.02	0
2	GAL	B	401	-	12,12,12	0.62	0	17,17,17	0.73	0
2	GAL	C	401	-	12,12,12	0.52	0	17,17,17	0.79	0
3	HFK	A	402	-	26,30,30	4.47	10 (38%)	24,44,44	4.02	10 (41%)
3	HFK	B	402	-	26,30,30	4.52	10 (38%)	24,44,44	4.11	11 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	HGE	C	402	-	18,18,18	1.82	3 (16%)	22,23,23	1.78	5 (22%)
3	HFK	C	403	-	26,30,30	4.49	10 (38%)	24,44,44	4.38	10 (41%)

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
2	GAL	A	401	-	-	1/2/22/22	0/1/1/1
2	GAL	B	401	-	-	2/2/22/22	0/1/1/1
2	GAL	C	401	-	-	1/2/22/22	0/1/1/1
3	HFK	A	402	-	-	2/2/43/43	0/5/5/5
3	HFK	B	402	-	-	2/2/43/43	0/5/5/5
4	HGE	C	402	-	-	2/11/21/21	0/2/2/2
3	HFK	C	403	-	-	2/2/43/43	0/5/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	HFK	C06-C07	13.48	1.54	1.37
3	A	402	HFK	C06-C07	13.37	1.54	1.37
3	B	402	HFK	C06-C07	13.35	1.54	1.37
3	B	402	HFK	C15-N16	9.97	1.52	1.36
3	A	402	HFK	C15-N16	9.63	1.52	1.36
3	C	403	HFK	C15-N16	9.40	1.51	1.36
3	B	402	HFK	C15-N14	8.89	1.53	1.30
3	A	402	HFK	C15-N14	8.84	1.53	1.30
3	C	403	HFK	C15-N14	8.80	1.53	1.30
3	C	403	HFK	O01-C02	7.59	1.38	1.23
3	B	402	HFK	O01-C02	7.48	1.38	1.23
3	A	402	HFK	O01-C02	7.43	1.38	1.23
3	B	402	HFK	C06-N16	5.90	1.47	1.37
3	A	402	HFK	C06-N16	5.64	1.46	1.37
3	C	403	HFK	C06-N16	5.48	1.46	1.37
3	C	403	HFK	C03-C02	5.33	1.57	1.50
4	C	402	HGE	C8-N	5.29	1.48	1.37
3	A	402	HFK	C03-C02	5.14	1.57	1.50
3	B	402	HFK	C03-C02	4.99	1.57	1.50
3	B	402	HFK	C18-N17	4.53	1.44	1.36
3	C	403	HFK	C18-N17	4.42	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	HFK	C18-N17	4.29	1.44	1.36
4	C	402	HGE	O-C2	3.71	1.41	1.33
3	C	403	HFK	C02-C07	3.45	1.56	1.46
3	A	402	HFK	C02-C07	3.32	1.56	1.46
3	B	402	HFK	C02-C07	3.23	1.56	1.46
3	C	403	HFK	C08-N14	2.93	1.49	1.46
3	B	402	HFK	C05-C06	2.86	1.54	1.49
3	C	403	HFK	C05-C06	2.73	1.54	1.49
3	A	402	HFK	C05-C06	2.65	1.54	1.49
3	A	402	HFK	C08-N14	2.55	1.49	1.46
4	C	402	HGE	O-C1	-2.49	1.38	1.46
3	B	402	HFK	C08-N14	2.27	1.48	1.46

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	HFK	C08-C07-C06	-10.86	109.50	121.75
3	A	402	HFK	C08-C07-C06	-10.30	110.13	121.75
3	C	403	HFK	C08-C07-C06	-9.32	111.24	121.75
3	C	403	HFK	C02-C07-C06	-8.64	110.96	119.17
3	C	403	HFK	O01-C02-C03	-8.36	107.17	120.86
3	C	403	HFK	C05-C06-C07	-8.29	112.04	122.97
3	B	402	HFK	O01-C02-C03	-7.83	108.03	120.86
3	A	402	HFK	O01-C02-C03	-7.77	108.13	120.86
3	B	402	HFK	O01-C02-C07	-6.91	112.02	121.54
3	C	403	HFK	C15-N16-C06	-6.87	112.44	120.67
3	B	402	HFK	C05-C06-C07	-6.85	113.94	122.97
3	C	403	HFK	N16-C15-N14	-6.63	112.79	123.88
3	A	402	HFK	O01-C02-C07	-6.51	112.58	121.54
3	A	402	HFK	C05-C06-C07	-6.47	114.44	122.97
3	A	402	HFK	N16-C15-N14	-6.08	113.70	123.88
3	A	402	HFK	C15-N16-C06	-5.97	113.52	120.67
3	B	402	HFK	N16-C15-N14	-5.65	114.44	123.88
3	B	402	HFK	N17-C15-N14	-5.58	108.53	117.81
3	C	403	HFK	O01-C02-C07	-5.33	114.20	121.54
3	A	402	HFK	N17-C15-N14	-5.16	109.23	117.81
3	B	402	HFK	C15-N16-C06	-5.05	114.62	120.67
3	C	403	HFK	N17-C15-N14	-4.71	109.98	117.81
4	C	402	HGE	O-C2-C3	4.39	120.36	112.10
3	B	402	HFK	C02-C07-C06	-3.99	115.37	119.17
3	A	402	HFK	C05-C06-N16	-3.54	109.89	115.34
3	B	402	HFK	C05-C06-N16	-3.34	110.21	115.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	HFK	C02-C07-C06	-3.31	116.03	119.17
4	C	402	HGE	C5-C4-C3	3.13	115.62	110.41
3	C	403	HFK	C05-C06-N16	-2.95	110.80	115.34
3	A	402	HFK	C18-N17-C15	-2.87	120.12	126.49
4	C	402	HGE	C11-N2-C8	2.80	120.56	116.86
3	B	402	HFK	C18-N17-C15	-2.70	120.49	126.49
4	C	402	HGE	O-C2-O1	-2.35	119.68	124.13
3	B	402	HFK	C03-C02-C07	-2.27	113.12	117.36
4	C	402	HGE	C4-C5-N	2.14	115.52	111.10
3	C	403	HFK	C18-N17-C15	-2.07	121.89	126.49

There are no chirality outliers.

All (12) torsion outliers are listed below:

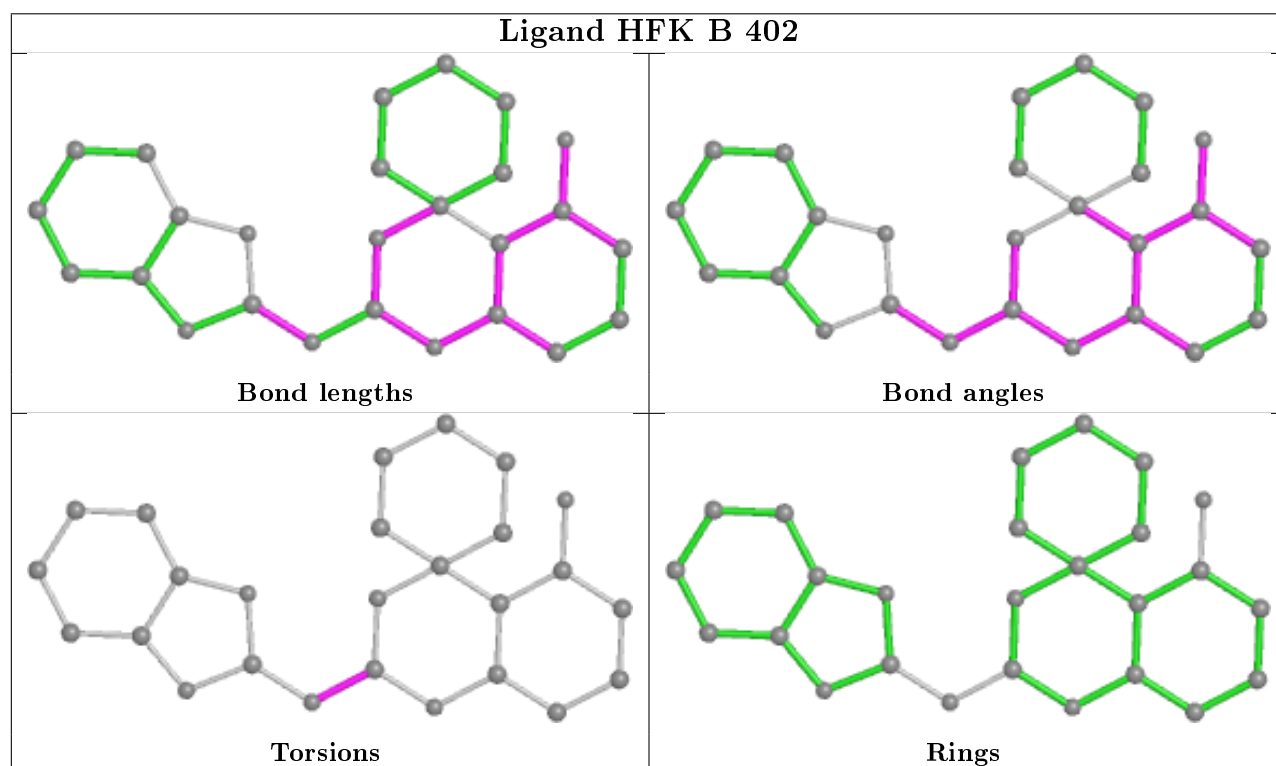
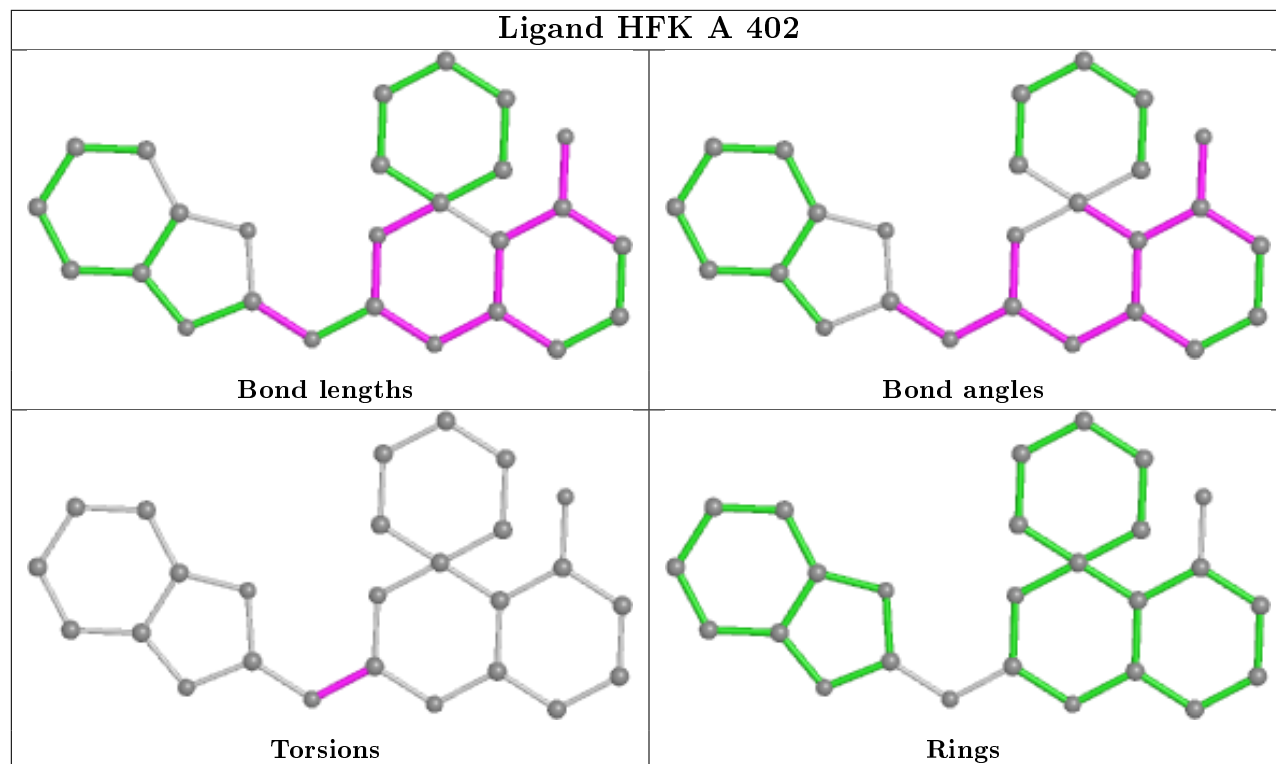
Mol	Chain	Res	Type	Atoms
3	A	402	HFK	N14-C15-N17-C18
3	B	402	HFK	N14-C15-N17-C18
4	C	402	HGE	C9-C8-N-C6
3	C	403	HFK	N14-C15-N17-C18
2	B	401	GAL	O5-C5-C6-O6
2	C	401	GAL	O5-C5-C6-O6
4	C	402	HGE	N2-C8-N-C6
2	A	401	GAL	O5-C5-C6-O6
2	B	401	GAL	C4-C5-C6-O6
3	A	402	HFK	N16-C15-N17-C18
3	B	402	HFK	N16-C15-N17-C18
3	C	403	HFK	N16-C15-N17-C18

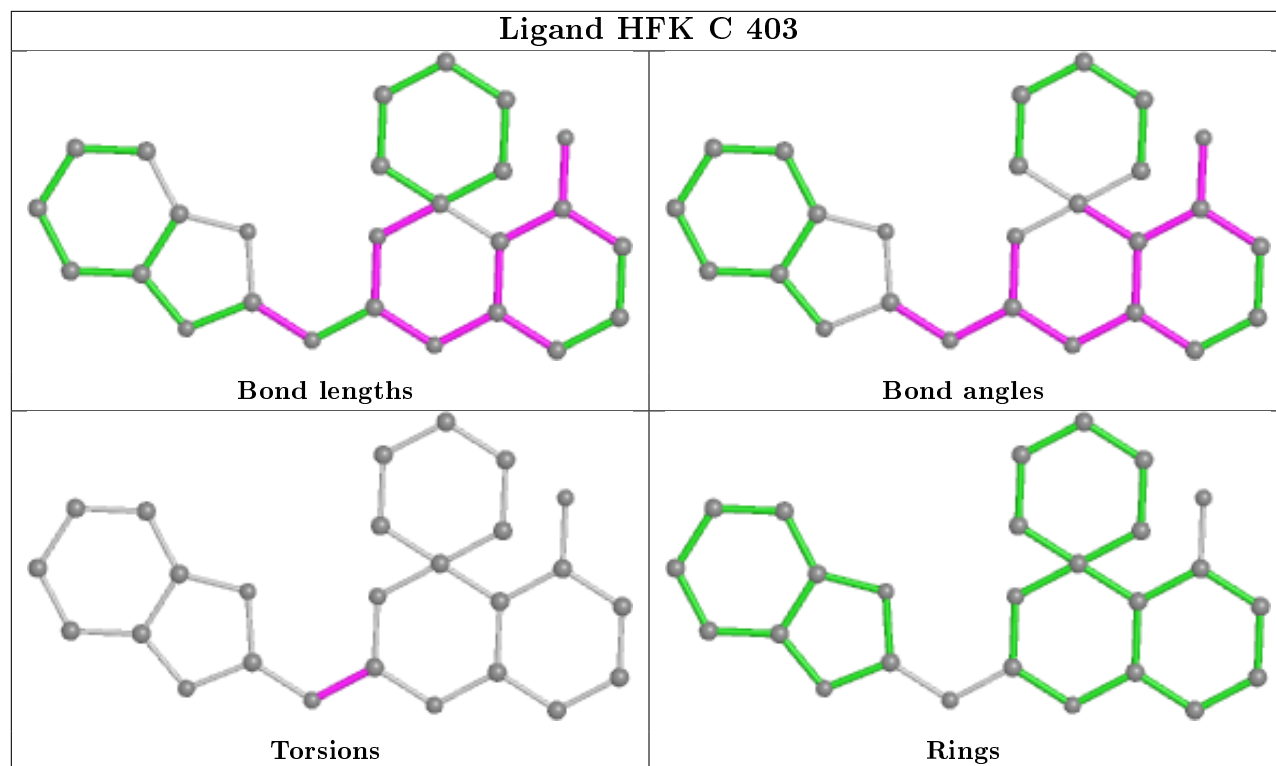
There are no ring outliers.

No monomer is involved in short contacts.

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 than 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.





## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	391/391 (100%)	0.01	3 (0%)	86 90	24, 40, 64, 98	0
1	B	385/391 (98%)	0.22	7 (1%)	68 76	31, 46, 79, 105	0
1	C	390/391 (99%)	0.44	21 (5%)	25 34	28, 49, 100, 125	0
1	D	357/391 (91%)	0.62	31 (8%)	10 16	27, 57, 108, 142	0
All	All	1523/1564 (97%)	0.32	62 (4%)	37 46	24, 47, 93, 142	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	120	ALA	10.2
1	C	275	PHE	6.2
1	C	368	ILE	5.6
1	D	373	GLY	5.2
1	D	103	THR	4.9
1	D	71	GLY	4.6
1	C	246	VAL	4.2
1	C	265	ALA	4.2
1	D	231	LEU	4.0
1	C	231	LEU	3.6
1	C	266	ALA	3.1
1	C	364	ALA	3.1
1	C	188	PHE	3.0
1	A	9	VAL	3.0
1	C	365	MET	3.0
1	D	107	ALA	2.9
1	D	119	ALA	2.9
1	B	9	VAL	2.9
1	D	47	TYR	2.9
1	D	176	SER	2.9
1	C	360	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	367	HIS	2.8
1	D	72	LEU	2.7
1	A	372	TYR	2.7
1	B	26	ALA	2.7
1	D	128	VAL	2.6
1	B	7	PRO	2.6
1	D	64	VAL	2.6
1	A	3	ALA	2.5
1	C	263	LEU	2.5
1	C	270	VAL	2.5
1	D	88	LEU	2.5
1	C	251	GLY	2.4
1	D	104	PRO	2.4
1	D	177	PHE	2.4
1	D	78	THR	2.4
1	D	12	LEU	2.4
1	B	128	VAL	2.4
1	D	114	ILE	2.4
1	C	214	SER	2.3
1	C	269	LEU	2.3
1	B	27	GLU	2.3
1	D	13	LEU	2.3
1	B	188	PHE	2.3
1	D	254	SER	2.3
1	D	67	PRO	2.3
1	C	308	VAL	2.3
1	D	30	LEU	2.3
1	D	375	THR	2.2
1	C	358	ALA	2.2
1	D	214	SER	2.2
1	D	233	SER	2.2
1	C	250	LEU	2.2
1	D	91	PRO	2.1
1	C	300	TYR	2.1
1	D	174	GLU	2.1
1	C	333	LEU	2.1
1	D	230	SER	2.1
1	D	152	PHE	2.1
1	D	116	TYR	2.0
1	B	88	LEU	2.0
1	D	232	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

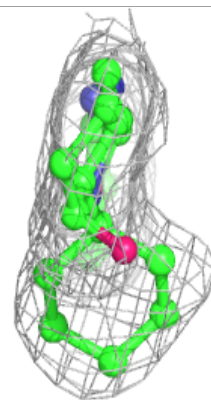
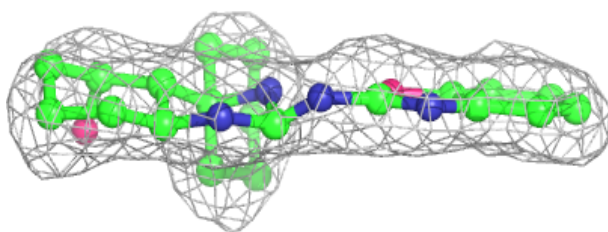
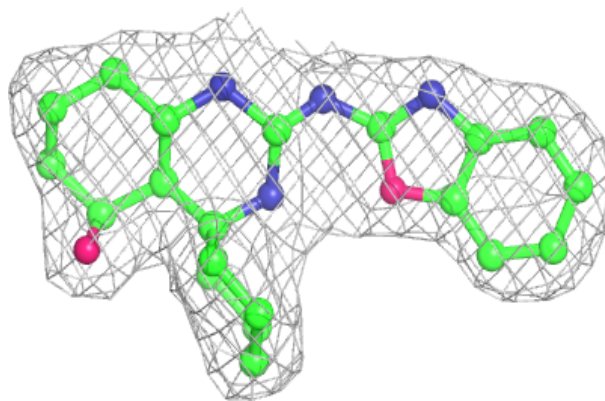
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	HGE	C	402	17/17	0.70	0.30	87,88,102,102	0
3	HFK	B	402	26/26	0.85	0.15	49,54,58,80	0
2	GAL	B	401	12/12	0.89	0.12	32,37,43,45	0
3	HFK	C	403	26/26	0.89	0.15	47,49,61,68	0
3	HFK	A	402	26/26	0.90	0.12	35,38,47,54	0
2	GAL	A	401	12/12	0.92	0.12	23,27,32,40	0
2	GAL	C	401	12/12	0.93	0.12	31,37,39,41	0

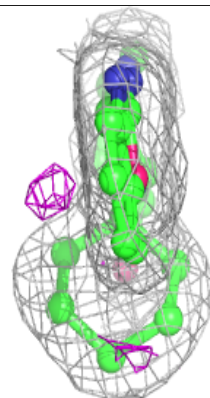
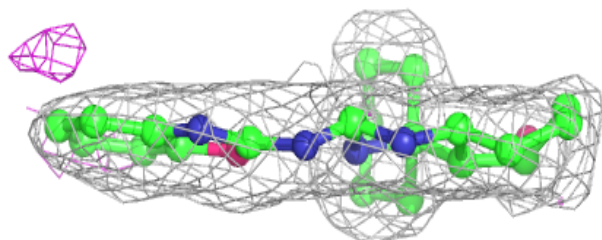
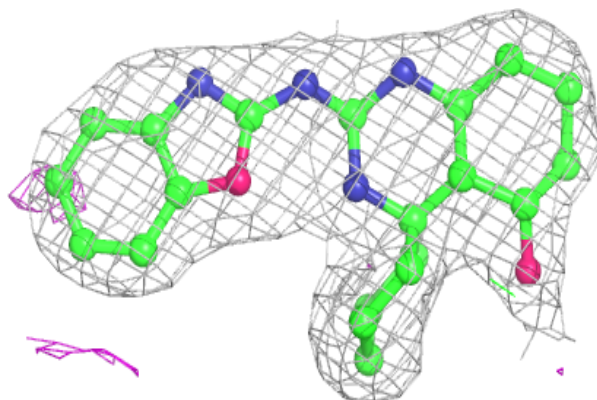
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around HFK B 402:**

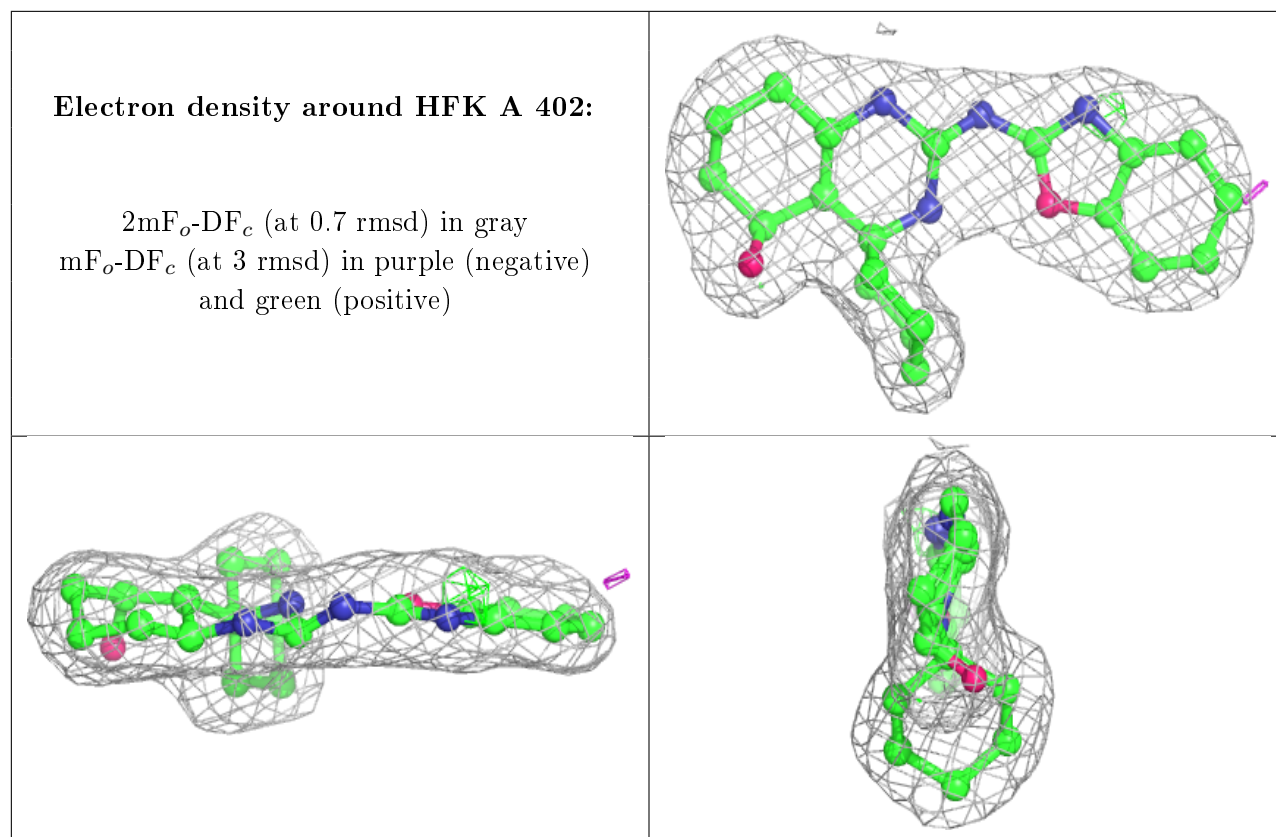
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around HFK C 403:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.