



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:02 AM UTC

PDB ID : 6ZGV / pdb_00006zgv
Title : Structure of human galactokinase 1 bound with 2-(4-chlorophenyl)-N-(pyrimidin-2-yl)acetamide
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 : 2020-06-20
Resolution : 2.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

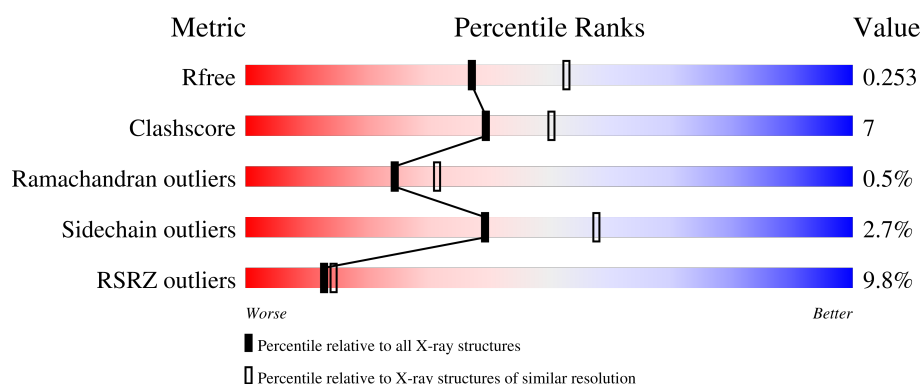
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	399	14% 76% 18% ...
1	B	399	9% 80% 16% ..
1	D	399	13% 78% 14% • 7%
1	E	399	2% 87% 10% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11450 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	388	Total	C	N	O	S	0	0	0
			2685	1687	474	508	16			
1	B	387	Total	C	N	O	S	0	0	0
			2746	1727	484	520	15			
1	E	391	Total	C	N	O	S	0	0	0
			2851	1788	507	540	16			
1	D	372	Total	C	N	O	S	0	0	0
			2600	1631	462	494	13			

There are 40 discrepancies between the modelled and reference sequences:

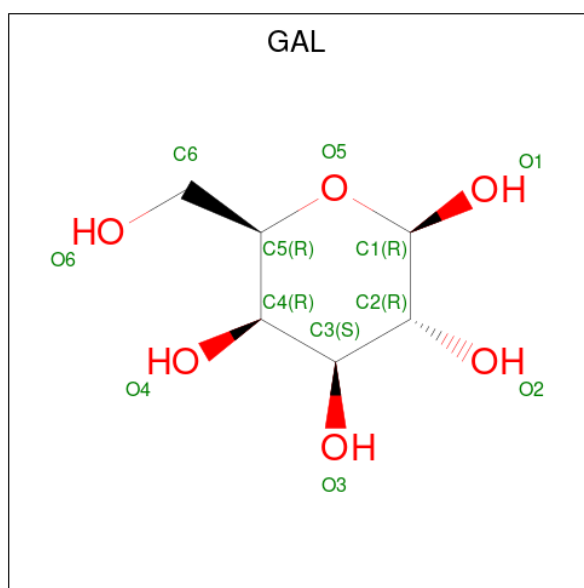
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP P51570
A	-5	ALA	-	expression tag	UNP P51570
A	-4	HIS	-	expression tag	UNP P51570
A	-3	HIS	-	expression tag	UNP P51570
A	-2	HIS	-	expression tag	UNP P51570
A	-1	HIS	-	expression tag	UNP P51570
A	0	HIS	-	expression tag	UNP P51570
A	1	HIS	-	expression tag	UNP P51570
A	252	ALA	LYS	engineered mutation	UNP P51570
A	253	ALA	GLU	engineered mutation	UNP P51570
B	-6	MET	-	initiating methionine	UNP P51570
B	-5	ALA	-	expression tag	UNP P51570
B	-4	HIS	-	expression tag	UNP P51570
B	-3	HIS	-	expression tag	UNP P51570
B	-2	HIS	-	expression tag	UNP P51570
B	-1	HIS	-	expression tag	UNP P51570
B	0	HIS	-	expression tag	UNP P51570
B	1	HIS	-	expression tag	UNP P51570
B	252	ALA	LYS	engineered mutation	UNP P51570
B	253	ALA	GLU	engineered mutation	UNP P51570
E	-6	MET	-	initiating methionine	UNP P51570

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	ALA	-	expression tag	UNP P51570
E	-4	HIS	-	expression tag	UNP P51570
E	-3	HIS	-	expression tag	UNP P51570
E	-2	HIS	-	expression tag	UNP P51570
E	-1	HIS	-	expression tag	UNP P51570
E	0	HIS	-	expression tag	UNP P51570
E	1	HIS	-	expression tag	UNP P51570
E	252	ALA	LYS	engineered mutation	UNP P51570
E	253	ALA	GLU	engineered mutation	UNP P51570
D	-6	MET	-	initiating methionine	UNP P51570
D	-5	ALA	-	expression tag	UNP P51570
D	-4	HIS	-	expression tag	UNP P51570
D	-3	HIS	-	expression tag	UNP P51570
D	-2	HIS	-	expression tag	UNP P51570
D	-1	HIS	-	expression tag	UNP P51570
D	0	HIS	-	expression tag	UNP P51570
D	1	HIS	-	expression tag	UNP P51570
D	252	ALA	LYS	engineered mutation	UNP P51570
D	253	ALA	GLU	engineered mutation	UNP P51570

- Molecule 2 is beta-D-galactopyranose (CCD ID: GAL) (formula: C₆H₁₂O₆).



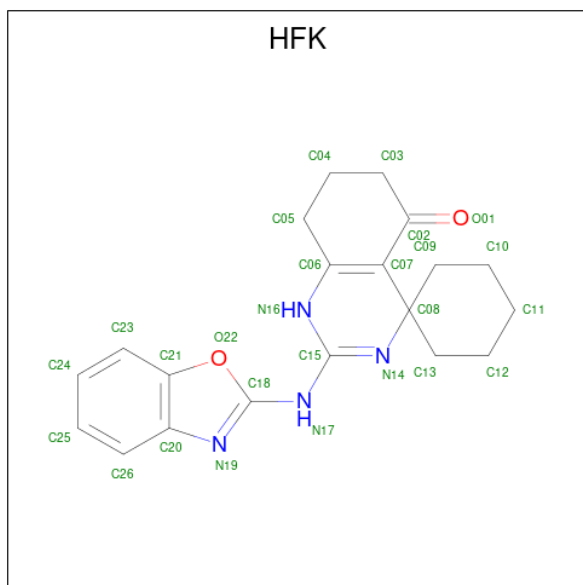
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

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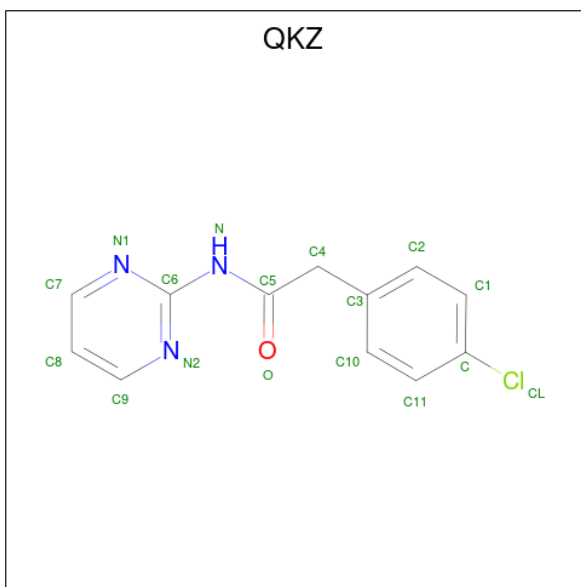
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is 2-(1,3-benzoxazol-2-ylamino)spiro[1,6,7,8-tetrahydroquinazoline-4,1'-cyclohexane]-5-one (CCD ID: HFK) (formula: $C_{20}H_{22}N_4O_2$).



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	E	1	Total	C	N	O	0	0
			26	20	4	2		

- Molecule 4 is 2-(4-chlorophenyl)- {N}-pyrimidin-2-yl-ethanamide (CCD ID: QKZ) (formula: $C_{12}H_{10}ClN_3O$) (labeled as "Ligand of Interest" by depositor).



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

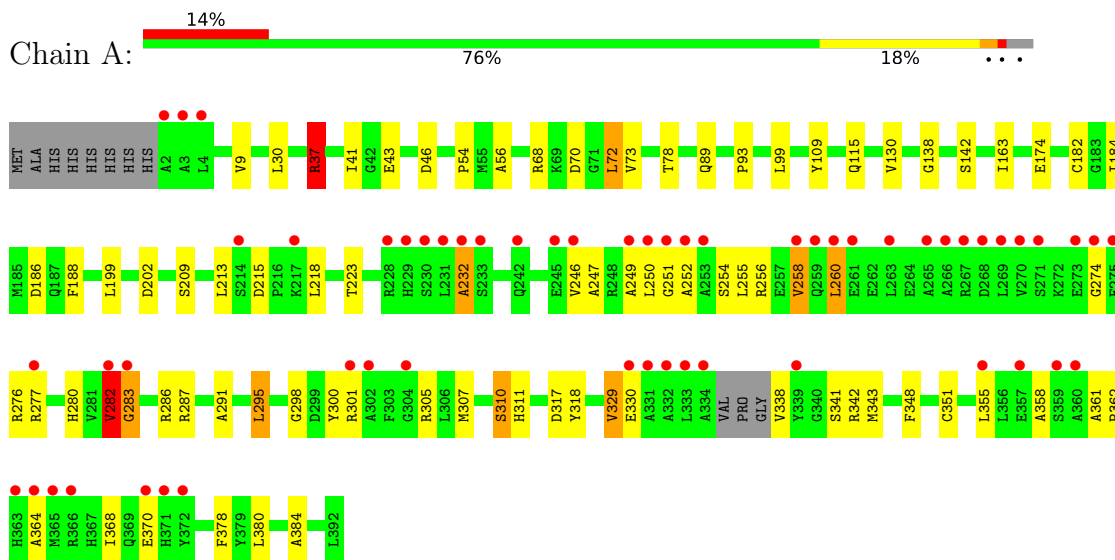
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	90	Total	O	0	0
			90	90		
5	B	82	Total	O	0	0
			82	82		
5	E	157	Total	O	0	0
			157	157		
5	D	108	Total	O	0	0
			108	108		

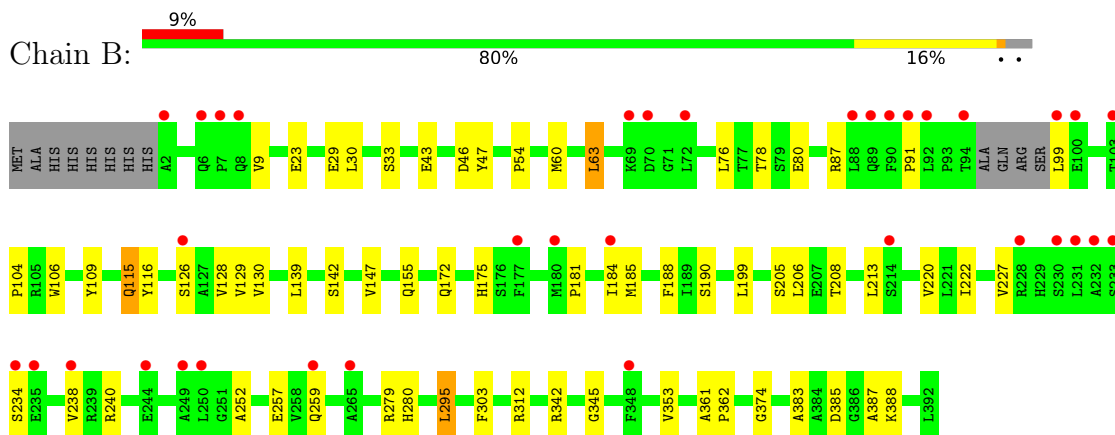
3 Residue-property plots

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.

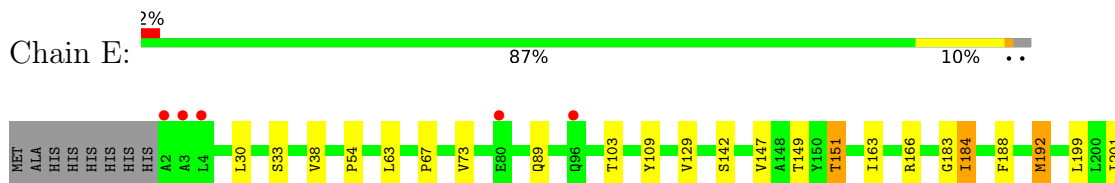
• Molecule 1: Galactokinase

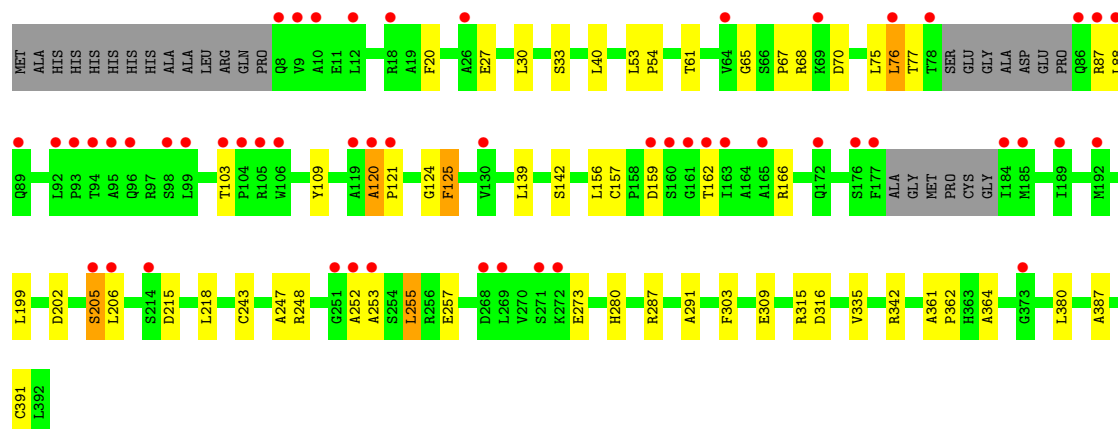


• Molecule 1: Galactokinase



• Molecule 1: Galactokinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.56Å 114.46Å 121.01Å 90.00° 100.39° 90.00°	Depositor
Resolution (Å)	72.46 – 2.30 72.46 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (72.46-2.30) 99.1 (72.46-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.207 , 0.246 (Not available) , 0.253	Depositor DCC
R_{free} test set	5314 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11450	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 4.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, GAL, QKZ

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	1.30	10/2733 (0.4%)	1.55	6/3736 (0.2%)
1	B	1.16	1/2799 (0.0%)	1.54	9/3821 (0.2%)
1	D	1.19	2/2644 (0.1%)	1.55	6/3607 (0.2%)
1	E	1.15	0/2904	1.47	5/3953 (0.1%)
All	All	1.20	13/11080 (0.1%)	1.53	26/15117 (0.2%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	125	PHE	C-O	9.01	1.34	1.23
1	A	282	VAL	C-N	8.77	1.46	1.33
1	A	282	VAL	C-O	8.67	1.33	1.24
1	A	310	SER	C-O	8.12	1.33	1.24
1	A	286	ARG	C-O	8.07	1.34	1.24
1	A	298	GLY	C-O	6.51	1.32	1.23
1	B	374	GLY	C-O	6.14	1.29	1.23
1	A	301	ARG	C-O	6.00	1.31	1.24
1	A	41	ILE	C-O	5.64	1.30	1.24
1	A	295	LEU	C-O	5.62	1.31	1.24
1	A	305	ARG	C-O	5.27	1.31	1.24
1	A	370	GLU	C-O	5.21	1.30	1.24
1	D	124	GLY	C-O	5.03	1.28	1.23

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	LEU	CA-C-N	-8.58	110.14	122.06
1	B	139	LEU	C-N-CA	-8.58	110.14	122.06
1	B	280	HIS	CA-CB-CG	-7.30	106.50	113.80
1	B	46	ASP	CA-CB-CG	6.57	119.17	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	280	HIS	CA-CB-CG	-6.34	107.46	113.80
1	A	37	ARG	CG-CD-NE	-6.31	98.12	112.00
1	D	139	LEU	CA-C-N	6.22	132.23	122.78
1	D	139	LEU	C-N-CA	6.22	132.23	122.78
1	A	46	ASP	CA-CB-CG	6.20	118.80	112.60
1	B	139	LEU	N-CA-C	-6.14	101.37	110.46
1	E	149	THR	N-CA-C	-6.14	104.50	111.07
1	A	282	VAL	CB-CA-C	5.89	119.75	112.04
1	E	301	ARG	N-CA-C	-5.50	105.29	111.28
1	A	280	HIS	CA-CB-CG	-5.46	108.34	113.80
1	E	183	GLY	CA-C-O	-5.29	116.76	122.47
1	E	67	PRO	CA-C-O	-5.23	115.29	121.67
1	D	273	GLU	N-CA-C	-5.21	105.28	111.69
1	D	205	SER	CA-C-O	-5.18	114.86	120.81
1	B	345	GLY	CA-C-N	5.15	125.66	120.00
1	B	345	GLY	C-N-CA	5.15	125.66	120.00
1	B	279	ARG	N-CA-C	-5.14	105.76	111.36
1	B	312	ARG	N-CA-C	-5.10	105.72	111.28
1	A	358	ALA	CA-C-N	5.09	127.35	120.38
1	A	358	ALA	C-N-CA	5.09	127.35	120.38
1	D	280	HIS	N-CA-C	-5.04	105.68	111.07
1	E	103	THR	CB-CA-C	5.02	115.64	108.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2685	0	2511	48	0
1	B	2746	0	2601	34	0
1	D	2600	0	2433	40	0
1	E	2851	0	2787	23	0
2	A	12	0	11	0	0
2	B	12	0	12	0	0
2	E	12	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	26	0	0	0	0
3	B	26	0	0	0	0
3	E	26	0	0	0	0
4	D	17	0	0	0	0
5	A	90	0	0	1	0
5	B	82	0	0	1	0
5	D	108	0	0	0	0
5	E	157	0	0	1	0
All	All	11450	0	10366	144	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 7.

All (144) 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:87:ARG:O	1:D:88:LEU:HD23	1.65	0.96
1:A:274:GLY:O	1:A:276:ARG:O	1.97	0.83
1:D:248:ARG:HA	1:D:252:ALA:HB2	1.61	0.82
1:D:159:ASP:O	1:D:159:ASP:OD1	1.99	0.81
1:B:23:GLU:OE1	1:B:87:ARG:NH2	2.16	0.79
1:E:147:VAL:O	1:E:151:THR:HG23	1.86	0.75
1:A:311:HIS:HD2	1:A:343:MET:H	1.34	0.73
1:D:120:ALA:HB3	1:D:121:PRO:HD3	1.73	0.70
1:A:72:LEU:C	1:A:72:LEU:HD12	2.16	0.70
1:B:188:PHE:CE1	1:B:208:THR:HG21	2.26	0.70
1:D:315:ARG:NH1	1:D:316:ASP:OD1	2.23	0.70
1:D:248:ARG:CA	1:D:252:ALA:HB2	2.21	0.69
1:D:253:ALA:HB3	1:D:257:GLU:HG3	1.75	0.67
1:D:202:ASP:O	1:D:205:SER:O	2.15	0.65
1:D:159:ASP:OD1	1:D:159:ASP:C	2.40	0.64
1:E:361:ALA:HB3	1:E:362:PRO:HD3	1.80	0.64
1:A:213:LEU:CD1	1:A:295:LEU:HD11	2.28	0.63
1:A:54:PRO:HD2	1:A:199:LEU:O	1.99	0.62
1:B:99:LEU:CB	1:B:115:GLN:HE21	2.12	0.62
1:A:223:THR:O	1:A:351:CYS:HA	2.00	0.61
1:E:147:VAL:O	1:E:151:THR:CG2	2.47	0.61
1:D:252:ALA:O	1:D:253:ALA:C	2.39	0.61
1:A:78:THR:OG1	1:A:130:VAL:HG12	2.01	0.60
1:D:248:ARG:N	1:D:252:ALA:HB2	2.16	0.60
1:B:43:GLU:HB2	1:B:342:ARG:NH2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ALA:C	1:A:251:GLY:H	2.11	0.59
1:B:23:GLU:CD	1:B:87:ARG:NH2	2.61	0.58
1:D:162:THR:O	1:D:166:ARG:HG3	2.03	0.58
1:E:163:ILE:HG21	1:E:192:MET:SD	2.42	0.58
1:A:247:ALA:HB1	1:A:252:ALA:O	2.03	0.58
1:A:218:LEU:HD11	1:A:355:LEU:HD11	1.85	0.58
1:D:247:ALA:HB1	1:D:252:ALA:HA	1.86	0.57
1:B:252:ALA:HB1	1:B:257:GLU:HB2	1.87	0.57
1:D:54:PRO:HD2	1:D:199:LEU:O	2.05	0.57
1:D:361:ALA:HB3	1:D:362:PRO:HD3	1.88	0.56
1:E:151:THR:HG21	1:E:387:ALA:HB1	1.87	0.55
1:E:273:GLU:O	1:E:277:ARG:HG2	2.07	0.55
1:E:218:LEU:HD11	1:E:355:LEU:HG	1.89	0.55
1:D:215:ASP:CG	1:D:218:LEU:HD13	2.32	0.54
1:B:30:LEU:HD21	1:B:155:GLN:HB3	1.90	0.53
1:E:261:GLU:OE1	5:E:501:HOH:O	2.19	0.52
1:B:99:LEU:CB	1:B:115:GLN:NE2	2.73	0.52
1:B:385:ASP:OD2	1:B:388:LYS:NZ	2.37	0.52
1:A:68:ARG:CZ	1:A:72:LEU:HD11	2.39	0.52
1:A:364:ALA:O	1:A:368:ILE:HG12	2.10	0.52
1:A:277:ARG:HA	1:A:318:TYR:HD1	1.76	0.51
1:D:67:PRO:HB3	1:D:156:LEU:HD22	1.92	0.51
1:B:9:VAL:HG22	1:B:60:MET:HE3	1.92	0.51
1:D:315:ARG:NH1	1:D:316:ASP:CG	2.69	0.51
1:A:368:ILE:HB	1:A:378:PHE:HZ	1.75	0.51
1:A:260:LEU:HD12	1:A:260:LEU:O	2.11	0.50
1:A:37:ARG:NH2	1:A:138:GLY:O	2.45	0.50
1:B:147:VAL:HG21	1:B:190:SER:HB3	1.94	0.50
1:D:361:ALA:HB3	1:D:362:PRO:CD	2.41	0.50
1:B:80:GLU:CB	5:B:549:HOH:O	2.59	0.50
1:E:54:PRO:HD2	1:E:199:LEU:O	2.12	0.49
1:D:68:ARG:NH1	1:D:70:ASP:OD2	2.42	0.49
1:E:30:LEU:CD2	1:D:391:CYS:HB2	2.43	0.49
1:E:109:TYR:CE1	1:E:142:SER:HB2	2.47	0.48
1:B:33:SER:O	1:B:387:ALA:HA	2.13	0.48
1:A:277:ARG:HA	1:A:318:TYR:CD1	2.49	0.48
1:D:247:ALA:C	1:D:252:ALA:HB2	2.39	0.48
1:A:250:LEU:HD12	1:A:250:LEU:N	2.29	0.47
1:A:218:LEU:HD22	1:A:300:TYR:CE1	2.49	0.47
1:A:72:LEU:C	1:A:72:LEU:CD1	2.87	0.47
1:B:222:ILE:HD12	1:B:222:ILE:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:ALA:HB1	1:E:269:LEU:HD12	1.97	0.47
1:A:184:ILE:O	1:A:188:PHE:HB2	2.14	0.47
1:A:307:MET:O	1:A:310:SER:HB3	2.15	0.47
1:A:311:HIS:CD2	1:A:343:MET:H	2.23	0.47
1:A:109:TYR:CE1	1:A:142:SER:HB2	2.50	0.47
1:E:322:CYS:HB2	1:E:323:PRO:HD2	1.97	0.47
1:D:335:VAL:HG21	1:D:364:ALA:HA	1.97	0.47
1:B:109:TYR:CE1	1:B:142:SER:HB2	2.50	0.46
1:D:87:ARG:O	1:D:88:LEU:CD2	2.52	0.46
1:E:356:LEU:HD23	1:E:356:LEU:N	2.31	0.45
1:E:38:VAL:HG23	1:E:344:THR:HG21	1.97	0.45
1:A:56:ALA:HB3	1:A:384:ALA:O	2.16	0.45
1:B:234:SER:O	1:B:238:VAL:HG23	2.17	0.44
1:A:213:LEU:HD13	1:A:295:LEU:HD21	1.98	0.44
1:D:243:CYS:HB3	1:D:255:LEU:HD22	1.99	0.44
1:A:361:ALA:HB1	1:A:380:LEU:HD11	1.98	0.44
1:B:175:HIS:CD2	1:B:181:PRO:HA	2.52	0.44
1:A:277:ARG:N	1:A:317:ASP:OD1	2.50	0.44
1:B:43:GLU:HB2	1:B:342:ARG:HH22	1.81	0.44
1:E:63:LEU:CD1	1:E:129:VAL:HG22	2.48	0.44
1:B:29:GLU:C	1:B:30:LEU:HD12	2.43	0.44
1:B:213:LEU:HD12	1:B:383:ALA:HB2	1.99	0.43
1:D:20:PHE:CE2	1:D:65:GLY:HA2	2.53	0.43
1:D:76:LEU:C	1:D:76:LEU:HD13	2.43	0.43
1:A:37:ARG:HD3	1:A:186:ASP:OD1	2.18	0.43
1:A:70:ASP:OD1	1:A:72:LEU:HG	2.18	0.43
1:B:47:TYR:CE1	1:B:240:ARG:HG2	2.52	0.43
1:D:121:PRO:HD2	1:D:157:CYS:SG	2.57	0.43
1:B:54:PRO:HD2	1:B:199:LEU:O	2.18	0.43
1:A:329:VAL:O	1:A:330:GLU:C	2.61	0.43
1:B:205:SER:O	1:B:206:LEU:HB2	2.18	0.43
1:B:361:ALA:N	1:B:362:PRO:CD	2.82	0.43
1:A:93:PRO:HB3	1:A:115:GLN:HE22	1.84	0.43
1:B:78:THR:OG1	1:B:130:VAL:HG12	2.18	0.43
1:D:68:ARG:HG2	1:D:125:PHE:N	2.34	0.43
1:A:255:LEU:O	1:A:256:ARG:C	2.60	0.43
1:D:315:ARG:NH1	1:D:316:ASP:OD2	2.52	0.43
1:B:184:ILE:O	1:B:185:MET:C	2.61	0.43
1:D:33:SER:HA	1:D:61:THR:O	2.18	0.43
1:A:255:LEU:O	1:A:258:VAL:N	2.47	0.42
1:D:291:ALA:HB1	1:D:303:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ASP:CG	1:A:256:ARG:HH22	2.27	0.42
1:E:184:ILE:O	1:E:188:PHE:HB2	2.19	0.42
1:E:223:THR:O	1:E:351:CYS:HA	2.19	0.42
1:A:218:LEU:HD22	1:A:300:TYR:CZ	2.53	0.42
1:B:295:LEU:HD13	1:B:303:PHE:CD2	2.55	0.42
1:D:53:LEU:HD12	1:D:53:LEU:HA	1.88	0.42
1:A:43:GLU:HB2	1:A:342:ARG:NH2	2.34	0.42
1:E:163:ILE:HD13	1:E:166:ARG:HH11	1.83	0.42
1:A:246:VAL:O	1:A:250:LEU:HD13	2.20	0.42
1:A:184:ILE:HD12	1:A:184:ILE:C	2.43	0.42
1:B:63:LEU:CD1	1:B:129:VAL:HG22	2.50	0.42
1:D:109:TYR:CE1	1:D:142:SER:HB2	2.55	0.42
1:D:40:LEU:O	1:D:342:ARG:HD3	2.20	0.42
1:A:99:LEU:H	1:A:115:GLN:NE2	2.18	0.41
1:A:163:ILE:HG13	5:A:551:HOH:O	2.19	0.41
1:B:76:LEU:O	1:B:128:VAL:HA	2.20	0.41
1:E:199:LEU:HD23	1:E:201:ILE:HD11	2.01	0.41
1:D:70:ASP:OD1	1:D:70:ASP:C	2.63	0.41
1:D:202:ASP:O	1:D:206:LEU:HA	2.20	0.41
1:A:232:ALA:HA	1:A:348:PHE:CD2	2.54	0.41
1:B:23:GLU:CD	1:B:87:ARG:HH22	2.23	0.41
1:A:174:GLU:HG2	1:A:182:CYS:SG	2.61	0.41
1:A:361:ALA:N	1:A:362:PRO:CD	2.83	0.41
1:B:116:TYR:CE2	1:B:172:GLN:HG2	2.56	0.41
1:D:380:LEU:HD23	1:D:380:LEU:HA	1.88	0.41
1:B:63:LEU:HD11	1:B:129:VAL:HG22	2.02	0.41
1:E:73:VAL:O	1:E:89:GLN:HA	2.20	0.41
1:D:287:ARG:HD3	1:D:309:GLU:HB3	2.03	0.41
1:D:33:SER:O	1:D:387:ALA:HA	2.21	0.41
1:A:282:VAL:O	1:A:283:GLY:C	2.64	0.41
1:A:287:ARG:O	1:A:291:ALA:HB2	2.21	0.41
1:B:104:PRO:HB2	1:B:106:TRP:CD1	2.55	0.41
1:E:33:SER:O	1:E:387:ALA:HA	2.21	0.40
1:A:43:GLU:HB2	1:A:342:ARG:HH22	1.87	0.40
1:A:73:VAL:O	1:A:89:GLN:HA	2.20	0.40
1:B:220:VAL:CG1	1:B:353:VAL:HG23	2.52	0.40
1:E:219:ALA:O	1:E:356:LEU:HD23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	384/399 (96%)	354 (92%)	26 (7%)	4 (1%)	12	15
1	B	383/399 (96%)	368 (96%)	13 (3%)	2 (0%)	24	31
1	D	366/399 (92%)	339 (93%)	25 (7%)	2 (0%)	24	31
1	E	389/399 (98%)	381 (98%)	8 (2%)	0	100	100
All	All	1522/1596 (95%)	1442 (95%)	72 (5%)	8 (0%)	24	31

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	103	THR
1	A	254	SER
1	A	283	GLY
1	B	115	GLN
1	A	232	ALA
1	B	91	PRO
1	D	120	ALA
1	A	215	ASP

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	247/315 (78%)	236 (96%)	11 (4%)	24	37
1	B	262/315 (83%)	257 (98%)	5 (2%)	50	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	241/315 (76%)	235 (98%)	6 (2%)	42 60
1	E	286/315 (91%)	280 (98%)	6 (2%)	47 66
All	All	1036/1260 (82%)	1008 (97%)	28 (3%)	39 58

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	30	LEU
1	A	37	ARG
1	A	72	LEU
1	A	209	SER
1	A	258	VAL
1	A	260	LEU
1	A	282	VAL
1	A	329	VAL
1	A	338	VAL
1	A	341	SER
1	B	63	LEU
1	B	126	SER
1	B	227	VAL
1	B	259	GLN
1	B	295	LEU
1	E	151	THR
1	E	184	ILE
1	E	192	MET
1	E	264	GLU
1	E	282	VAL
1	E	355	LEU
1	D	27	GLU
1	D	30	LEU
1	D	75	LEU
1	D	76	LEU
1	D	77	THR
1	D	255	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN

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Mol	Chain	Res	Type
1	A	115	GLN
1	A	172	GLN
1	A	311	HIS
1	B	49	GLN
1	B	86	GLN
1	B	115	GLN
1	E	226	ASN
1	E	327	GLN
1	E	367	HIS
1	D	194	GLN
1	D	226	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
3	HFK	B	402	-	29,30,30	2.81	8 (27%)	32,44,44	1.96	8 (25%)
3	HFK	A	402	-	29,30,30	2.70	8 (27%)	32,44,44	1.70	10 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	QKZ	D	401	-	18,18,18	1.48	1 (5%)	23,23,23	1.08	1 (4%)
2	GAL	A	401	-	12,12,12	0.61	0	17,17,17	2.19	5 (29%)
2	GAL	E	401	-	12,12,12	1.06	0	17,17,17	2.78	6 (35%)
2	GAL	B	401	-	12,12,12	1.07	1 (8%)	17,17,17	1.71	5 (29%)
3	HFK	E	402	-	29,30,30	2.26	9 (31%)	32,44,44	2.04	11 (34%)

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	HFK	B	402	-	-	2/4/43/43	0/5/5/5
3	HFK	A	402	-	-	2/4/43/43	0/5/5/5
4	QKZ	D	401	-	-	0/8/8/8	0/2/2/2
2	GAL	A	401	-	-	2/2/22/22	0/1/1/1
2	GAL	E	401	-	-	2/2/22/22	0/1/1/1
2	GAL	B	401	-	-	1/2/22/22	0/1/1/1
3	HFK	E	402	-	-	2/4/43/43	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	HFK	C06-C07	10.34	1.50	1.37
3	A	402	HFK	C06-C07	10.29	1.50	1.37
3	E	402	HFK	C06-C07	6.62	1.45	1.37
3	A	402	HFK	C15-N14	5.76	1.45	1.30
3	B	402	HFK	C15-N14	5.51	1.44	1.30
3	E	402	HFK	C15-N14	5.39	1.44	1.30
4	D	401	QKZ	C6-N2	4.41	1.40	1.34
3	E	402	HFK	C15-N16	4.07	1.43	1.36
3	B	402	HFK	C05-C06	3.79	1.55	1.49
3	B	402	HFK	C15-N16	3.74	1.42	1.36
3	A	402	HFK	C18-N19	3.59	1.36	1.30
3	A	402	HFK	C18-N17	3.48	1.43	1.36
3	B	402	HFK	C15-N17	3.44	1.45	1.37
3	B	402	HFK	C18-N19	3.24	1.35	1.30
3	E	402	HFK	C05-C06	3.19	1.55	1.49
3	B	402	HFK	O22-C21	3.16	1.43	1.38
3	B	402	HFK	C18-N17	3.15	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	HFK	C15-N17	3.14	1.44	1.37
3	E	402	HFK	C20-N19	-2.81	1.34	1.39
3	E	402	HFK	C15-N17	2.66	1.43	1.37
3	E	402	HFK	C08-N14	2.54	1.49	1.46
3	A	402	HFK	C26-C20	2.52	1.43	1.40
3	A	402	HFK	C05-C06	2.42	1.53	1.49
3	E	402	HFK	C18-N17	2.36	1.41	1.36
3	A	402	HFK	C15-N16	2.28	1.40	1.36
2	B	401	GAL	C4-C3	2.11	1.57	1.52
3	E	402	HFK	C06-N16	2.02	1.40	1.37

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	GAL	C1-O5-C5	-7.17	99.78	113.65
2	E	401	GAL	C1-C2-C3	-5.79	98.54	110.36
3	B	402	HFK	C07-C06-N16	-5.75	117.47	122.11
2	A	401	GAL	C1-O5-C5	-5.74	102.55	113.65
3	E	402	HFK	C07-C06-N16	-5.21	117.90	122.11
2	A	401	GAL	C1-C2-C3	-4.60	100.96	110.36
3	B	402	HFK	C23-C21-C20	-4.12	118.61	123.62
3	E	402	HFK	C09-C10-C11	3.85	117.35	111.35
3	B	402	HFK	O22-C21-C23	3.78	134.45	126.49
2	E	401	GAL	O1-C1-C2	3.74	119.84	108.98
3	E	402	HFK	C23-C21-C20	-3.48	119.39	123.62
3	A	402	HFK	C02-C07-C06	-3.44	116.13	119.18
2	B	401	GAL	C1-C2-C3	-3.41	103.39	110.36
3	E	402	HFK	C05-C06-N16	3.39	120.28	115.46
3	E	402	HFK	N17-C15-N14	3.29	124.10	117.96
2	E	401	GAL	C3-C4-C5	3.23	116.09	110.23
3	B	402	HFK	O22-C18-N19	-3.13	109.94	115.57
3	E	402	HFK	O22-C21-C23	3.00	132.79	126.49
3	E	402	HFK	C13-C12-C11	2.91	115.89	111.35
3	A	402	HFK	O22-C18-N19	-2.79	110.55	115.57
2	B	401	GAL	O5-C5-C6	2.75	113.25	106.44
3	A	402	HFK	C04-C03-C02	-2.71	108.37	113.57
2	A	401	GAL	O1-C1-C2	2.70	116.80	108.98
3	A	402	HFK	O22-C21-C23	2.65	132.06	126.49
3	E	402	HFK	O22-C18-N19	-2.59	110.92	115.57
3	A	402	HFK	C13-C12-C11	2.59	115.38	111.35
3	E	402	HFK	N17-C15-N16	-2.58	113.63	117.96
3	A	402	HFK	N17-C15-N14	2.56	122.74	117.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	GAL	C1-O5-C5	-2.56	108.70	113.65
2	B	401	GAL	O2-C2-C1	2.54	115.12	109.25
3	B	402	HFK	C08-C07-C06	-2.48	118.95	121.75
3	A	402	HFK	C09-C10-C11	2.42	115.12	111.35
4	D	401	QKZ	C2-C1-C	-2.40	116.82	119.24
2	A	401	GAL	O5-C1-C2	-2.38	106.11	110.30
2	E	401	GAL	O6-C6-C5	-2.37	103.28	111.33
3	A	402	HFK	C07-C06-N16	-2.35	120.22	122.11
3	B	402	HFK	N17-C18-N19	-2.26	122.16	128.58
3	E	402	HFK	N17-C18-N19	-2.24	122.21	128.58
3	B	402	HFK	C02-C07-C06	-2.24	117.19	119.18
2	E	401	GAL	O1-C1-O5	-2.20	103.87	110.41
3	B	402	HFK	C05-C06-N16	2.15	118.52	115.46
3	E	402	HFK	C20-N19-C18	2.14	108.36	104.13
3	A	402	HFK	C08-C07-C06	-2.12	119.35	121.75
2	A	401	GAL	O5-C5-C6	2.11	111.68	106.44
2	B	401	GAL	O6-C6-C5	-2.10	104.19	111.33
3	A	402	HFK	C23-C21-C20	-2.03	121.15	123.62

There are no chirality outliers.

All (11) torsion outliers are listed below:

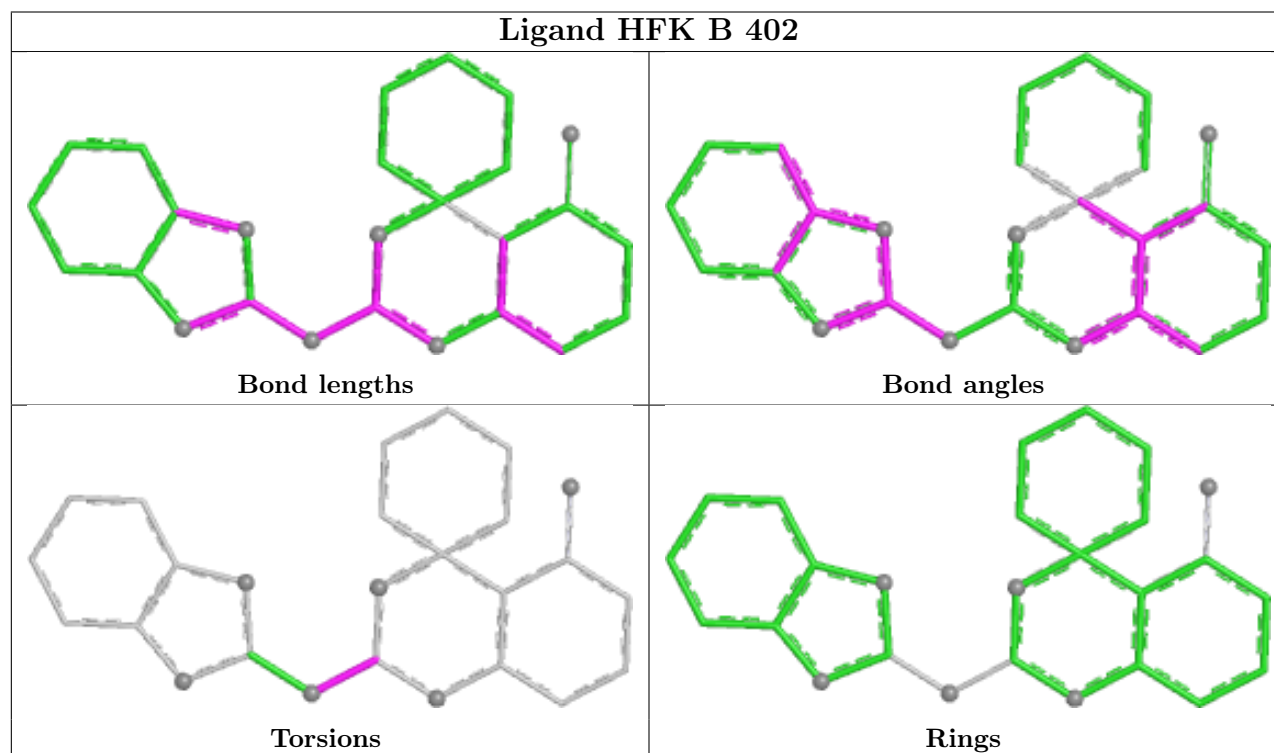
Mol	Chain	Res	Type	Atoms
2	E	401	GAL	O5-C5-C6-O6
2	A	401	GAL	O5-C5-C6-O6
2	A	401	GAL	C4-C5-C6-O6
2	B	401	GAL	O5-C5-C6-O6
2	E	401	GAL	C4-C5-C6-O6
3	A	402	HFK	N14-C15-N17-C18
3	A	402	HFK	N16-C15-N17-C18
3	B	402	HFK	N16-C15-N17-C18
3	E	402	HFK	N16-C15-N17-C18
3	B	402	HFK	N14-C15-N17-C18
3	E	402	HFK	N14-C15-N17-C18

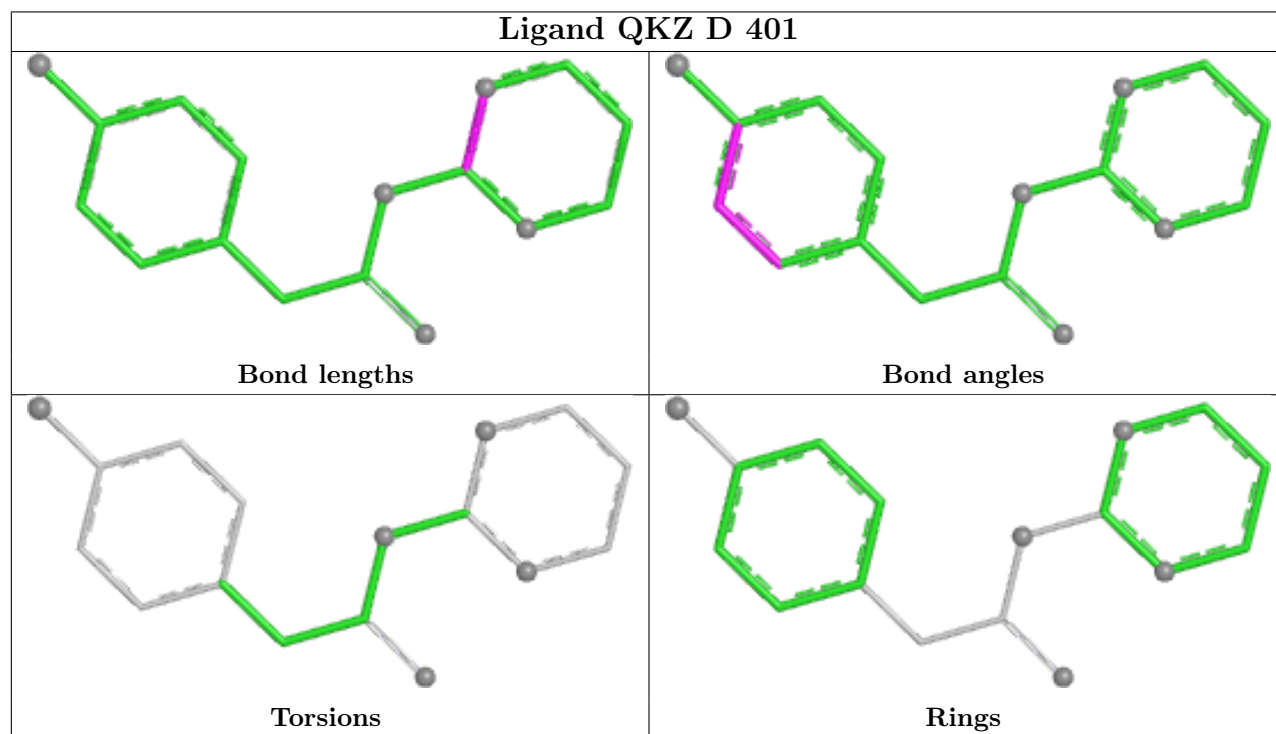
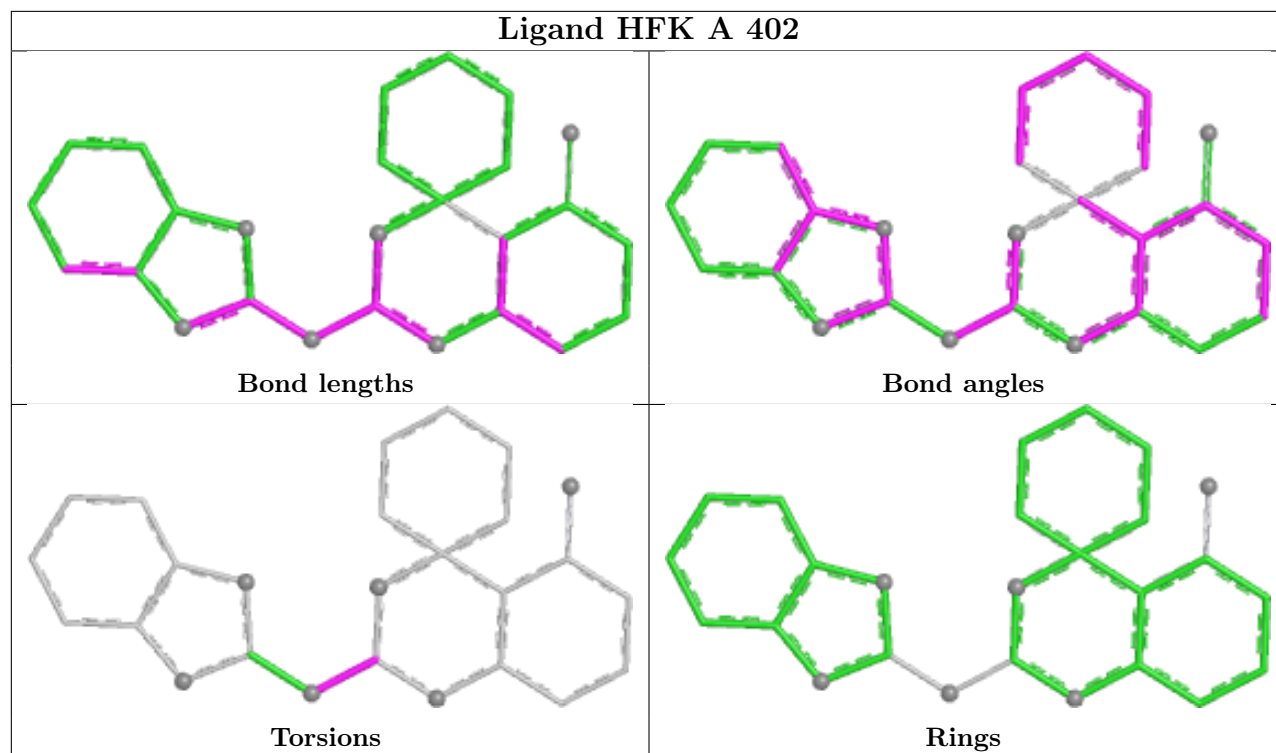
There are no ring outliers.

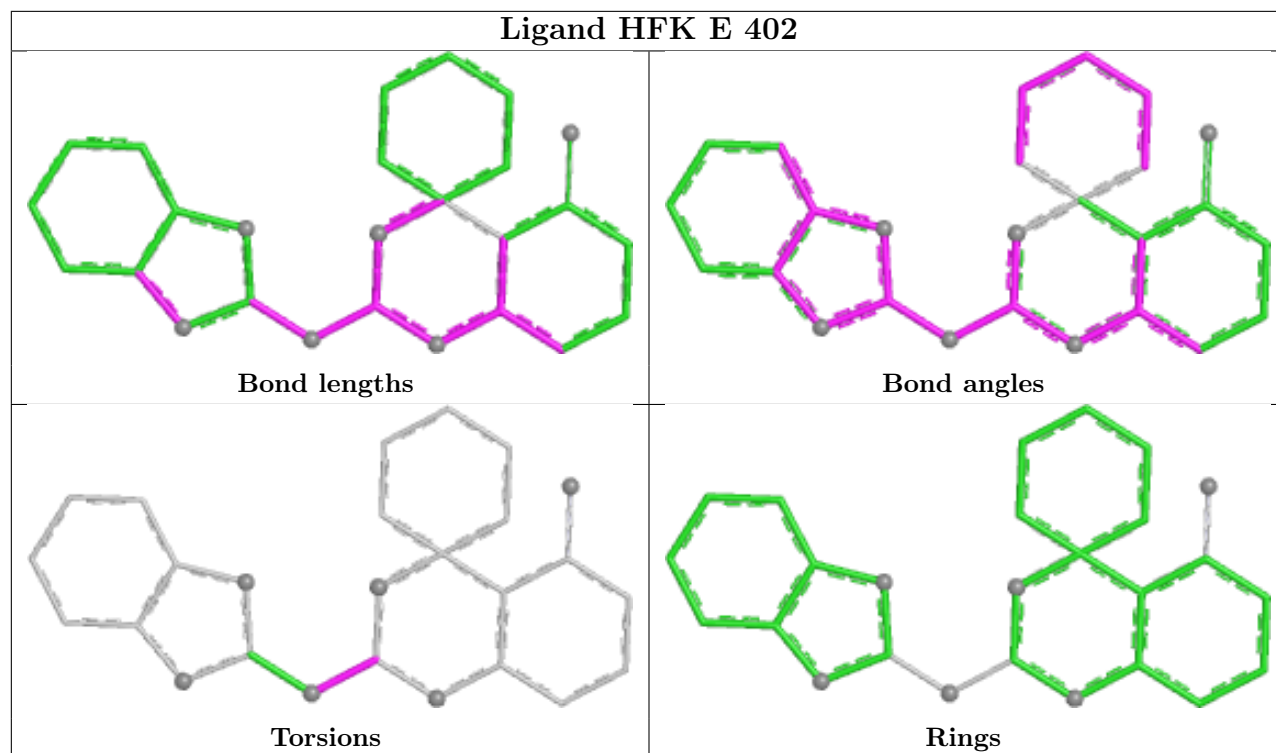
No monomer is involved in short contacts.

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, 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	388/399 (97%)	0.72	57 (14%) 6 6	26, 52, 101, 138	0
1	B	387/399 (96%)	0.58	35 (9%) 15 16	28, 51, 89, 106	0
1	D	372/399 (93%)	0.73	53 (14%) 6 7	25, 53, 101, 138	0
1	E	391/399 (97%)	-0.04	6 (1%) 72 73	24, 39, 63, 76	0
All	All	1538/1596 (96%)	0.49	151 (9%) 13 14	24, 48, 95, 138	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	252	ALA	6.8
1	A	2	ALA	6.3
1	B	94	THR	6.0
1	D	106	TRP	5.7
1	A	233	SER	5.5
1	B	2	ALA	5.4
1	A	370	GLU	5.0
1	B	232	ALA	5.0
1	A	275	PHE	4.8
1	B	99	LEU	4.7
1	A	269	LEU	4.6
1	A	270	VAL	4.4
1	D	120	ALA	4.4
1	B	230	SER	4.4
1	A	334	ALA	4.4
1	B	233	SER	4.4
1	A	283	GLY	4.4
1	B	231	LEU	4.2
1	A	268	ASP	4.2
1	D	121	PRO	4.2
1	A	259	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	261	GLU	4.0
1	D	163	ILE	3.9
1	B	92	LEU	3.8
1	B	6	GLN	3.8
1	D	251	GLY	3.8
1	B	103	THR	3.7
1	D	103	THR	3.7
1	A	263	LEU	3.7
1	D	99	LEU	3.7
1	D	8	GLN	3.6
1	A	230	SER	3.6
1	A	273	GLU	3.6
1	A	359	SER	3.5
1	D	9	VAL	3.5
1	E	2	ALA	3.5
1	D	184	ILE	3.5
1	D	78	THR	3.5
1	D	119	ALA	3.5
1	A	249	ALA	3.4
1	B	228	ARG	3.4
1	A	260	LEU	3.3
1	A	232	ALA	3.3
1	D	253	ALA	3.3
1	D	87	ARG	3.3
1	B	214	SER	3.3
1	D	214	SER	3.3
1	A	339	TYR	3.3
1	A	333	LEU	3.2
1	D	268	ASP	3.2
1	D	185	MET	3.2
1	A	363	HIS	3.1
1	A	253	ALA	3.1
1	D	10	ALA	3.1
1	D	165	ALA	3.1
1	D	105	ARG	3.0
1	D	64	VAL	3.0
1	D	104	PRO	3.0
1	B	249	ALA	3.0
1	A	282	VAL	3.0
1	A	301	ARG	2.9
1	D	269	LEU	2.9
1	D	89	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	8	GLN	2.9
1	E	80	GLU	2.9
1	D	271	SER	2.8
1	A	265	ALA	2.8
1	A	229	HIS	2.8
1	D	93	PRO	2.8
1	D	161	GLY	2.8
1	B	100	GLU	2.8
1	A	231	LEU	2.7
1	A	372	TYR	2.7
1	B	91	PRO	2.7
1	B	259	GLN	2.7
1	D	92	LEU	2.7
1	A	3	ALA	2.6
1	D	76	LEU	2.6
1	A	360	ALA	2.6
1	B	90	PHE	2.6
1	D	96	GLN	2.6
1	D	86	GLN	2.5
1	D	172	GLN	2.5
1	B	72	LEU	2.5
1	A	214	SER	2.5
1	A	4	LEU	2.5
1	D	26	ALA	2.5
1	B	177	PHE	2.5
1	A	246	VAL	2.5
1	D	177	PHE	2.4
1	B	89	GLN	2.4
1	B	238	VAL	2.4
1	B	69	LYS	2.4
1	A	365	MET	2.4
1	B	88	LEU	2.4
1	E	268	ASP	2.4
1	A	252	ALA	2.4
1	E	4	LEU	2.4
1	D	159	ASP	2.4
1	A	266	ALA	2.4
1	D	160	SER	2.4
1	A	250	LEU	2.4
1	D	373	GLY	2.3
1	D	176	SER	2.3
1	A	267	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	331	ALA	2.3
1	B	180	MET	2.3
1	D	18	ARG	2.3
1	A	242	GLN	2.3
1	A	274	GLY	2.3
1	A	364	ALA	2.3
1	A	258	VAL	2.3
1	B	250	LEU	2.3
1	A	271	SER	2.3
1	A	251	GLY	2.2
1	A	277	ARG	2.2
1	A	366	ARG	2.2
1	B	265	ALA	2.2
1	D	95	ALA	2.2
1	B	126	SER	2.2
1	D	206	LEU	2.2
1	B	7	PRO	2.2
1	A	245	GLU	2.2
1	A	355	LEU	2.2
1	D	12	LEU	2.2
1	A	330	GLU	2.2
1	D	69	LYS	2.2
1	A	302	ALA	2.2
1	B	70	ASP	2.1
1	D	192	MET	2.1
1	A	304	GLY	2.1
1	A	332	ALA	2.1
1	B	234	SER	2.1
1	B	184	ILE	2.1
1	D	272	LYS	2.1
1	A	371	HIS	2.1
1	A	217	LYS	2.1
1	A	357	GLU	2.1
1	D	130	VAL	2.1
1	B	348	PHE	2.1
1	A	228	ARG	2.1
1	D	162	THR	2.1
1	E	3	ALA	2.1
1	E	96	GLN	2.1
1	D	94	THR	2.0
1	B	235	GLU	2.0
1	B	244	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	98	SER	2.0
1	D	205	SER	2.0
1	D	88	LEU	2.0
1	D	189	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

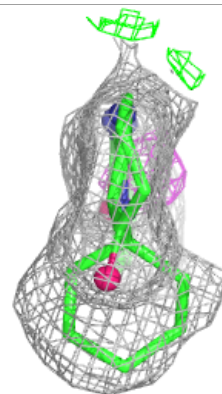
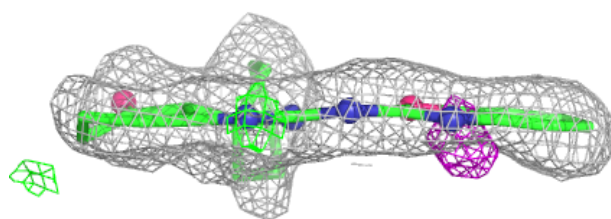
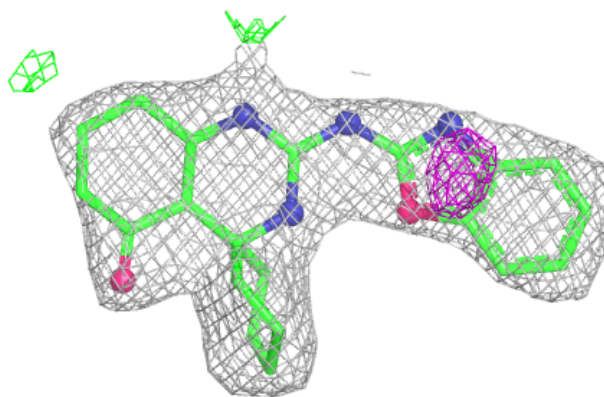
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HFK	B	402	26/26	0.86	0.16	59,64,71,72	0
2	GAL	B	401	12/12	0.89	0.11	37,46,49,54	0
4	QKZ	D	401	17/17	0.91	0.12	42,48,69,70	0
3	HFK	A	402	26/26	0.93	0.10	46,57,63,65	0
3	HFK	E	402	26/26	0.94	0.08	36,40,46,48	0
2	GAL	A	401	12/12	0.95	0.06	37,42,46,46	0
2	GAL	E	401	12/12	0.96	0.06	23,27,32,39	0

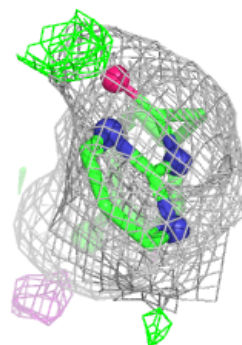
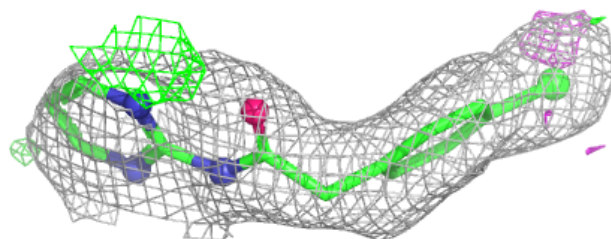
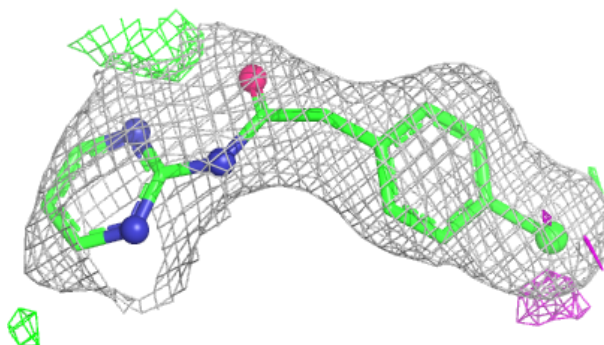
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

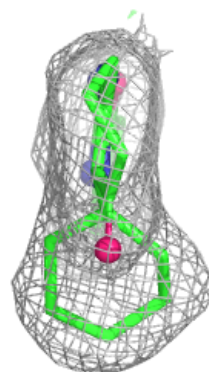
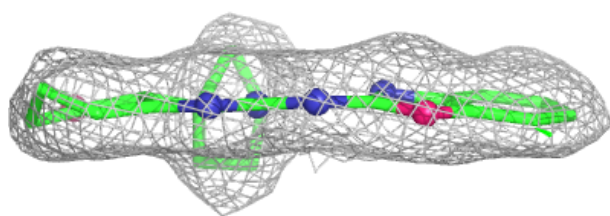
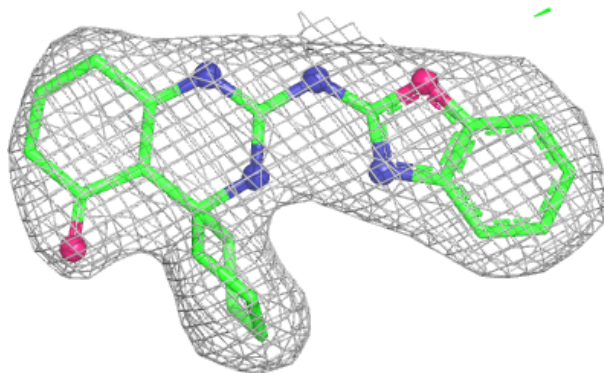
**Electron density around QKZ D 401:**

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

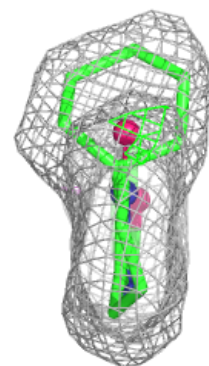
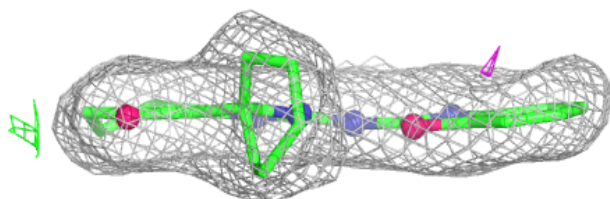
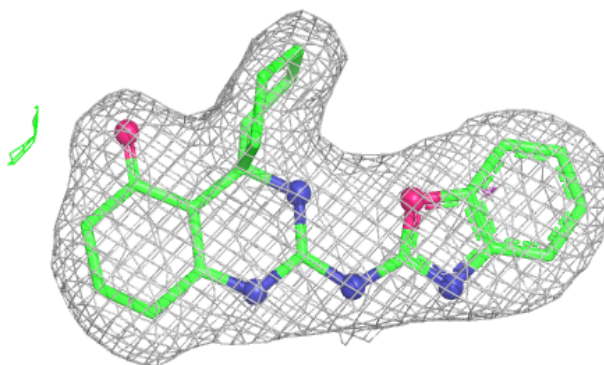


Electron density around HFK A 402:

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

**Electron density around HFK E 402:**

$2mF_o - DF_c$ (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.