



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:47 AM UTC

PDB ID : 6ZGY / pdb_00006zgy
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:

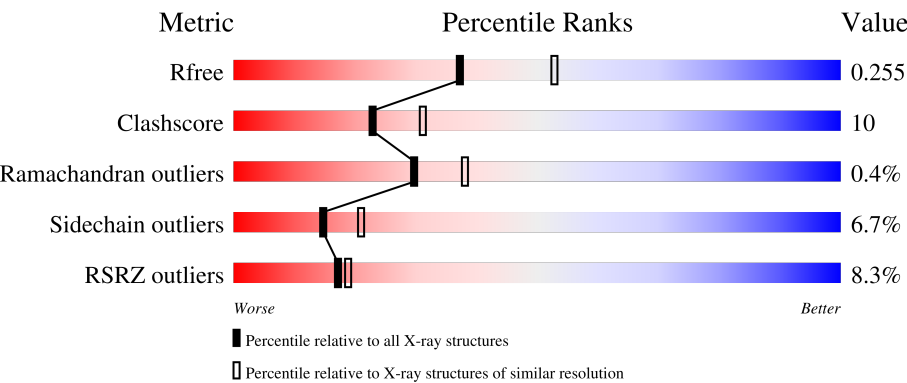
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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	12% 74% 19% • •
1	B	399	6% 75% 19% • •
1	D	399	14% 65% 23% • 8%
1	E	399	% 82% 14% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	QL5	A	403	-	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11641 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	1	0
			2799	1761	494	527	17			
1	B	391	Total	C	N	O	S	0	0	0
			2834	1775	505	538	16			
1	E	391	Total	C	N	O	S	0	2	0
			2865	1797	509	543	16			
1	D	369	Total	C	N	O	S	0	0	0
			2549	1597	447	492	13			

There are 40 discrepancies between the modelled and reference sequences:

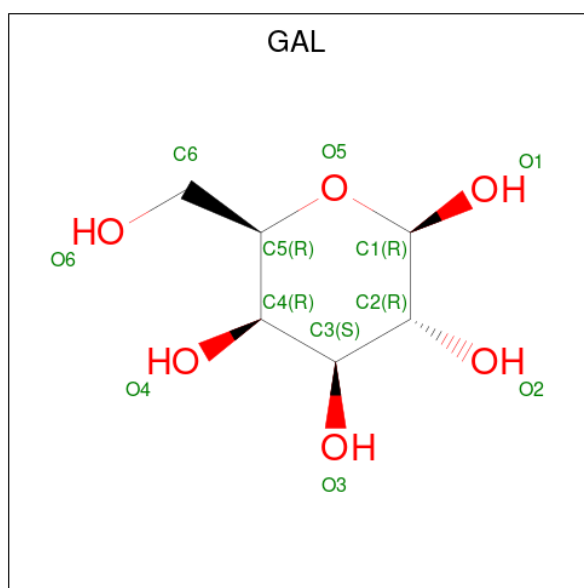
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP P51570
A	-5	ALA	-	expression tag	UNP P51570
A	-4	HIS	-	expression tag	UNP P51570
A	-3	HIS	-	expression tag	UNP P51570
A	-2	HIS	-	expression tag	UNP P51570
A	-1	HIS	-	expression tag	UNP P51570
A	0	HIS	-	expression tag	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

Continued on next page...

Continued from previous page...

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).



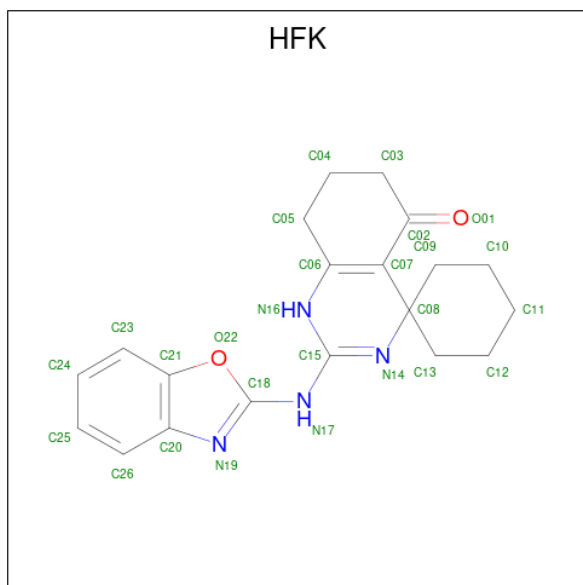
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

Continued on next page...

Continued from previous page...

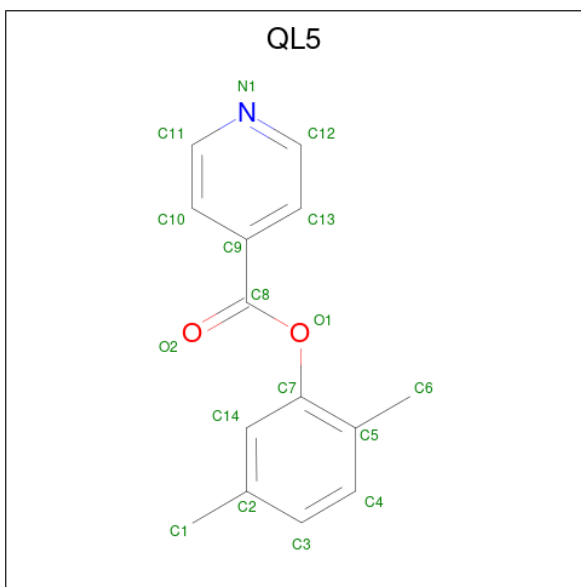
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			12	6	6		

- 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 (2,5-dimethylphenyl) pyridine-4-carboxylate (CCD ID: QL5) (formula: $C_{14}H_{13}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	14	1	2		
4	B	1	Total	C	N	O	0	0
			17	14	1	2		

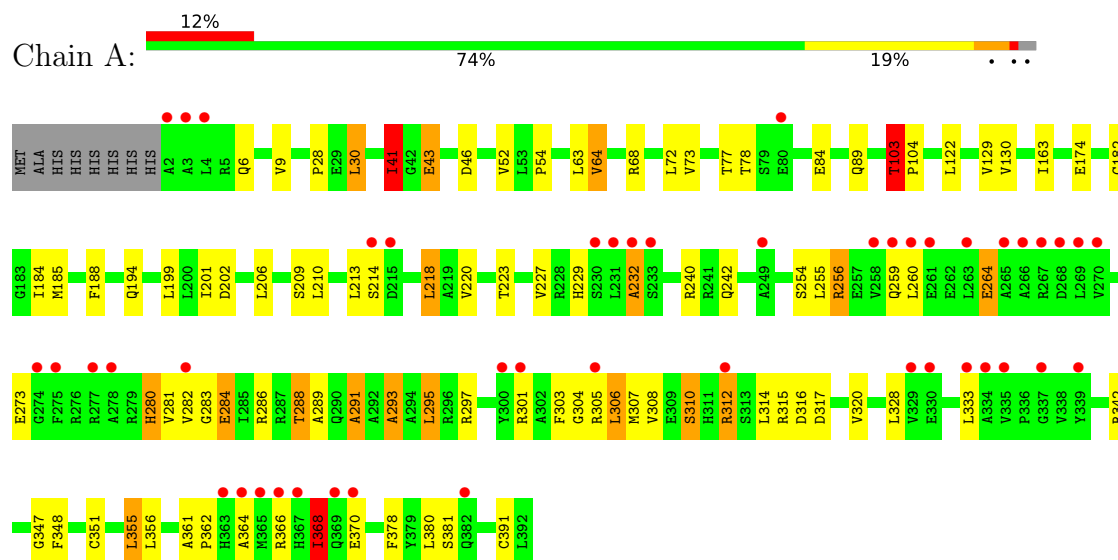
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	102	Total	O	0	0
			102	102		
5	B	100	Total	O	0	0
			100	100		
5	E	163	Total	O	0	0
			163	163		
5	D	81	Total	O	0	0
			81	81		

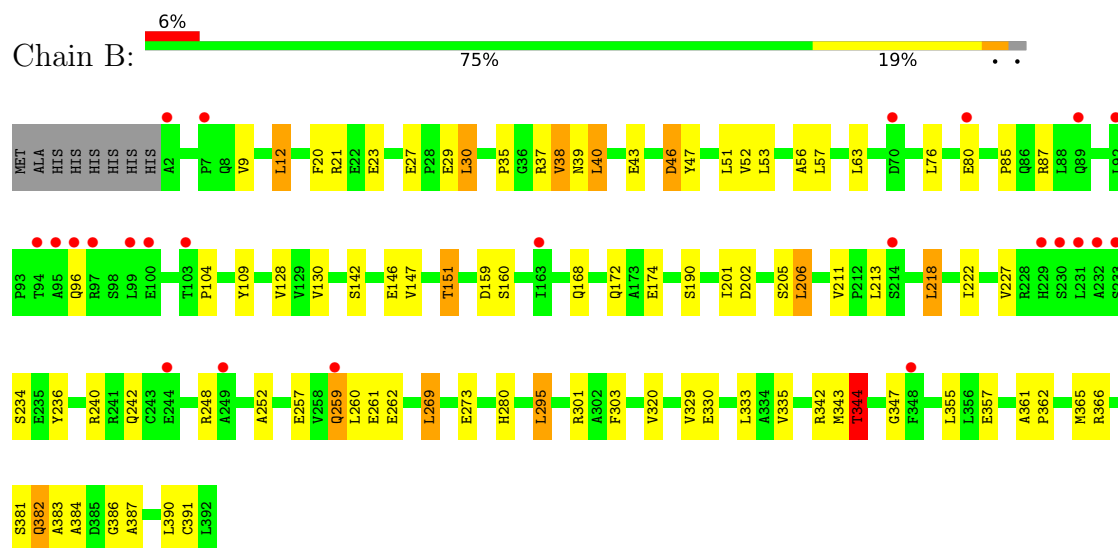
3 Residue-property plots

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.

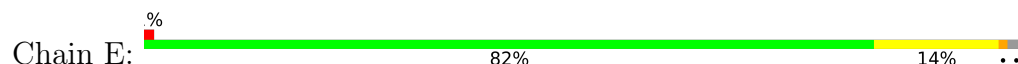
• Molecule 1: Galactokinase



• Molecule 1: Galactokinase

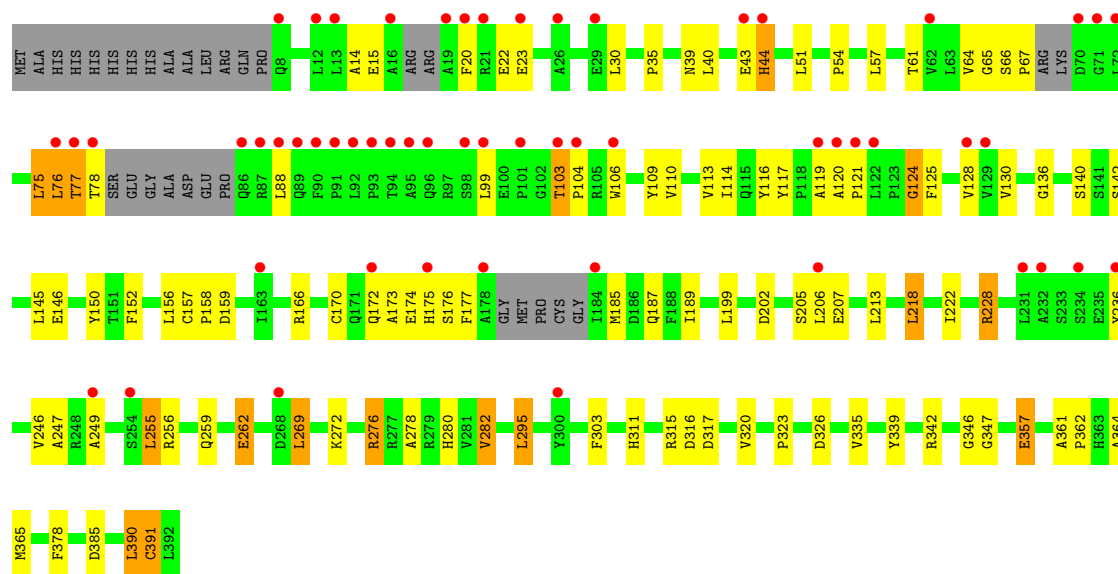


• Molecule 1: Galactokinase





● 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	73.31Å 114.63Å 120.82Å 90.00° 100.60° 90.00°	Depositor
Resolution (Å)	118.76 – 2.30 118.76 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (118.76-2.30) 99.6 (118.76-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.206 , 0.254 0.210 , 0.255	Depositor DCC
R_{free} test set	7384 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11641	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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, QL5

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	1.34	10/2855 (0.4%)	1.62	29/3895 (0.7%)
1	B	1.21	5/2888 (0.2%)	1.57	12/3934 (0.3%)
1	D	1.24	5/2588 (0.2%)	1.60	7/3533 (0.2%)
1	E	1.17	1/2925 (0.0%)	1.53	13/3981 (0.3%)
All	All	1.24	21/11256 (0.2%)	1.58	61/15343 (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	1
1	D	0	1
All	All	0	2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	306	LEU	C-O	16.84	1.43	1.24
1	A	301	ARG	C-O	10.33	1.36	1.24
1	D	124	GLY	C-O	9.49	1.36	1.23
1	A	312	ARG	C-O	8.38	1.33	1.24
1	B	23	GLU	CG-CD	8.29	1.72	1.52
1	A	310	SER	C-O	7.73	1.33	1.24
1	A	305	ARG	C-O	7.39	1.33	1.24
1	B	23	GLU	CD-OE2	7.17	1.39	1.25
1	D	125	PHE	C-O	6.50	1.32	1.24
1	D	66	SER	C-O	6.41	1.30	1.24
1	E	67	PRO	C-O	-6.34	1.16	1.23
1	D	249	ALA	C-O	6.19	1.31	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	295	LEU	C-O	6.10	1.31	1.24
1	D	44	HIS	CE1-NE2	6.05	1.38	1.32
1	A	288	THR	C-O	5.78	1.30	1.24
1	B	343	MET	C-O	5.70	1.30	1.23
1	A	286	ARG	C-O	5.62	1.30	1.24
1	A	293	ALA	C-O	5.17	1.30	1.24
1	A	291	ALA	C-O	5.10	1.30	1.24
1	B	87	ARG	CZ-NH1	5.02	1.39	1.32
1	B	335	VAL	N-CA	5.02	1.50	1.46

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	280	HIS	CA-CB-CG	-9.07	104.73	113.80
1	B	87	ARG	CG-CD-NE	-8.77	92.71	112.00
1	E	391	CYS	CB-CA-C	8.39	123.79	110.19
1	D	391	CYS	CB-CA-C	8.37	123.55	109.48
1	A	282	VAL	O-C-N	8.27	129.89	121.87
1	A	306	LEU	O-C-N	8.12	130.73	122.12
1	A	310	SER	CA-C-O	-7.96	112.11	120.55
1	B	23	GLU	CB-CG-CD	7.82	125.89	112.60
1	A	310	SER	O-C-N	7.75	130.34	122.12
1	B	344	THR	CB-CA-C	-7.61	94.90	109.66
1	A	46	ASP	CA-CB-CG	7.35	119.95	112.60
1	E	344	THR	CB-CA-C	-7.33	95.43	109.66
1	B	46	ASP	CA-CB-CG	7.33	119.93	112.60
1	A	240	ARG	CG-CD-NE	-7.20	96.16	112.00
1	A	103	THR	CB-CA-C	6.86	117.57	109.47
1	E	41	ILE	CA-C-O	-6.43	116.35	120.66
1	E	84	GLU	CB-CG-CD	6.26	123.25	112.60
1	A	366	ARG	CA-C-N	6.21	129.07	120.63
1	A	366	ARG	C-N-CA	6.21	129.07	120.63
1	A	84	GLU	CB-CA-C	6.19	117.78	108.86
1	E	46	ASP	CA-CB-CG	6.15	118.75	112.60
1	D	259	GLN	CB-CA-C	6.14	119.91	109.53
1	A	312	ARG	O-C-N	6.10	128.59	122.12
1	E	123	PRO	CA-C-N	6.07	127.06	120.44
1	E	123	PRO	C-N-CA	6.07	127.06	120.44
1	E	67	PRO	CA-C-O	-5.93	114.44	121.67
1	A	366	ARG	N-CA-C	-5.84	104.60	110.97
1	E	391	CYS	CA-CB-SG	-5.79	101.08	114.40
1	D	158	PRO	N-CA-C	5.72	119.84	111.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	13	LEU	CA-C-N	5.67	127.81	120.44
1	E	13	LEU	C-N-CA	5.67	127.81	120.44
1	D	280	HIS	CA-CB-CG	-5.64	108.16	113.80
1	A	306	LEU	CA-C-O	-5.63	114.58	120.55
1	A	368	ILE	CA-C-O	-5.55	115.63	121.41
1	B	344	THR	N-CA-CB	5.55	120.19	111.20
1	A	283	GLY	CA-C-O	-5.47	115.09	121.00
1	D	391	CYS	CA-CB-SG	-5.45	101.86	114.40
1	B	330	GLU	CB-CG-CD	5.44	121.85	112.60
1	D	262	GLU	N-CA-C	-5.32	105.38	111.07
1	E	301	ARG	N-CA-C	-5.26	105.46	111.14
1	A	306	LEU	N-CA-C	-5.22	105.59	111.28
1	A	46	ASP	CB-CA-C	5.21	119.07	110.88
1	A	301	ARG	O-C-N	5.21	129.00	122.23
1	A	284	GLU	O-C-N	5.21	127.43	122.07
1	A	281	VAL	N-CA-C	-5.18	105.27	110.30
1	E	347	GLY	CA-C-O	-5.17	117.13	122.25
1	A	280	HIS	N-CA-C	-5.15	105.35	110.97
1	A	240	ARG	CB-CA-C	5.13	118.94	110.88
1	A	283	GLY	O-C-N	5.13	127.11	122.18
1	A	256	ARG	CA-C-N	5.12	128.79	120.60
1	A	256	ARG	C-N-CA	5.12	128.79	120.60
1	B	303	PHE	CA-C-N	5.11	125.61	119.94
1	B	303	PHE	C-N-CA	5.11	125.61	119.94
1	B	172	GLN	N-CA-C	-5.11	105.72	111.28
1	A	41	ILE	CB-CA-C	-5.09	106.96	111.74
1	A	77	THR	CA-CB-OG1	-5.07	102.00	109.60
1	D	99	LEU	CA-C-O	-5.03	116.73	122.01
1	A	229	HIS	CA-C-N	5.02	127.32	120.54
1	A	229	HIS	C-N-CA	5.02	127.32	120.54
1	B	248	ARG	CA-C-N	5.00	127.49	120.28
1	B	248	ARG	C-N-CA	5.00	127.49	120.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	SER	Peptide
1	D	124	GLY	Mainchain

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	2799	0	2695	67	0
1	B	2834	0	2730	57	0
1	D	2549	0	2370	73	0
1	E	2865	0	2803	35	0
2	A	12	0	12	1	0
2	B	12	0	12	1	0
2	E	12	0	11	0	0
3	A	26	0	0	0	0
3	B	26	0	0	0	0
3	E	26	0	0	0	0
4	A	17	0	0	12	0
4	B	17	0	0	3	0
5	A	102	0	0	0	0
5	B	100	0	0	2	0
5	D	81	0	0	4	0
5	E	163	0	0	2	0
All	All	11641	0	10633	226	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 10.

All (226) 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:39:ASN:HB2	5:D:422:HOH:O	1.63	0.99
1:A:218:LEU:HD11	4:A:403:QL5:O1	1.68	0.94
1:D:276:ARG:NH1	1:D:317:ASP:OD1	2.02	0.93
1:D:39:ASN:ND2	1:D:43:GLU:CB	2.32	0.92
1:A:259:GLN:CB	1:D:272:LYS:HE2	2.03	0.88
1:D:236:TYR:OH	1:D:346:GLY:O	1.95	0.84
1:B:259:GLN:HE21	1:B:262:GLU:H	1.26	0.82
1:D:103:THR:CB	1:D:104:PRO:HD2	2.15	0.76
1:D:103:THR:CB	1:D:104:PRO:CD	2.63	0.75
1:A:218:LEU:CD1	4:A:403:QL5:O1	2.35	0.74
1:D:136:GLY:O	1:D:228:ARG:NH1	2.22	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:SER:O	1:D:146:GLU:HG3	1.90	0.71
1:D:57:LEU:HD21	1:D:222:ILE:HD11	1.74	0.70
1:A:54:PRO:HD2	1:A:199:LEU:O	1.92	0.69
1:D:202:ASP:O	1:D:205:SER:O	2.11	0.68
1:E:39:ASN:O	1:E:344:THR:HG23	1.94	0.68
1:D:295:LEU:HD13	1:D:303:PHE:CD2	2.29	0.67
1:D:365:MET:HE2	1:D:378:PHE:HB2	1.76	0.67
1:D:276:ARG:HG2	1:D:276:ARG:HH11	1.59	0.66
1:B:259:GLN:NE2	1:B:261:GLU:HB2	2.11	0.64
1:A:72:LEU:C	1:A:72:LEU:HD12	2.22	0.64
1:E:172:GLN:NE2	1:E:176:SER:OG	2.30	0.63
1:E:218:LEU:HD11	1:E:355:LEU:HG	1.80	0.63
1:A:293:ALA:O	1:A:297:ARG:HG3	1.98	0.63
1:A:218:LEU:HD11	4:A:403:QL5:C8	2.29	0.63
1:B:39:ASN:O	1:B:344:THR:CG2	2.47	0.62
1:E:257:GLU:HG3	5:E:609:HOH:O	1.99	0.62
1:A:259:GLN:CB	1:D:272:LYS:CE	2.77	0.62
1:B:355:LEU:HD11	4:B:403:QL5:C14	2.29	0.62
1:B:160:SER:O	1:B:160:SER:OG	2.13	0.62
1:B:259:GLN:HE22	1:B:261:GLU:HB2	1.65	0.62
1:A:218:LEU:HD13	1:A:355:LEU:HD11	1.82	0.61
1:A:356:LEU:HD11	1:A:361:ALA:HA	1.83	0.61
1:B:151:THR:HG21	1:B:387:ALA:HB1	1.83	0.60
1:D:39:ASN:HD22	1:D:43:GLU:CB	2.14	0.60
1:A:289:ALA:HB1	1:D:269:LEU:HD22	1.83	0.60
1:D:54:PRO:HD2	1:D:199:LEU:O	2.01	0.60
1:D:76:LEU:C	1:D:76:LEU:HD23	2.27	0.60
1:A:304:GLY:O	1:A:307:MET:HB2	2.02	0.60
1:E:78:THR:OG1	1:E:130:VAL:HG12	2.02	0.60
1:E:151:THR:HG21	1:E:387:ALA:HB1	1.84	0.60
1:A:218:LEU:HD11	4:A:403:QL5:C7	2.32	0.59
1:D:121:PRO:HD2	1:D:157:CYS:SG	2.43	0.59
1:A:242:GLN:NE2	1:A:273:GLU:OE1	2.36	0.57
1:E:39:ASN:HB3	1:E:344:THR:HG22	1.85	0.57
1:B:218:LEU:HD13	4:B:403:QL5:C6	2.35	0.57
1:B:40:LEU:HB2	1:B:53:LEU:O	2.04	0.57
1:E:88:LEU:HD22	1:E:104:PRO:HD2	1.87	0.57
1:B:147:VAL:O	1:B:151:THR:CG2	2.53	0.56
1:D:315:ARG:HD2	1:D:316:ASP:OD1	2.05	0.56
1:E:147:VAL:O	1:E:151:THR:CG2	2.53	0.56
1:B:43:GLU:HB2	1:B:342:ARG:NH2	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:LEU:HD22	1:D:391:CYS:N	2.20	0.56
1:A:43:GLU:HB2	1:A:342:ARG:NH2	2.21	0.55
1:A:280:HIS:O	1:A:284:GLU:N	2.36	0.55
1:D:117:TYR:CE2	1:D:119:ALA:HB3	2.41	0.55
1:A:43:GLU:HB3	1:A:314:LEU:HD21	1.88	0.55
1:A:308:VAL:HG12	1:A:312:ARG:NH1	2.22	0.55
1:D:173:ALA:O	1:D:177:PHE:HB2	2.07	0.55
1:D:205:SER:O	1:D:207:GLU:N	2.40	0.55
1:E:39:ASN:O	1:E:344:THR:CG2	2.54	0.55
1:A:303:PHE:CG	4:A:403:QL5:C1	2.90	0.55
1:D:77:THR:OG1	1:D:78:THR:N	2.40	0.55
1:A:78:THR:OG1	1:A:130:VAL:HG12	2.06	0.54
1:D:205:SER:C	1:D:207:GLU:H	2.14	0.54
1:B:222:ILE:HD12	1:B:222:ILE:N	2.22	0.54
1:B:146:GLU:OE2	1:B:174:GLU:OE1	2.26	0.54
1:A:295:LEU:HD13	4:A:403:QL5:C2	2.38	0.54
1:B:12:LEU:HD22	1:B:130:VAL:CG2	2.38	0.54
1:B:259:GLN:NE2	1:B:262:GLU:H	2.02	0.53
1:E:163:ILE:HG21	1:E:192:MET:SD	2.48	0.53
1:A:223:THR:O	1:A:351:CYS:HA	2.08	0.53
1:D:365:MET:HE2	1:D:378:PHE:CB	2.38	0.53
1:B:38:VAL:HG22	1:B:57:LEU:HD21	1.91	0.53
1:E:147:VAL:O	1:E:151:THR:HG23	2.09	0.53
1:A:391:CYS:CB	1:B:30:LEU:HD22	2.40	0.52
1:B:211:VAL:HG11	1:B:295:LEU:HD13	1.91	0.52
1:B:109:TYR:CE1	1:B:142:SER:HB2	2.45	0.52
1:D:276:ARG:HH11	1:D:276:ARG:CG	2.23	0.52
1:D:76:LEU:O	1:D:128:VAL:HA	2.09	0.52
1:A:303:PHE:CD2	4:A:403:QL5:C1	2.93	0.52
1:E:54:PRO:HD2	1:E:199:LEU:O	2.10	0.52
1:D:109:TYR:O	1:D:113:VAL:HG23	2.10	0.51
1:D:39:ASN:CB	5:D:422:HOH:O	2.37	0.51
1:B:147:VAL:O	1:B:151:THR:HG23	2.10	0.51
1:B:259:GLN:HE21	1:B:262:GLU:N	2.03	0.51
1:E:23:GLU:CD	1:E:87:ARG:HE	2.19	0.51
1:D:323:PRO:HG3	5:D:452:HOH:O	2.11	0.51
1:D:61:THR:HG21	1:D:145:LEU:HA	1.93	0.50
1:E:100:GLU:HB2	1:E:101:PRO:HD2	1.93	0.50
1:D:120:ALA:HB3	1:D:121:PRO:HD3	1.93	0.50
1:B:29:GLU:C	1:B:30:LEU:HD23	2.36	0.50
1:A:28:PRO:HG3	1:A:64:VAL:CG1	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:VAL:HG22	1:B:201:ILE:HB	1.94	0.50
1:B:85:PRO:HD2	1:B:104:PRO:HG3	1.93	0.49
1:A:303:PHE:CD1	4:A:403:QL5:C1	2.96	0.49
1:A:223:THR:HG21	1:A:328:LEU:HD22	1.94	0.49
1:E:361:ALA:HB3	1:E:362:PRO:HD3	1.95	0.49
1:B:56:ALA:HB3	1:B:384:ALA:O	2.13	0.49
1:B:361:ALA:HB3	1:B:362:PRO:HD3	1.94	0.49
1:A:364:ALA:HB1	1:A:368:ILE:CD1	2.43	0.49
1:D:39:ASN:HD21	1:D:43:GLU:N	2.11	0.49
1:D:276:ARG:NH1	1:D:276:ARG:HG2	2.27	0.49
1:D:213:LEU:N	1:D:213:LEU:HD12	2.28	0.48
1:D:295:LEU:HD13	1:D:303:PHE:CE2	2.47	0.48
1:D:159:ASP:OD1	1:D:159:ASP:O	2.31	0.48
1:E:184:ILE:HG13	1:E:188:PHE:HD2	1.78	0.48
1:D:365:MET:HG2	1:D:378:PHE:CG	2.49	0.48
1:A:361:ALA:N	1:A:362:PRO:HD2	2.29	0.47
1:A:308:VAL:CG2	1:A:333:LEU:HD21	2.43	0.47
1:E:31:ALA:HB2	1:E:392:LEU:HD11	1.95	0.47
1:D:30:LEU:HD11	1:D:152:PHE:CE2	2.49	0.47
1:D:67:PRO:HB3	1:D:156:LEU:HD22	1.95	0.47
1:D:51:LEU:HD23	1:D:202:ASP:HA	1.96	0.47
1:D:185:MET:O	1:D:189:ILE:HG22	2.14	0.47
1:A:43:GLU:OE1	2:A:401:GAL:O6	2.23	0.47
1:B:12:LEU:HD22	1:B:130:VAL:HG23	1.95	0.47
1:E:49:GLN:NE2	1:E:204:ARG:HG3	2.30	0.47
1:B:259:GLN:HG3	1:B:262:GLU:HB2	1.97	0.47
1:E:49:GLN:HE21	1:E:204:ARG:HG3	1.79	0.47
1:A:291:ALA:HB1	1:A:303:PHE:CE1	2.51	0.46
1:B:76:LEU:O	1:B:128:VAL:HA	2.16	0.46
1:D:116:TYR:CE2	1:D:172:GLN:O	2.68	0.46
1:A:41:ILE:CD1	1:A:288:THR:HG23	2.45	0.46
1:B:147:VAL:O	1:B:151:THR:HG22	2.16	0.46
1:A:30:LEU:HD11	1:B:391:CYS:HB2	1.98	0.46
1:A:391:CYS:HB2	1:B:30:LEU:HD22	1.98	0.46
1:B:51:LEU:HD23	1:B:202:ASP:HA	1.98	0.46
1:D:320:VAL:O	1:D:347:GLY:HA3	2.16	0.46
1:A:364:ALA:O	1:A:368:ILE:N	2.34	0.45
1:B:242:GLN:NE2	1:B:273:GLU:OE1	2.49	0.45
1:A:194:GLN:HG3	1:A:210:LEU:CD1	2.47	0.45
1:A:303:PHE:CE2	4:A:403:QL5:C1	3.00	0.45
1:A:68:ARG:CZ	1:A:72:LEU:HD11	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:VAL:CG1	1:B:295:LEU:HD13	2.46	0.45
1:D:159:ASP:OD1	1:D:159:ASP:C	2.59	0.45
1:B:147:VAL:HG21	1:B:190:SER:HB3	1.98	0.44
1:E:147:VAL:O	1:E:151:THR:HG22	2.17	0.44
1:A:28:PRO:CB	1:A:64:VAL:HG13	2.48	0.44
1:A:380:LEU:HD23	1:A:380:LEU:HA	1.82	0.44
1:B:20:PHE:N	1:B:128:VAL:HG21	2.32	0.44
1:A:41:ILE:HD13	1:A:288:THR:HA	1.98	0.44
1:E:184:ILE:O	1:E:188:PHE:HB2	2.18	0.44
1:D:390:LEU:HD22	1:D:391:CYS:H	1.83	0.44
1:A:174:GLU:HG2	1:A:182:CYS:SG	2.58	0.44
1:E:8:GLN:CB	5:E:648:HOH:O	2.65	0.44
1:E:109:TYR:CE1	1:E:142:SER:HB2	2.52	0.44
1:D:174:GLU:O	1:D:176:SER:N	2.50	0.44
1:D:256:ARG:HG3	1:D:256:ARG:O	2.16	0.44
1:B:355:LEU:CD1	4:B:403:QL5:C14	2.95	0.44
1:D:20:PHE:CE2	1:D:65:GLY:HA2	2.52	0.44
1:A:218:LEU:HD21	4:A:403:QL5:C6	2.47	0.44
1:B:382:GLN:H	1:B:382:GLN:HG2	1.66	0.44
1:D:202:ASP:OD1	1:D:256:ARG:NH2	2.51	0.44
1:D:218:LEU:HD11	1:D:339:TYR:CE2	2.53	0.44
1:B:213:LEU:HD12	1:B:383:ALA:HB2	2.00	0.44
1:A:184:ILE:O	1:A:185:MET:C	2.61	0.43
1:B:252:ALA:HB1	1:B:257:GLU:HB2	1.99	0.43
1:A:255:LEU:O	1:A:256:ARG:C	2.61	0.43
1:A:320:VAL:O	1:A:347:GLY:HA3	2.18	0.43
1:D:44:HIS:HD2	1:D:236:TYR:HE1	1.66	0.43
1:D:110:VAL:O	1:D:114:ILE:HG13	2.18	0.43
1:B:159:ASP:OD1	1:B:159:ASP:C	2.62	0.43
1:E:39:ASN:N	1:E:344:THR:HG21	2.34	0.43
1:E:92:LEU:HD11	1:E:123:PRO:C	2.43	0.43
1:A:260:LEU:HD11	1:A:264:GLU:OE2	2.19	0.43
1:B:35:PRO:HG3	1:B:386:GLY:HA2	2.01	0.43
1:B:80:GLU:CB	5:B:574:HOH:O	2.66	0.43
1:B:39:ASN:O	1:B:344:THR:HG23	2.18	0.43
1:E:219:ALA:O	1:E:356:LEU:HD23	2.19	0.43
1:D:174:GLU:C	1:D:176:SER:H	2.27	0.43
1:A:163:ILE:HD12	1:A:188:PHE:CE1	2.54	0.42
1:A:194:GLN:HG3	1:A:210:LEU:HD11	2.01	0.42
1:A:306:LEU:O	1:A:310:SER:N	2.50	0.42
1:D:44:HIS:HD2	1:D:236:TYR:CE1	2.37	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:LEU:HD12	1:D:88:LEU:HD23	2.00	0.42
1:A:52:VAL:HG22	1:A:201:ILE:HB	2.00	0.42
1:E:39:ASN:H	1:E:344:THR:HG21	1.84	0.42
1:E:133:VAL:O	1:E:135:LEU:HD23	2.20	0.42
1:D:278:ALA:O	1:D:282:VAL:HG13	2.20	0.42
1:E:76:LEU:O	1:E:128:VAL:HA	2.18	0.42
1:E:92:LEU:HD11	1:E:124:GLY:N	2.35	0.42
1:A:232:ALA:HA	1:A:348:PHE:CD2	2.55	0.42
1:D:14:ALA:O	1:D:15:GLU:C	2.62	0.42
1:A:303:PHE:CE1	4:A:403:QL5:C1	3.02	0.42
1:B:47:TYR:CE1	1:B:240:ARG:HG2	2.54	0.42
1:B:205:SER:O	1:B:206:LEU:HB2	2.18	0.42
1:B:320:VAL:O	1:B:347:GLY:HA3	2.20	0.42
1:D:339:TYR:OH	1:D:357:GLU:OE2	2.27	0.42
1:E:199:LEU:HD11	1:E:208:THR:HB	2.01	0.42
1:A:364:ALA:O	1:A:368:ILE:HD12	2.21	0.41
1:E:199:LEU:HD23	1:E:201:ILE:HD11	2.02	0.41
1:D:35:PRO:HG3	1:D:385:ASP:O	2.19	0.41
1:E:356:LEU:HD23	1:E:356:LEU:N	2.35	0.41
1:B:236:TYR:HH	2:B:401:GAL:HO4	1.66	0.41
1:B:329:VAL:O	1:B:333:LEU:HG	2.20	0.41
1:A:202:ASP:O	1:A:206:LEU:N	2.49	0.41
1:D:150:TYR:CE1	1:D:166:ARG:HD3	2.56	0.41
1:A:163:ILE:HD12	1:A:188:PHE:HE1	1.85	0.41
1:B:151:THR:HB	5:B:505:HOH:O	2.21	0.41
1:A:260:LEU:O	1:A:260:LEU:HD12	2.21	0.41
1:B:269:LEU:HD12	1:B:269:LEU:HA	1.94	0.41
1:A:315:ARG:NH1	1:A:316:ASP:OD1	2.54	0.41
1:B:365:MET:O	1:B:366:ARG:C	2.63	0.41
1:E:246:VAL:O	1:E:250:LEU:HG	2.20	0.41
1:D:311:HIS:NE2	1:D:326:ASP:OD1	2.47	0.41
1:A:73:VAL:O	1:A:89:GLN:HA	2.21	0.41
1:B:37:ARG:C	1:B:37:ARG:HD2	2.45	0.41
1:B:43:GLU:HB2	1:B:342:ARG:HH22	1.85	0.41
1:D:152:PHE:CE1	1:D:156:LEU:HD11	2.56	0.41
1:D:170:CYS:HB2	1:D:187:GLN:HG2	2.03	0.41
1:D:246:VAL:O	1:D:247:ALA:C	2.63	0.41
1:A:52:VAL:HG23	1:A:54:PRO:HD3	2.01	0.41
1:A:291:ALA:O	1:A:303:PHE:CD1	2.74	0.41
1:A:368:ILE:HB	1:A:378:PHE:HZ	1.86	0.41
1:D:39:ASN:CG	5:D:422:HOH:O	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:LEU:HD12	1:D:255:LEU:HA	1.91	0.41
1:A:303:PHE:CZ	4:A:403:QL5:C1	3.03	0.40
1:B:21:ARG:HD2	1:B:27:GLU:OE2	2.22	0.40
1:A:103:THR:HA	1:A:104:PRO:HA	1.88	0.40
1:D:335:VAL:HG21	1:D:364:ALA:HA	2.03	0.40
1:A:63:LEU:HD11	1:A:129:VAL:HG22	2.03	0.40
1:A:368:ILE:CG2	1:A:378:PHE:HZ	2.34	0.40
1:D:361:ALA:HB3	1:D:362:PRO:HD3	2.02	0.40
1:B:46:ASP:HB3	1:B:52:VAL:HG11	2.04	0.40
1:D:40:LEU:O	1:D:342:ARG:HD3	2.20	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	390/399 (98%)	373 (96%)	16 (4%)	1 (0%)	36	46
1	B	389/399 (98%)	374 (96%)	14 (4%)	1 (0%)	36	46
1	D	359/399 (90%)	332 (92%)	23 (6%)	4 (1%)	11	13
1	E	391/399 (98%)	381 (97%)	10 (3%)	0	100	100
All	All	1529/1596 (96%)	1460 (96%)	63 (4%)	6 (0%)	30	38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	103	THR
1	D	175	HIS
1	B	96	GLN
1	D	206	LEU
1	A	232	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	106	TRP

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	272/315 (86%)	252 (93%)	20 (7%)	13	17
1	B	279/315 (89%)	257 (92%)	22 (8%)	11	15
1	D	234/315 (74%)	216 (92%)	18 (8%)	12	16
1	E	289/315 (92%)	277 (96%)	12 (4%)	26	40
All	All	1074/1260 (85%)	1002 (93%)	72 (7%)	15	21

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	9	VAL
1	A	30	LEU
1	A	41	ILE
1	A	43	GLU
1	A	64	VAL
1	A	103	THR
1	A	122	LEU
1	A	209	SER
1	A	213	LEU
1	A	218	LEU
1	A	220	VAL
1	A	227	VAL
1	A	254	SER
1	A	264	GLU
1	A	317	ASP
1	A	355	LEU
1	A	368	ILE
1	A	370	GLU
1	A	381	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	9	VAL
1	B	12	LEU
1	B	30	LEU
1	B	38	VAL
1	B	40	LEU
1	B	63	LEU
1	B	151	THR
1	B	168	GLN
1	B	206	LEU
1	B	218	LEU
1	B	227	VAL
1	B	234	SER
1	B	259	GLN
1	B	260	LEU
1	B	269	LEU
1	B	295	LEU
1	B	301	ARG
1	B	344	THR
1	B	357	GLU
1	B	381	SER
1	B	382	GLN
1	B	390	LEU
1	E	84	GLU
1	E	89	GLN
1	E	97	ARG
1	E	151	THR
1	E	168	GLN
1	E	184	ILE
1	E	213	LEU
1	E	264	GLU
1	E	282	VAL
1	E	344	THR
1	E	377	THR
1	E	390	LEU
1	D	22	GLU
1	D	23	GLU
1	D	64	VAL
1	D	75	LEU
1	D	76	LEU
1	D	77	THR
1	D	130	VAL
1	D	140	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	218	LEU
1	D	228	ARG
1	D	255	LEU
1	D	262	GLU
1	D	269	LEU
1	D	276	ARG
1	D	282	VAL
1	D	295	LEU
1	D	357	GLU
1	D	390	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	GLN
1	A	290	GLN
1	A	327	GLN
1	B	86	GLN
1	B	229	HIS
1	B	242	GLN
1	B	259	GLN
1	B	382	GLN
1	E	49	GLN
1	E	89	GLN
1	E	172	GLN
1	E	229	HIS
1	E	367	HIS
1	D	39	ASN
1	D	154	GLN
1	D	363	HIS

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 ⓘ

8 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	2.50	7 (24%)	32,44,44	2.09	8 (25%)
3	HFK	A	402	-	29,30,30	2.66	9 (31%)	32,44,44	2.48	14 (43%)
3	HFK	E	402	-	29,30,30	2.70	10 (34%)	32,44,44	2.06	8 (25%)
2	GAL	B	401	-	12,12,12	0.67	0	17,17,17	1.44	2 (11%)
2	GAL	A	401	-	12,12,12	0.74	0	17,17,17	2.32	2 (11%)
4	QL5	B	403	-	18,18,18	0.33	0	24,24,24	0.50	0
2	GAL	E	401	-	12,12,12	0.88	1 (8%)	17,17,17	3.30	5 (29%)
4	QL5	A	403	-	18,18,18	0.38	0	24,24,24	0.85	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HFK	B	402	-	-	2/4/43/43	0/5/5/5
3	HFK	A	402	-	-	3/4/43/43	0/5/5/5
3	HFK	E	402	-	-	2/4/43/43	0/5/5/5
2	GAL	B	401	-	-	1/2/22/22	0/1/1/1
2	GAL	A	401	-	-	2/2/22/22	0/1/1/1
4	QL5	B	403	-	-	2/8/8/8	0/2/2/2
2	GAL	E	401	-	-	1/2/22/22	0/1/1/1
4	QL5	A	403	-	-	0/8/8/8	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	402	HFK	C06-C07	10.01	1.49	1.37
3	A	402	HFK	C06-C07	9.45	1.49	1.37
3	B	402	HFK	C06-C07	9.13	1.48	1.37
3	A	402	HFK	C15-N14	5.62	1.45	1.30
3	B	402	HFK	C15-N14	5.60	1.44	1.30
3	E	402	HFK	C15-N14	5.15	1.43	1.30
3	E	402	HFK	C03-C02	3.95	1.56	1.50
3	A	402	HFK	C08-N14	3.92	1.50	1.46
3	B	402	HFK	C15-N16	3.51	1.42	1.36
3	A	402	HFK	C26-C20	3.50	1.45	1.40
3	B	402	HFK	C05-C06	3.48	1.55	1.49
3	E	402	HFK	C15-N16	3.32	1.42	1.36
3	E	402	HFK	C05-C06	3.21	1.55	1.49
3	A	402	HFK	C18-N17	3.12	1.42	1.36
3	B	402	HFK	C15-N17	3.09	1.44	1.37
3	A	402	HFK	C15-N17	2.98	1.44	1.37
3	E	402	HFK	C15-N17	2.76	1.43	1.37
3	A	402	HFK	C05-C06	2.75	1.54	1.49
3	B	402	HFK	C18-N19	2.67	1.34	1.30
3	E	402	HFK	C20-N19	-2.62	1.34	1.39
3	E	402	HFK	C18-N19	2.56	1.34	1.30
3	A	402	HFK	C15-N16	2.39	1.40	1.36
2	E	401	GAL	C4-C3	2.33	1.58	1.52
3	A	402	HFK	C13-C08	2.24	1.57	1.54
3	E	402	HFK	C06-N16	2.23	1.41	1.37
3	E	402	HFK	C13-C08	2.18	1.57	1.54
3	B	402	HFK	C18-N17	2.08	1.40	1.36

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	GAL	C1-O5-C5	-9.98	94.35	113.65
3	A	402	HFK	C02-C07-C06	-8.76	111.41	119.18
2	A	401	GAL	C1-O5-C5	-7.22	99.68	113.65
2	E	401	GAL	C1-C2-C3	-7.05	95.97	110.36
3	B	402	HFK	C02-C07-C06	-6.40	113.50	119.18
3	B	402	HFK	C07-C06-N16	-5.82	117.42	122.11
2	A	401	GAL	C1-C2-C3	-5.19	99.76	110.36
3	E	402	HFK	C07-C06-N16	-5.15	117.96	122.11
3	E	402	HFK	C23-C21-C20	-4.73	117.87	123.62
2	E	401	GAL	O1-C1-C2	4.00	120.60	108.98
3	E	402	HFK	N17-C15-N14	3.89	125.22	117.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	HFK	C05-C06-C07	-3.75	117.62	122.72
3	E	402	HFK	C09-C10-C11	3.54	116.86	111.35
3	A	402	HFK	N17-C15-N14	3.40	124.31	117.96
3	E	402	HFK	N17-C18-N19	-3.39	118.97	128.58
3	E	402	HFK	O22-C21-C23	3.27	133.37	126.49
3	B	402	HFK	O22-C21-C23	3.18	133.17	126.49
3	A	402	HFK	O22-C21-C23	3.13	133.07	126.49
3	B	402	HFK	C23-C21-C20	-3.07	119.88	123.62
3	A	402	HFK	C07-C06-N16	-3.07	119.64	122.11
3	A	402	HFK	C05-C06-N16	2.98	119.71	115.46
2	B	401	GAL	O5-C1-C2	-2.93	105.14	110.30
3	A	402	HFK	C04-C05-C06	-2.91	104.83	110.97
3	E	402	HFK	C05-C06-N16	2.82	119.48	115.46
3	A	402	HFK	O22-C21-C20	-2.76	105.92	107.80
3	A	402	HFK	O22-C18-N19	-2.74	110.65	115.57
3	A	402	HFK	C08-C07-C06	-2.69	118.72	121.75
2	B	401	GAL	C1-O5-C5	-2.60	108.62	113.65
3	B	402	HFK	C08-C07-C06	-2.58	118.84	121.75
2	E	401	GAL	C6-C5-C4	2.57	119.33	113.02
4	A	403	QL5	O1-C7-C5	2.51	122.62	117.89
3	B	402	HFK	C09-C10-C11	2.50	115.25	111.35
3	E	402	HFK	N17-C15-N16	-2.44	113.86	117.96
3	B	402	HFK	N17-C15-N14	2.34	122.32	117.96
3	B	402	HFK	N17-C18-N19	-2.33	121.96	128.58
2	E	401	GAL	C3-C4-C5	2.21	114.23	110.23
3	A	402	HFK	C23-C21-C20	-2.17	120.98	123.62
3	A	402	HFK	C18-N17-C15	-2.09	120.15	125.27
3	A	402	HFK	N17-C15-N16	-2.07	114.48	117.96
3	A	402	HFK	C26-C20-C21	-2.00	117.76	120.31

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	403	QL5	C9-C8-O1-C7
4	B	403	QL5	O2-C8-O1-C7
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	O5-C5-C6-O6
3	A	402	HFK	N14-C15-N17-C18
3	A	402	HFK	N16-C15-N17-C18

Continued on next page...

Continued from previous page...

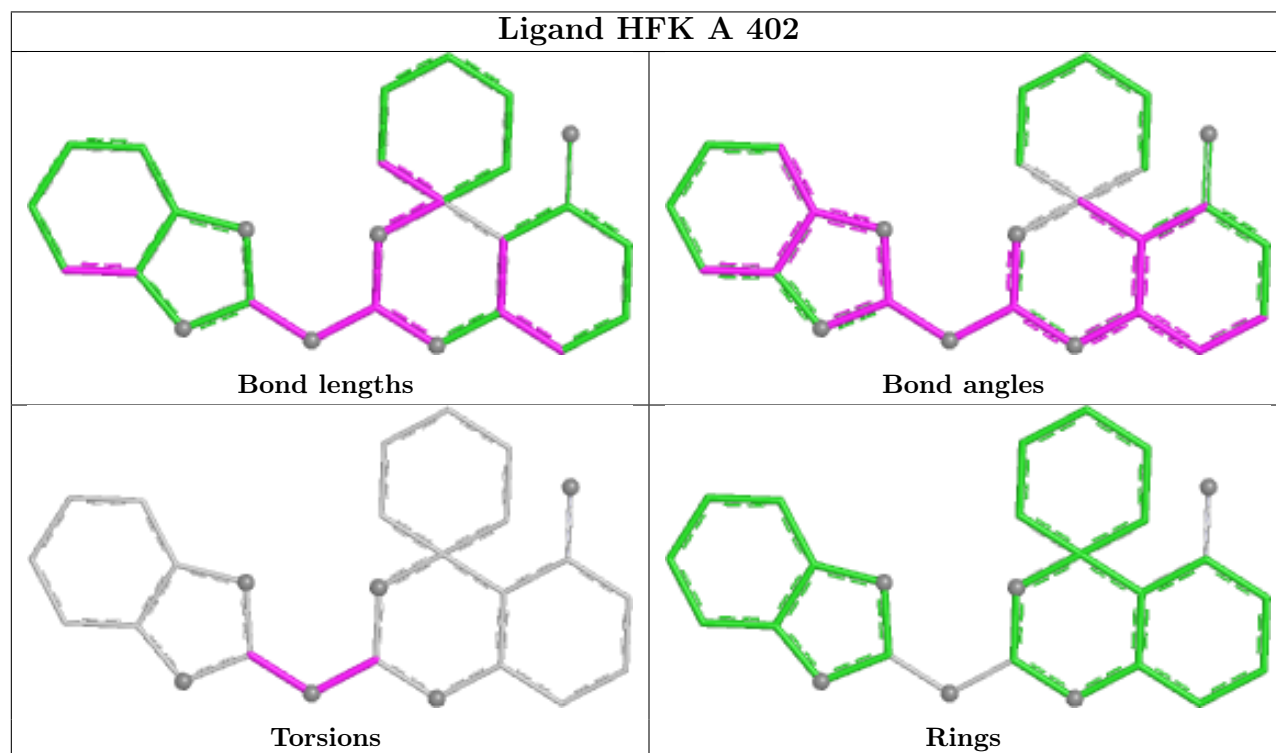
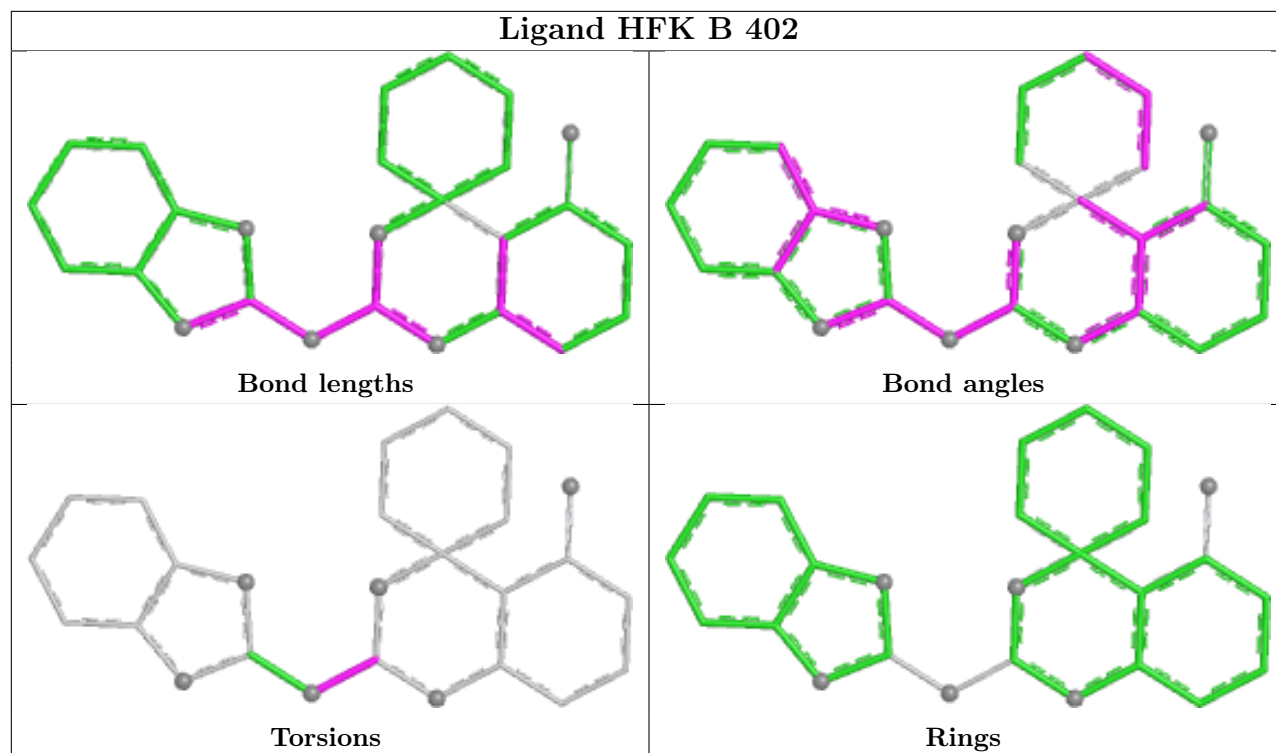
Mol	Chain	Res	Type	Atoms
3	B	402	HFK	N14-C15-N17-C18
3	B	402	HFK	N16-C15-N17-C18
3	E	402	HFK	N16-C15-N17-C18
3	E	402	HFK	N14-C15-N17-C18
3	A	402	HFK	O22-C18-N17-C15

There are no ring outliers.

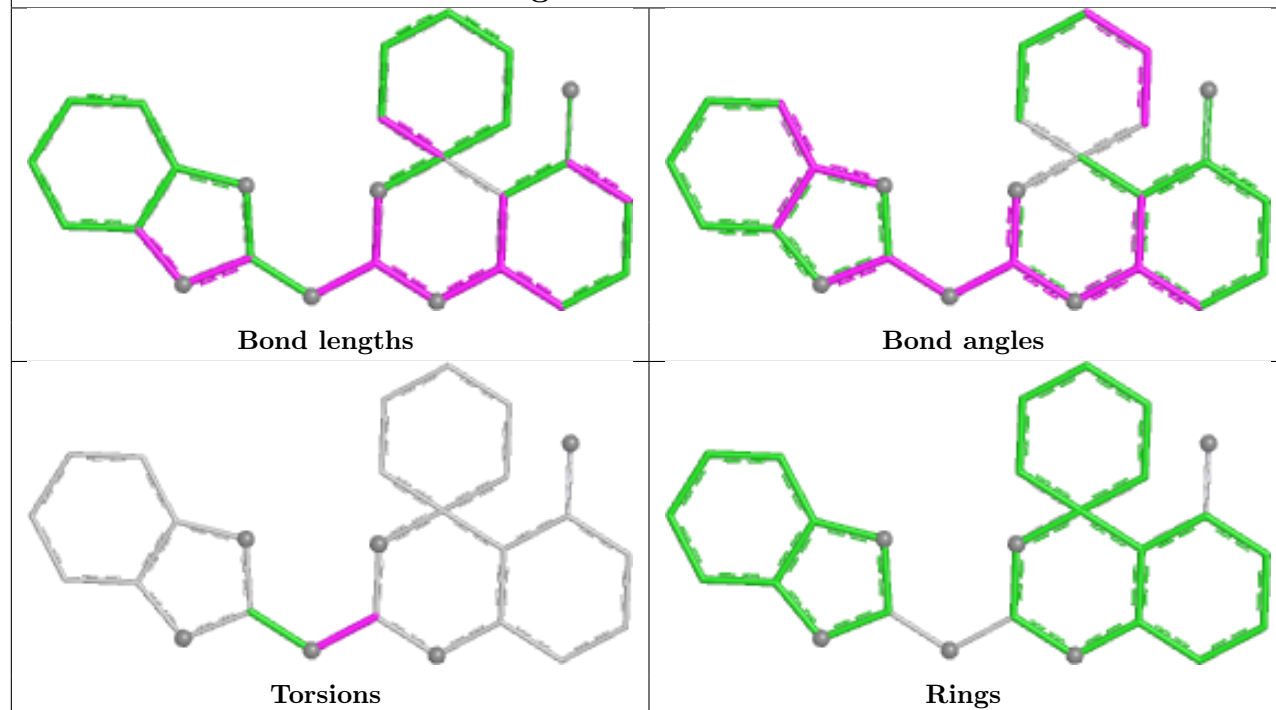
4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	GAL	1	0
2	A	401	GAL	1	0
4	B	403	QL5	3	0
4	A	403	QL5	12	0

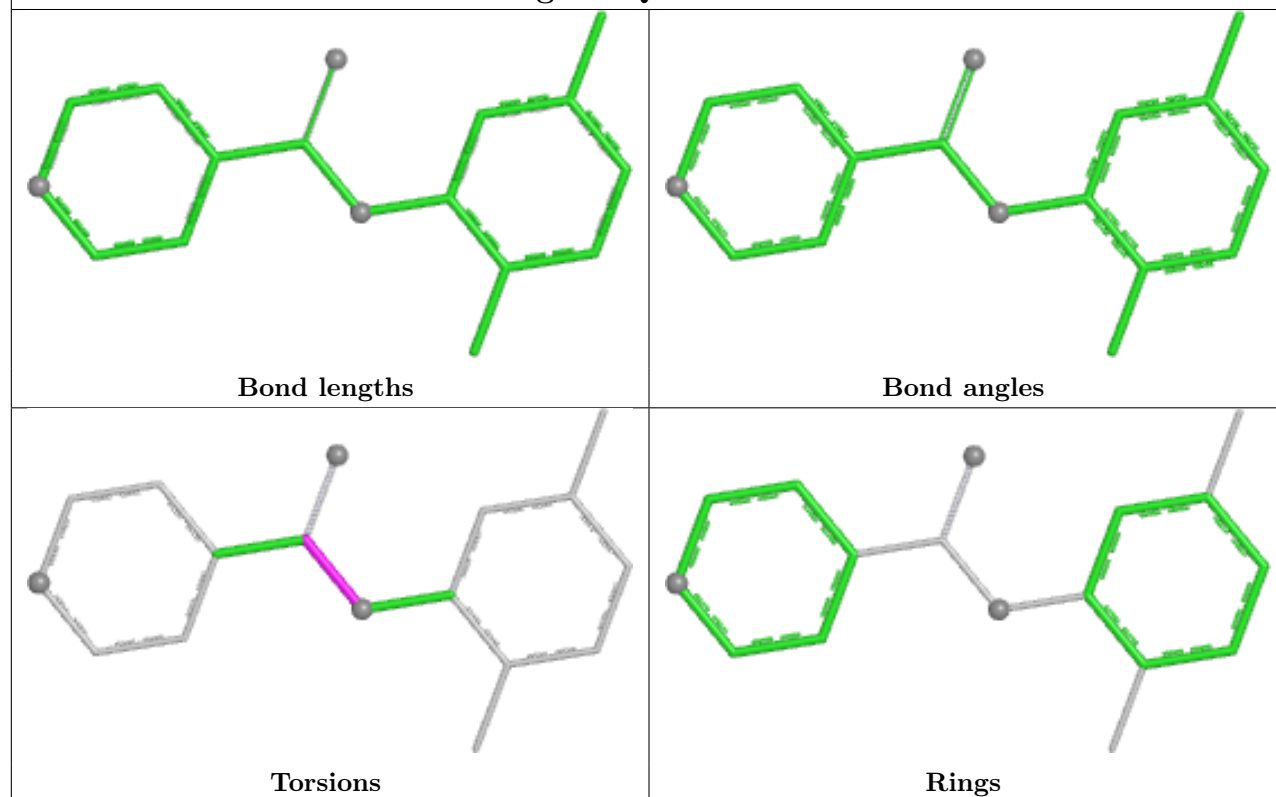
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

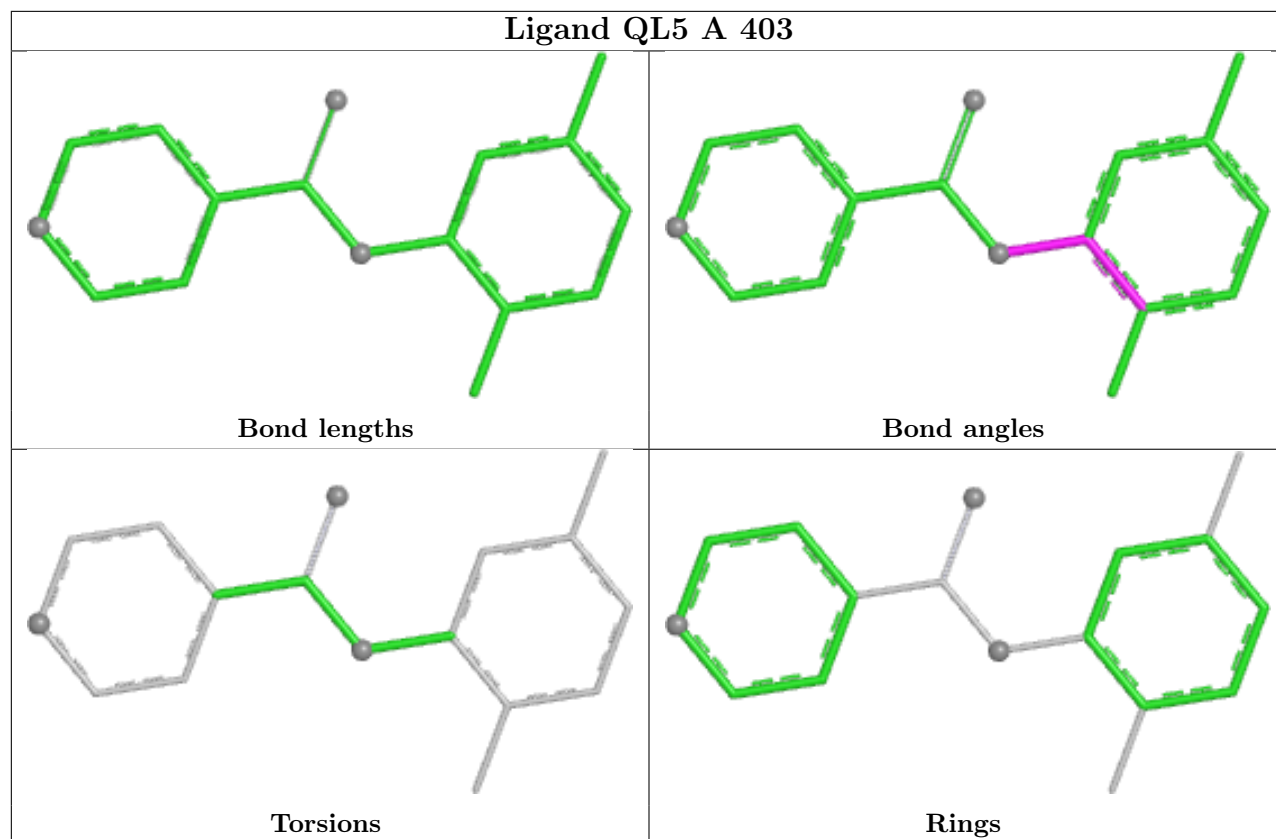


Ligand HFK E 402



Ligand QL5 B 403





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	391/399 (97%)	0.65	46 (11%) 9 10	29, 54, 101, 133	1 (0%)
1	B	391/399 (97%)	0.39	24 (6%) 27 29	31, 52, 86, 132	0
1	D	369/399 (92%)	0.87	56 (15%) 5 6	31, 59, 114, 155	0
1	E	391/399 (97%)	-0.02	2 (0%) 87 87	19, 42, 67, 76	2 (0%)
All	All	1542/1596 (96%)	0.47	128 (8%) 17 19	19, 51, 98, 155	3 (0%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	106	TRP	6.2
1	B	233	SER	4.8
1	D	19	ALA	4.7
1	D	99	LEU	4.6
1	A	233	SER	4.2
1	B	96	GLN	4.2
1	A	2	ALA	4.2
1	D	93	PRO	3.9
1	A	274	GLY	3.8
1	D	120	ALA	3.7
1	D	121	PRO	3.7
1	B	214	SER	3.7
1	D	78	THR	3.7
1	A	268	ASP	3.6
1	D	88	LEU	3.6
1	A	263	LEU	3.6
1	D	43	GLU	3.6
1	B	103	THR	3.5
1	A	366	ARG	3.5
1	B	95	ALA	3.4
1	D	178	ALA	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	269	LEU	3.4
1	A	369	GLN	3.4
1	B	99	LEU	3.4
1	B	231	LEU	3.3
1	D	184	ILE	3.3
1	D	95	ALA	3.2
1	D	72	LEU	3.2
1	D	231	LEU	3.2
1	A	230	SER	3.2
1	B	97	ARG	3.2
1	D	254	SER	3.1
1	B	89	GLN	3.1
1	D	236	TYR	3.1
1	D	96	GLN	3.1
1	A	266	ALA	3.1
1	A	282	VAL	3.1
1	D	76	LEU	3.1
1	D	70	ASP	3.0
1	D	94	THR	3.0
1	D	104	PRO	3.0
1	D	98	SER	3.0
1	A	305	ARG	2.9
1	D	89	GLN	2.9
1	D	86	GLN	2.9
1	B	80	GLU	2.9
1	A	249	ALA	2.9
1	A	370	GLU	2.9
1	A	215	ASP	2.9
1	D	122	LEU	2.8
1	B	2	ALA	2.8
1	E	2	ALA	2.8
1	A	365	MET	2.8
1	D	91	PRO	2.8
1	D	8	GLN	2.8
1	D	92	LEU	2.8
1	D	206	LEU	2.8
1	B	232	ALA	2.8
1	A	270	VAL	2.8
1	D	163	ILE	2.8
1	A	80	GLU	2.8
1	A	260	LEU	2.8
1	D	62	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	363	HIS	2.7
1	A	312	ARG	2.7
1	B	92	LEU	2.7
1	B	229	HIS	2.7
1	D	90	PHE	2.7
1	A	382	GLN	2.7
1	A	330	GLU	2.7
1	A	275	PHE	2.6
1	A	300	TYR	2.6
1	D	232	ALA	2.6
1	D	249	ALA	2.6
1	D	29	GLU	2.6
1	D	172	GLN	2.6
1	A	3	ALA	2.6
1	D	77	THR	2.6
1	D	268	ASP	2.6
1	A	334	ALA	2.5
1	D	87	ARG	2.5
1	A	265	ALA	2.5
1	A	278	ALA	2.5
1	A	337	GLY	2.5
1	D	44	HIS	2.5
1	A	367	HIS	2.5
1	A	329	VAL	2.5
1	D	300	TYR	2.5
1	D	234	SER	2.4
1	B	259	GLN	2.4
1	D	23	GLU	2.4
1	B	100	GLU	2.4
1	B	230	SER	2.3
1	A	231	LEU	2.3
1	A	267	ARG	2.3
1	A	339	TYR	2.3
1	B	249	ALA	2.3
1	D	119	ALA	2.3
1	A	258	VAL	2.3
1	A	335	VAL	2.3
1	D	13	LEU	2.2
1	D	101	PRO	2.2
1	D	71	GLY	2.2
1	D	26	ALA	2.2
1	B	94	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	348	PHE	2.2
1	D	20	PHE	2.2
1	D	128	VAL	2.2
1	B	7	PRO	2.2
1	A	261	GLU	2.2
1	A	4	LEU	2.2
1	A	259	GLN	2.2
1	B	70	ASP	2.1
1	B	244	GLU	2.1
1	A	214	SER	2.1
1	A	333	LEU	2.1
1	D	129	VAL	2.1
1	A	232	ALA	2.1
1	A	364	ALA	2.1
1	B	163	ILE	2.1
1	D	175	HIS	2.1
1	A	277	ARG	2.1
1	A	301	ARG	2.1
1	D	103	THR	2.0
1	E	213	LEU	2.0
1	D	12	LEU	2.0
1	D	16	ALA	2.0
1	D	21	ARG	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.

Continued on next page...

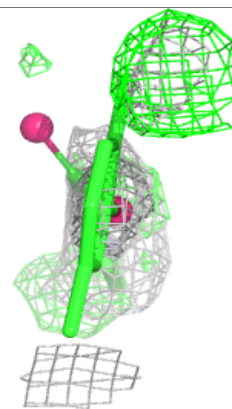
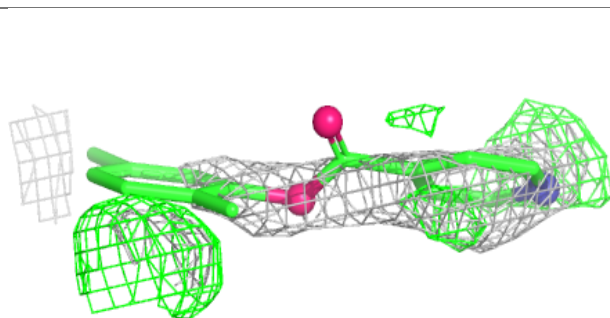
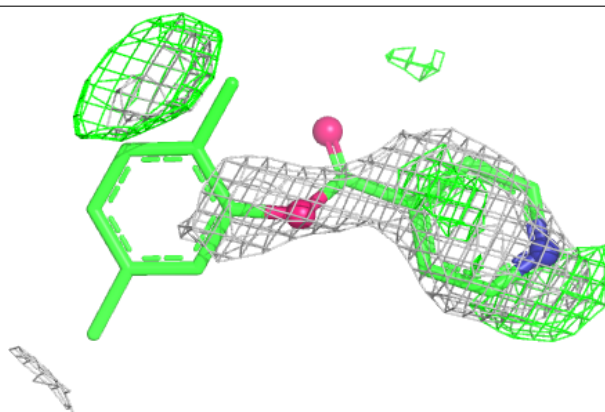
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	QL5	A	403	17/17	0.74	0.50	36,37,44,47	17
4	QL5	B	403	17/17	0.84	0.48	42,44,46,47	17
3	HFK	A	402	26/26	0.89	0.14	50,60,66,72	0
3	HFK	B	402	26/26	0.89	0.14	58,64,72,74	0
2	GAL	B	401	12/12	0.93	0.08	34,40,44,49	0
3	HFK	E	402	26/26	0.94	0.10	41,45,52,54	0
2	GAL	E	401	12/12	0.95	0.07	25,28,33,36	0
2	GAL	A	401	12/12	0.95	0.06	38,43,46,46	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.

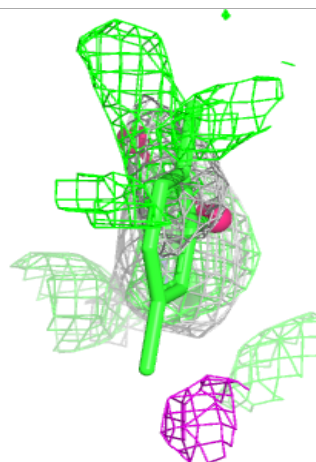
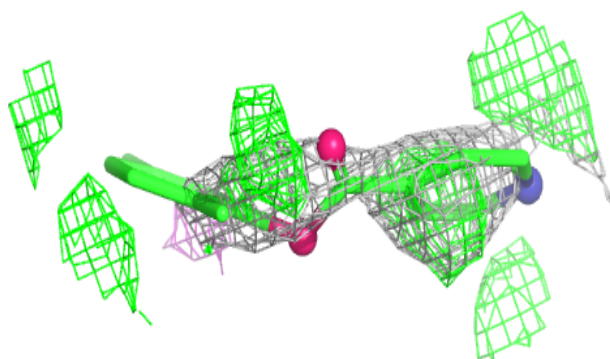
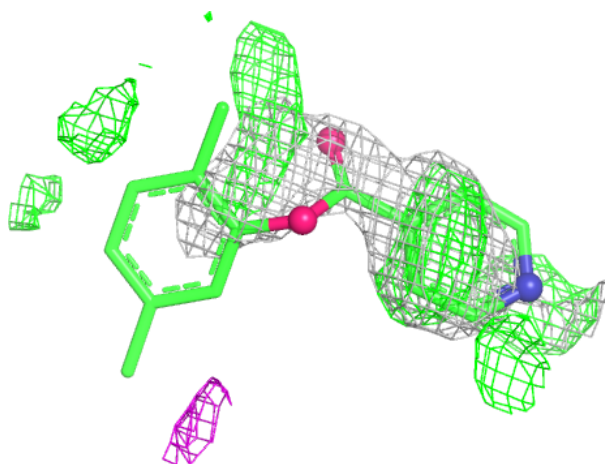
Electron density around QL5 A 403:

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



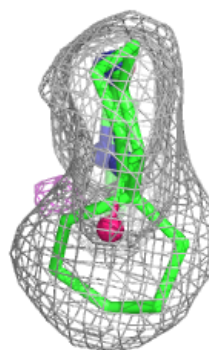
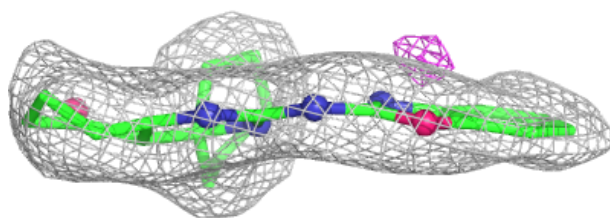
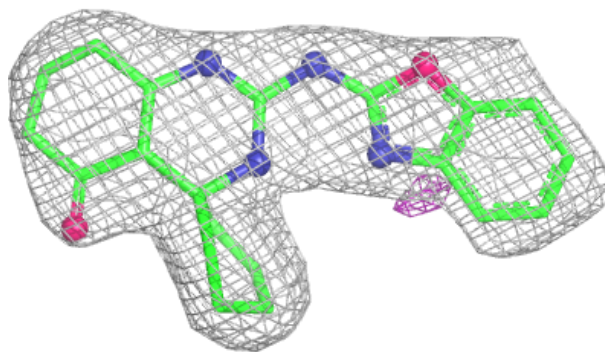
Electron density around QL5 B 403:

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

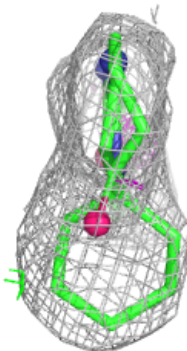
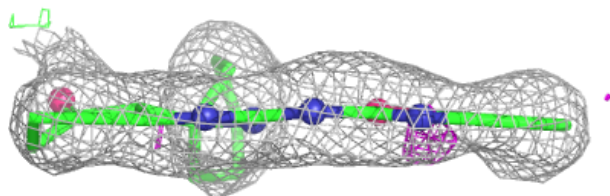
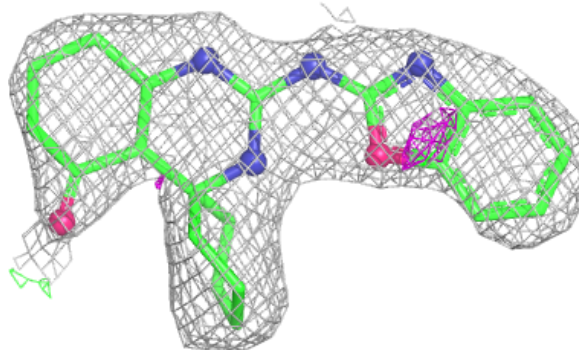


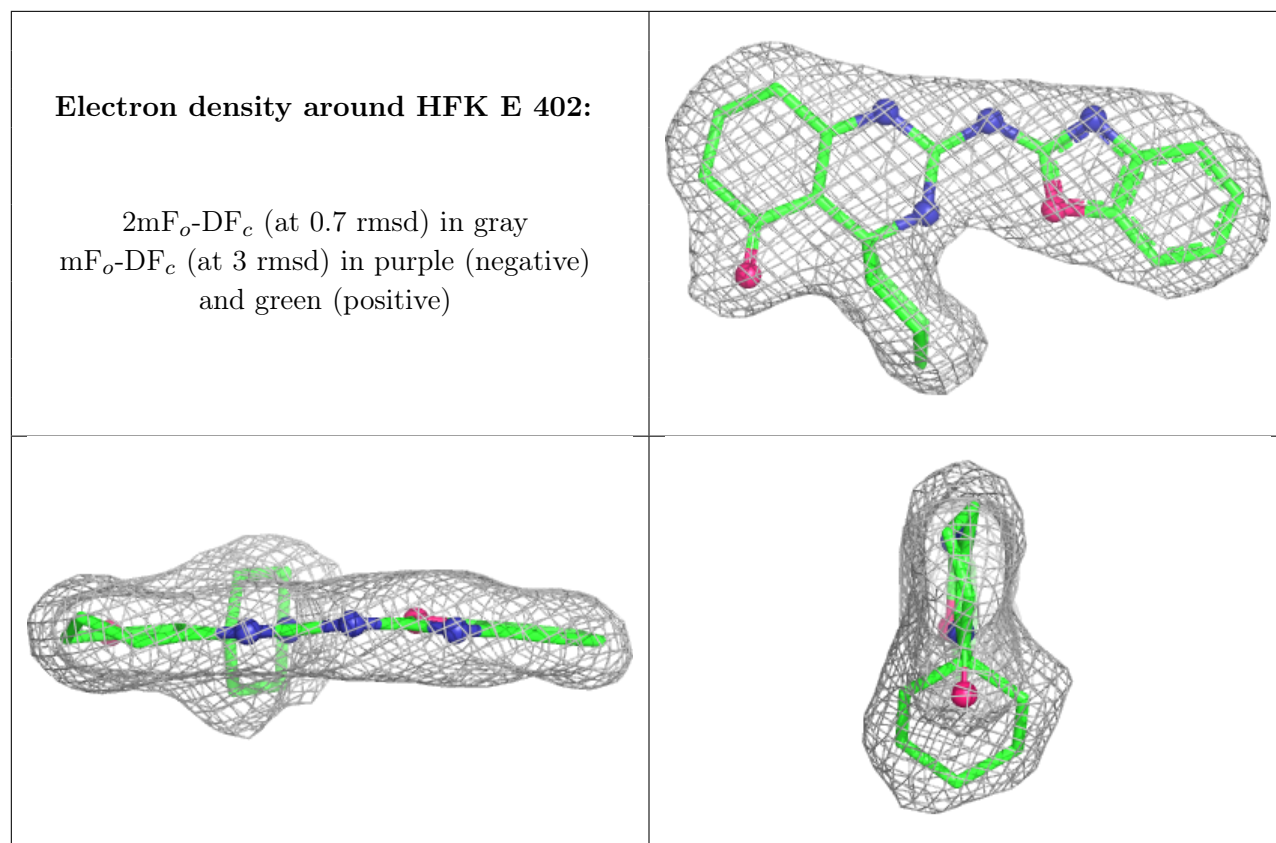
Electron density around HFK A 402:

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

**Electron density around HFK 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.