



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:31 AM UTC

PDB ID : 6QJE / pdb_00006qje
Title : Structure of human galactokinase 1 bound with 4-{[2-(Methylsulfonyl)-1H-imidazol-1-yl]methyl}-1,3-thiazole
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 : 2019-01-24
Resolution : 2.40 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

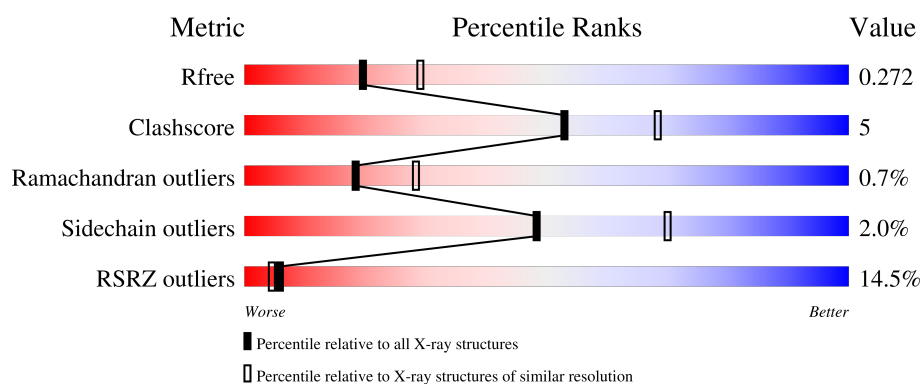
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	392	 4% 91% 8% ..
1	B	392	 17% 88% 12% .
1	C	392	 15% 88% 9% ..
1	D	392	 20% 77% 12% . 10%

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	J4Q	B	403	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11053 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.

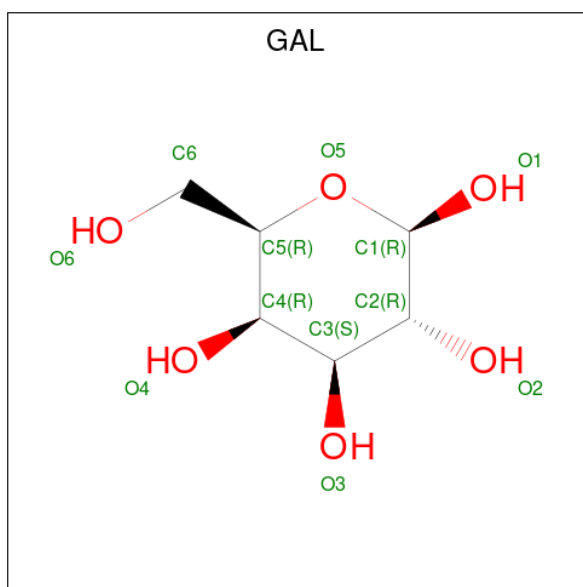
- Molecule 1 is a protein called Galactokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			2831	1777	503	535	16			
1	B	392	Total	C	N	O	S	0	0	0
			2729	1709	480	525	15			
1	C	384	Total	C	N	O	S	0	0	0
			2714	1708	479	512	15			
1	D	352	Total	C	N	O	S	0	0	0
			2443	1533	435	462	13			

There are 12 discrepancies between the modelled and reference sequences:

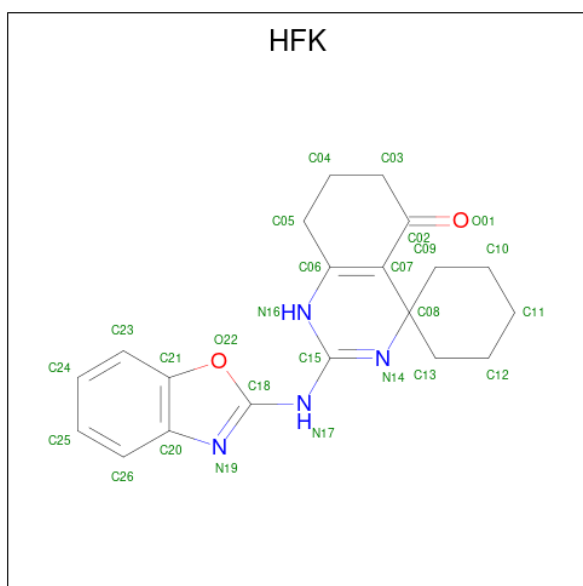
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	expression tag	UNP P51570
A	252	ALA	LYS	engineered mutation	UNP P51570
A	253	ALA	GLU	engineered mutation	UNP P51570
B	1	HIS	-	expression tag	UNP P51570
B	252	ALA	LYS	engineered mutation	UNP P51570
B	253	ALA	GLU	engineered mutation	UNP P51570
C	1	HIS	-	expression tag	UNP P51570
C	252	ALA	LYS	engineered mutation	UNP P51570
C	253	ALA	GLU	engineered mutation	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).



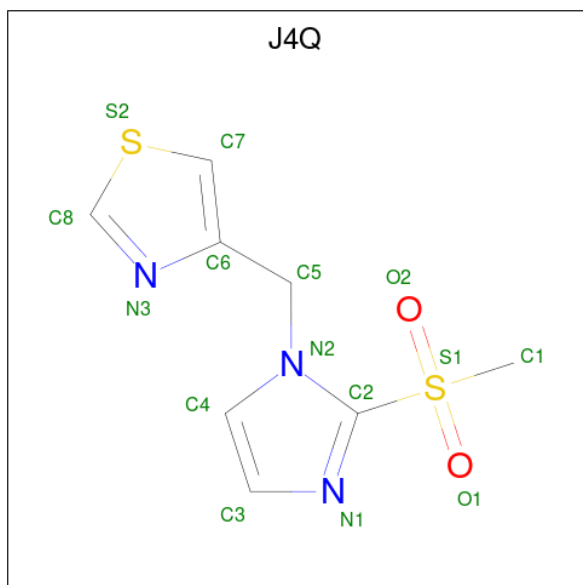
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is 2-(1,3-benzoxazol-2-ylamino)spiro[1,6,7,8-tetrahydroquinazoline-4,1'-cyclohexane]-5-one (CCD ID: HFK) (formula: C₂₀H₂₂N₄O₂).



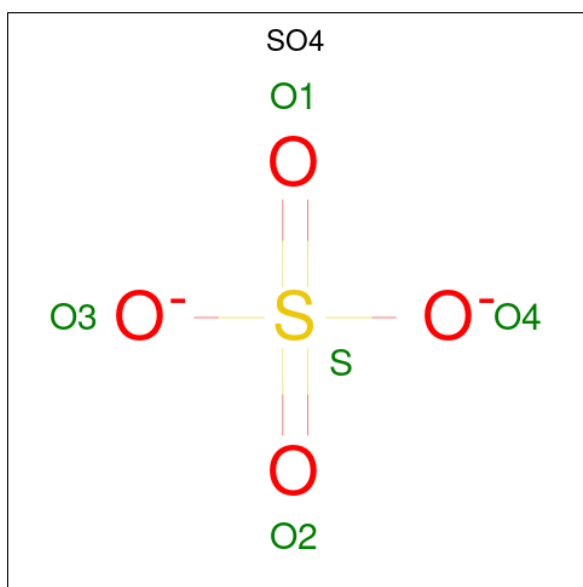
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			26	20	4	2		
3	B	1	Total	C	N	O	0	0
			26	20	4	2		
3	C	1	Total	C	N	O	0	0
			26	20	4	2		

- Molecule 4 is 4-[(2-methylsulfonylimidazol-1-yl)methyl]-1,3-thiazole (CCD ID: J4Q) (formula: $C_8H_9N_3O_2S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	3	2	2		
4	B	1	Total	C	N	O	S	0	0
			15	8	3	2	2		
4	D	1	Total	C	N	O	S	0	0
			15	8	3	2	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		

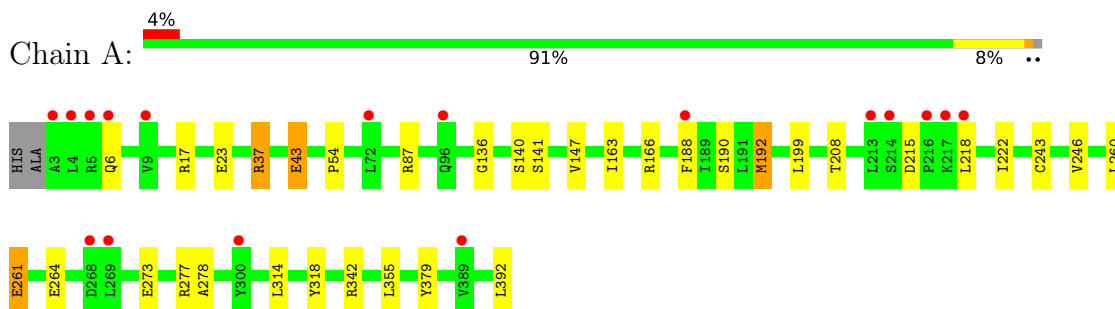
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	81	Total	O	0	0
			81	81		
6	B	45	Total	O	0	0
			45	45		
6	C	18	Total	O	0	0
			18	18		
6	D	28	Total	O	0	0
			28	28		

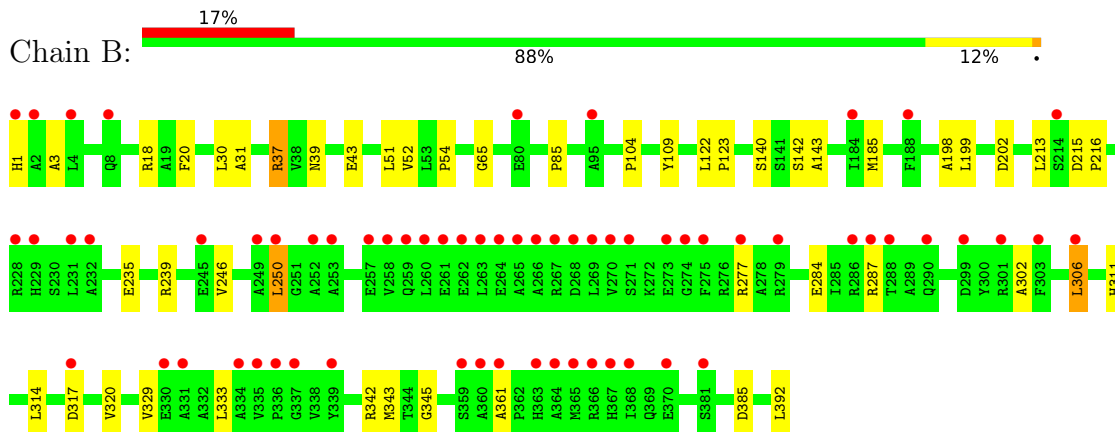
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

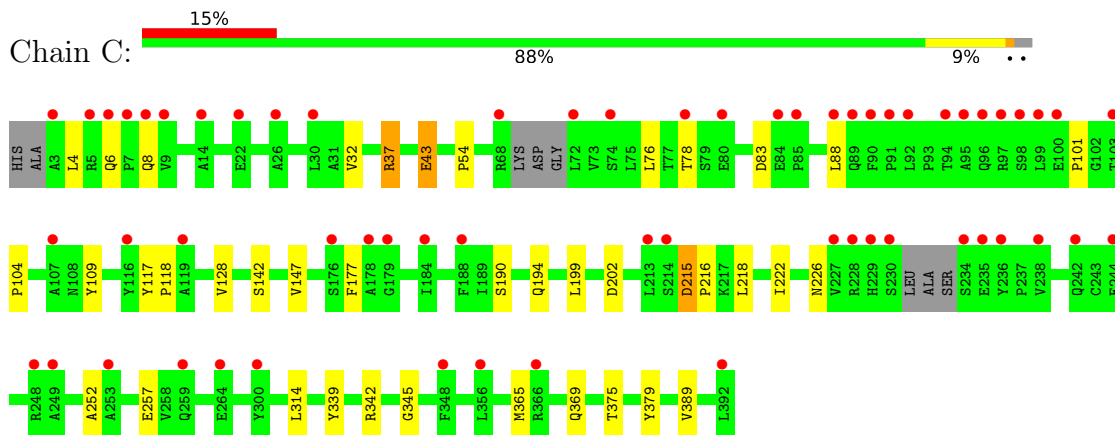
• Molecule 1: Galactokinase



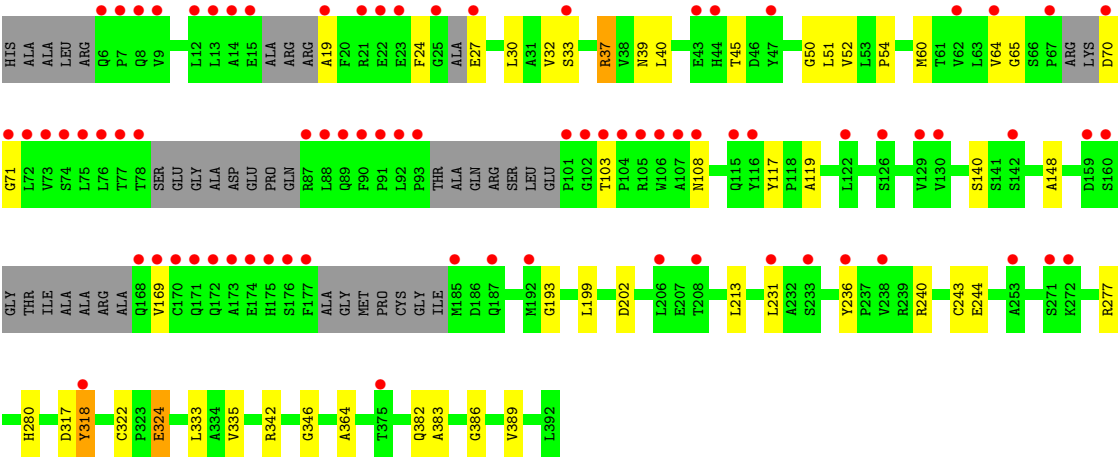
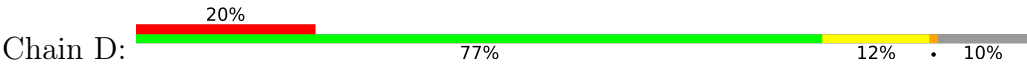
• Molecule 1: Galactokinase



• 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	73.70Å 114.87Å 121.04Å 90.00° 100.56° 90.00°	Depositor
Resolution (Å)	82.65 – 2.40 82.65 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (82.65-2.40) 99.6 (82.65-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.217 , 0.269 0.224 , 0.272	Depositor DCC
R_{free} test set	6310 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.4	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	0.94	EDS
Total number of atoms	11053	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HFK, SO4, J4Q, 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	0.35	0/2885	0.75	0/3928
1	B	0.34	0/2780	0.75	0/3798
1	C	0.33	0/2765	0.77	0/3772
1	D	0.34	0/2481	0.79	3/3378 (0.1%)
All	All	0.34	0/10911	0.77	3/14876 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	65	GLY	N-CA-C	5.50	118.28	110.74
1	D	27	GLU	CA-C-N	5.48	125.68	120.31
1	D	27	GLU	C-N-CA	5.48	125.68	120.31

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	2831	0	2736	22	0
1	B	2729	0	2540	29	0
1	C	2714	0	2567	20	0
1	D	2443	0	2251	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	12	0	12	0	0
2	B	12	0	12	0	0
2	C	12	0	12	0	0
3	A	26	0	0	1	0
3	B	26	0	0	0	0
3	C	26	0	0	0	0
4	A	15	0	0	2	0
4	B	15	0	0	2	0
4	D	15	0	0	5	0
5	C	5	0	0	0	0
6	A	81	0	0	2	0
6	B	45	0	0	1	0
6	C	18	0	0	2	0
6	D	28	0	0	6	0
All	All	11053	0	10130	104	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 5.

All (104) 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)
4:D:401:J4Q:C6	4:D:401:J4Q:N3	1.74	1.30
4:A:403:J4Q:N3	4:A:403:J4Q:C6	1.73	1.23
4:B:403:J4Q:N3	4:B:403:J4Q:C6	1.73	1.18
1:A:37:ARG:NH2	1:A:140:SER:OG	2.02	0.91
1:D:52:VAL:HG12	1:D:54:PRO:HD3	1.56	0.87
1:A:261:GLU:OE2	6:A:501:HOH:O	2.00	0.77
1:D:333:LEU:O	6:D:502:HOH:O	2.02	0.75
1:D:70:ASP:N	6:D:505:HOH:O	2.19	0.74
1:D:19:ALA:N	6:D:506:HOH:O	2.20	0.74
1:D:60:MET:SD	6:D:504:HOH:O	2.47	0.73
1:D:213:LEU:O	4:D:401:J4Q:O1	2.07	0.71
1:A:23:GLU:OE1	1:A:87:ARG:NH2	2.25	0.70
1:A:136:GLY:O	6:A:502:HOH:O	2.11	0.68
1:D:108:ASN:O	6:D:503:HOH:O	2.12	0.67
1:D:382:GLN:HB3	4:D:401:J4Q:C4	2.25	0.66
1:C:226:ASN:ND2	1:C:375:THR:O	2.24	0.65
1:C:37:ARG:HH22	1:C:345:GLY:HA2	1.62	0.64
1:D:37:ARG:NH2	1:D:39:ASN:OD1	2.31	0.63
1:B:37:ARG:NH1	1:B:140:SER:OG	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:VAL:HG12	1:C:389:VAL:HG22	1.82	0.61
4:D:401:J4Q:N3	4:D:401:J4Q:C5	2.60	0.61
1:B:284:GLU:HA	1:B:287:ARG:HD2	1.84	0.60
1:C:252:ALA:HB1	1:C:257:GLU:HB2	1.85	0.58
1:C:4:LEU:HB2	1:C:365:MET:HE1	1.87	0.57
1:B:39:ASN:CG	1:B:185:MET:HE1	2.30	0.57
1:D:243:CYS:SG	1:D:318:TYR:OH	2.54	0.57
1:B:198:ALA:HB2	1:B:213:LEU:HD22	1.87	0.56
1:D:280:HIS:HB3	1:D:318:TYR:CD2	2.40	0.56
1:D:280:HIS:HB3	1:D:318:TYR:HD2	1.70	0.56
4:A:403:J4Q:N3	4:A:403:J4Q:C5	2.60	0.54
1:B:277:ARG:N	1:B:317:ASP:OD2	2.38	0.54
1:A:215:ASP:HB3	1:A:218:LEU:HB3	1.89	0.54
1:B:39:ASN:HB2	1:B:185:MET:HE1	1.91	0.53
1:A:273:GLU:O	1:A:277:ARG:HG2	2.10	0.52
1:C:43:GLU:HB2	1:C:342:ARG:NH2	2.26	0.51
4:B:403:J4Q:N3	4:B:403:J4Q:C5	2.65	0.51
1:A:222:ILE:HB	1:A:379:TYR:HB2	1.93	0.51
1:D:51:LEU:HD23	1:D:202:ASP:HA	1.92	0.51
1:B:385:ASP:OD1	6:B:501:HOH:O	2.18	0.51
1:D:54:PRO:HD2	1:D:199:LEU:O	2.10	0.50
1:D:240:ARG:O	1:D:244:GLU:HG3	2.12	0.50
1:A:243:CYS:SG	1:A:318:TYR:OH	2.63	0.50
1:C:202:ASP:OD2	6:C:501:HOH:O	2.20	0.49
1:B:235:GLU:OE1	1:B:239:ARG:NH2	2.45	0.49
1:A:246:VAL:HG11	1:A:278:ALA:HB2	1.96	0.48
1:A:260:LEU:O	1:A:264:GLU:HG2	2.13	0.48
1:D:33:SER:OG	6:D:504:HOH:O	2.19	0.48
1:A:43:GLU:HB3	1:A:314:LEU:HD21	1.95	0.48
1:A:54:PRO:HD2	1:A:199:LEU:O	2.14	0.48
1:C:83:ASP:OD1	1:C:83:ASP:N	2.44	0.48
1:A:163:ILE:HG21	1:A:192:MET:HG3	1.95	0.48
1:A:188:PHE:CE2	1:A:208:THR:HG21	2.49	0.48
1:D:37:ARG:HH11	1:D:140:SER:HB2	1.79	0.47
1:B:54:PRO:HD2	1:B:199:LEU:O	2.14	0.47
1:D:117:TYR:CE2	1:D:119:ALA:HB3	2.50	0.47
1:A:261:GLU:H	1:A:261:GLU:CD	2.22	0.47
1:B:51:LEU:HD23	1:B:202:ASP:HA	1.95	0.46
1:C:147:VAL:HG21	1:C:190:SER:HB3	1.96	0.46
1:D:335:VAL:HG21	1:D:364:ALA:HA	1.96	0.46
1:C:369:GLN:NE2	6:C:502:HOH:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:HIS:C	1:B:3:ALA:H	2.24	0.46
1:B:39:ASN:CB	1:B:185:MET:HE1	2.45	0.46
1:C:76:LEU:HB3	1:C:128:VAL:HG22	1.97	0.46
1:C:218:LEU:HD11	1:C:339:TYR:HE2	1.79	0.46
1:D:236:TYR:OH	1:D:346:GLY:O	2.28	0.46
1:B:37:ARG:NH2	1:B:345:GLY:HA2	2.31	0.46
1:B:246:VAL:O	1:B:250:LEU:HB2	2.16	0.46
1:A:43:GLU:HB2	1:A:342:ARG:NH2	2.31	0.45
1:D:45:THR:HB	1:D:50:GLY:HA3	1.98	0.45
1:C:101:PRO:HG3	1:C:177:PHE:HA	1.99	0.45
1:B:43:GLU:HB2	1:B:342:ARG:NH2	2.31	0.45
1:D:193:GLY:O	1:D:386:GLY:N	2.49	0.45
1:D:40:LEU:O	1:D:342:ARG:HD3	2.16	0.44
1:B:54:PRO:HB3	1:B:185:MET:CE	2.48	0.44
1:B:320:VAL:HG23	1:B:343:MET:HE1	2.00	0.44
1:D:322:CYS:SG	1:D:324:GLU:HG2	2.57	0.44
1:B:20:PHE:CE2	1:B:65:GLY:HA2	2.54	0.43
1:D:383:ALA:H	4:D:401:J4Q:C4	2.31	0.43
1:A:17:ARG:HE	1:A:392:LEU:HD13	1.83	0.43
1:C:117:TYR:HA	1:C:118:PRO:HD3	1.74	0.43
1:B:43:GLU:HB3	1:B:314:LEU:HD21	2.00	0.43
1:C:43:GLU:HB3	1:C:314:LEU:HD21	2.01	0.43
1:A:37:ARG:O	1:A:37:ARG:HG3	2.15	0.43
1:A:147:VAL:HG21	1:A:190:SER:HB3	1.99	0.42
1:C:109:TYR:CE1	1:C:142:SER:HB2	2.54	0.42
1:B:302:ALA:O	1:B:306:LEU:HB2	2.19	0.42
1:C:222:ILE:HB	1:C:379:TYR:HB2	2.01	0.42
1:C:54:PRO:HD2	1:C:199:LEU:O	2.19	0.41
1:B:215:ASP:HA	1:B:216:PRO:HD3	1.91	0.41
1:C:215:ASP:HA	1:C:216:PRO:HD2	1.86	0.41
1:B:140:SER:HB3	1:B:143:ALA:HB3	2.02	0.41
1:B:31:ALA:HB2	1:B:392:LEU:HD11	2.02	0.41
1:B:85:PRO:HD2	1:B:104:PRO:HD3	2.03	0.41
1:D:32:VAL:HG12	1:D:389:VAL:HG22	2.03	0.41
1:B:333:LEU:HD12	1:B:333:LEU:HA	1.91	0.41
1:B:52:VAL:HG21	1:B:185:MET:HG3	2.03	0.41
1:B:311:HIS:CE1	1:B:329:VAL:HG21	2.56	0.41
1:A:141:SER:HB2	3:A:402:HFK:N19	2.36	0.40
1:C:88:LEU:HD13	1:C:104:PRO:HD2	2.03	0.40
1:A:163:ILE:HG12	1:A:166:ARG:NH1	2.37	0.40
1:B:109:TYR:CE1	1:B:142:SER:HB2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:LEU:HD12	1:B:123:PRO:HD2	2.02	0.40
1:D:277:ARG:NH1	1:D:317:ASP:O	2.54	0.40
1:A:37:ARG:NH2	1:A:140:SER:HG	2.16	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	388/392 (99%)	378 (97%)	9 (2%)	1 (0%)	36	50
1	B	390/392 (100%)	373 (96%)	16 (4%)	1 (0%)	36	50
1	C	378/392 (96%)	357 (94%)	18 (5%)	3 (1%)	16	25
1	D	336/392 (86%)	312 (93%)	19 (6%)	5 (2%)	8	12
All	All	1492/1568 (95%)	1420 (95%)	62 (4%)	10 (1%)	18	28

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	103	THR
1	D	148	ALA
1	B	361	ALA
1	A	6	GLN
1	C	8	GLN
1	C	6	GLN
1	C	215	ASP
1	D	24	PHE
1	D	169	VAL
1	D	71	GLY

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	278/309 (90%)	273 (98%)	5 (2%)	51	73
1	B	252/309 (82%)	247 (98%)	5 (2%)	48	70
1	C	256/309 (83%)	252 (98%)	4 (2%)	55	76
1	D	221/309 (72%)	215 (97%)	6 (3%)	39	62
All	All	1007/1236 (82%)	987 (98%)	20 (2%)	48	70

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	43	GLU
1	A	192	MET
1	A	261	GLU
1	A	355	LEU
1	B	18	ARG
1	B	30	LEU
1	B	37	ARG
1	B	250	LEU
1	B	306	LEU
1	C	37	ARG
1	C	43	GLU
1	C	78	THR
1	C	194	GLN
1	D	30	LEU
1	D	37	ARG
1	D	64	VAL
1	D	231	LEU
1	D	318	TYR
1	D	324	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	367	HIS
1	C	39	ASN
1	D	363	HIS
1	D	371	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 ⓘ

10 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	$\# Z > 2$
5	SO4	C	403	-	4,4,4	0.23	0	6,6,6	0.11	0
2	GAL	C	401	-	12,12,12	0.48	0	17,17,17	0.80	0
3	HFK	C	402	-	29,30,30	4.32	15 (51%)	32,44,44	4.42	16 (50%)
4	J4Q	B	403	-	15,16,16	4.99	10 (66%)	15,23,23	5.29	8 (53%)
2	GAL	A	401	-	12,12,12	0.73	0	17,17,17	0.92	0
3	HFK	A	402	-	29,30,30	4.24	15 (51%)	32,44,44	4.52	18 (56%)
4	J4Q	A	403	-	15,16,16	5.00	9 (60%)	15,23,23	4.73	7 (46%)
4	J4Q	D	401	-	15,16,16	4.98	9 (60%)	15,23,23	4.53	8 (53%)
2	GAL	B	401	-	12,12,12	0.45	0	17,17,17	0.86	0
3	HFK	B	402	-	29,30,30	4.28	15 (51%)	32,44,44	4.44	19 (59%)

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	C	401	-	-	1/2/22/22	0/1/1/1
3	HFK	C	402	-	-	2/4/43/43	0/5/5/5
4	J4Q	B	403	-	-	6/9/10/10	0/2/2/2
2	GAL	A	401	-	-	2/2/22/22	0/1/1/1
3	HFK	A	402	-	-	2/4/43/43	0/5/5/5
4	J4Q	A	403	-	-	3/9/10/10	0/2/2/2
4	J4Q	D	401	-	-	1/9/10/10	0/2/2/2
2	GAL	B	401	-	-	2/2/22/22	0/1/1/1
3	HFK	B	402	-	-	2/4/43/43	0/5/5/5

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	401	J4Q	C6-N3	13.83	1.74	1.38
4	B	403	J4Q	C6-N3	13.58	1.73	1.38
4	A	403	J4Q	C6-N3	13.58	1.73	1.38
3	A	402	HFK	C06-C07	12.41	1.52	1.37
3	B	402	HFK	C06-C07	12.21	1.52	1.37
3	C	402	HFK	C06-C07	12.15	1.52	1.37
3	C	402	HFK	C15-N16	11.05	1.54	1.36
3	B	402	HFK	C15-N16	10.62	1.53	1.36
3	A	402	HFK	C15-N16	10.48	1.53	1.36
4	A	403	J4Q	O2-S1	7.82	1.52	1.43
4	B	403	J4Q	O2-S1	7.80	1.52	1.43
3	B	402	HFK	C15-N14	7.66	1.50	1.30
3	C	402	HFK	C15-N14	7.51	1.49	1.30
3	A	402	HFK	C15-N14	7.50	1.49	1.30
4	D	401	J4Q	O2-S1	7.49	1.51	1.43
4	A	403	J4Q	O1-S1	7.45	1.51	1.43
4	B	403	J4Q	O1-S1	7.28	1.51	1.43
4	D	401	J4Q	O1-S1	7.12	1.51	1.43
3	C	402	HFK	O01-C02	6.33	1.35	1.23
3	B	402	HFK	O01-C02	6.20	1.35	1.23
3	A	402	HFK	O01-C02	6.00	1.35	1.23
3	C	402	HFK	C06-N16	5.92	1.46	1.37
3	B	402	HFK	C06-N16	5.72	1.46	1.37
3	C	402	HFK	C18-N17	5.68	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	J4Q	C5-C6	-5.61	1.42	1.50
3	A	402	HFK	C06-N16	5.58	1.46	1.37
3	B	402	HFK	C18-N17	5.52	1.47	1.36
4	D	401	J4Q	C5-C6	-5.49	1.42	1.50
3	A	402	HFK	C18-N17	5.37	1.46	1.36
4	B	403	J4Q	C5-C6	-5.15	1.43	1.50
3	B	402	HFK	C25-C24	4.05	1.47	1.38
3	C	402	HFK	C25-C24	4.03	1.47	1.38
3	A	402	HFK	C02-C07	3.96	1.58	1.46
3	B	402	HFK	C02-C07	3.96	1.58	1.46
3	C	402	HFK	C02-C07	3.94	1.58	1.46
3	A	402	HFK	C03-C02	3.88	1.56	1.50
3	A	402	HFK	C25-C24	3.87	1.46	1.38
3	C	402	HFK	C03-C02	3.68	1.55	1.50
3	B	402	HFK	C03-C02	3.55	1.55	1.50
3	B	402	HFK	C23-C21	3.51	1.46	1.39
3	C	402	HFK	C23-C21	3.44	1.46	1.39
3	B	402	HFK	C08-N14	3.28	1.49	1.46
3	A	402	HFK	C23-C21	3.21	1.46	1.39
3	A	402	HFK	C08-N14	3.04	1.49	1.46
3	B	402	HFK	C21-C20	2.95	1.42	1.38
4	B	403	J4Q	C2-S1	2.94	1.80	1.78
4	A	403	J4Q	C5-N2	-2.82	1.42	1.46
3	A	402	HFK	C21-C20	2.78	1.41	1.38
3	C	402	HFK	C08-N14	2.77	1.49	1.46
4	D	401	J4Q	C5-N2	-2.75	1.42	1.46
4	B	403	J4Q	C1-S1	2.73	1.79	1.75
3	C	402	HFK	C21-C20	2.68	1.41	1.38
3	A	402	HFK	C05-C06	2.65	1.54	1.49
4	D	401	J4Q	C1-S1	2.64	1.79	1.75
4	A	403	J4Q	C4-C3	2.62	1.41	1.35
3	A	402	HFK	C15-N17	-2.56	1.32	1.37
4	D	401	J4Q	C4-C3	2.56	1.41	1.35
3	C	402	HFK	C05-C06	2.55	1.53	1.49
3	B	402	HFK	C05-C06	2.47	1.53	1.49
4	B	403	J4Q	C5-N2	-2.46	1.43	1.46
4	D	401	J4Q	C7-S2	-2.46	1.62	1.70
4	B	403	J4Q	C4-C3	2.45	1.40	1.35
4	A	403	J4Q	C7-S2	-2.43	1.63	1.70
4	B	403	J4Q	C7-S2	-2.35	1.63	1.70
4	D	401	J4Q	C8-S2	-2.28	1.64	1.70
3	C	402	HFK	C15-N17	-2.27	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	HFK	C15-N17	-2.27	1.32	1.37
4	A	403	J4Q	C8-S2	-2.14	1.65	1.70
4	B	403	J4Q	C8-S2	-2.13	1.65	1.70
3	C	402	HFK	C04-C05	2.13	1.58	1.52
4	A	403	J4Q	C1-S1	2.12	1.78	1.75
3	B	402	HFK	C04-C05	2.12	1.58	1.52
3	A	402	HFK	C04-C05	2.09	1.58	1.52

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	J4Q	C7-S2-C8	12.62	105.06	89.47
4	B	403	J4Q	C7-S2-C8	12.37	104.75	89.47
4	D	401	J4Q	C7-S2-C8	12.09	104.40	89.47
3	C	402	HFK	C07-C06-N16	-11.42	112.89	122.11
3	A	402	HFK	C02-C07-C06	-11.13	109.30	119.18
3	B	402	HFK	C07-C06-N16	-9.76	114.23	122.11
3	A	402	HFK	C07-C06-N16	-9.71	114.27	122.11
3	B	402	HFK	C02-C07-C06	-9.69	110.58	119.18
4	B	403	J4Q	O2-S1-O1	-9.46	107.38	118.26
3	B	402	HFK	O01-C02-C03	-8.53	106.89	120.87
3	A	402	HFK	O01-C02-C03	-8.46	107.00	120.87
3	C	402	HFK	C08-C07-C06	-8.27	112.42	121.75
3	C	402	HFK	O01-C02-C07	-8.12	110.64	121.53
3	C	402	HFK	C02-C07-C06	-7.85	112.22	119.18
3	C	402	HFK	O01-C02-C03	-7.80	108.09	120.87
3	C	402	HFK	N16-C15-N14	-7.61	110.14	123.63
4	D	401	J4Q	O2-S1-O1	-7.60	109.51	118.26
3	B	402	HFK	N16-C15-N14	-7.51	110.32	123.63
3	B	402	HFK	O01-C02-C07	-7.50	111.47	121.53
3	A	402	HFK	N17-C15-N16	-7.25	105.77	117.96
3	A	402	HFK	N16-C15-N14	-7.14	110.96	123.63
4	B	403	J4Q	C7-C6-N3	-7.11	104.44	115.13
3	B	402	HFK	C08-C07-C06	-6.97	113.89	121.75
3	B	402	HFK	C05-C06-C07	-6.82	113.43	122.72
3	A	402	HFK	O01-C02-C07	-6.82	112.39	121.53
4	B	403	J4Q	S2-C8-N3	-6.80	104.93	115.58
4	D	401	J4Q	S2-C8-N3	-6.71	105.07	115.58
3	A	402	HFK	C08-C07-C06	-6.66	114.23	121.75
4	A	403	J4Q	O2-S1-O1	-6.64	110.62	118.26
3	C	402	HFK	C05-C06-C07	-6.56	113.79	122.72
4	A	403	J4Q	C7-C6-N3	-6.32	105.63	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	J4Q	S2-C8-N3	-6.27	105.77	115.58
3	B	402	HFK	N17-C15-N16	-6.26	107.44	117.96
3	A	402	HFK	C05-C06-C07	-6.16	114.33	122.72
3	A	402	HFK	C05-C06-N16	-5.94	107.02	115.46
3	B	402	HFK	C05-C06-N16	-5.52	107.61	115.46
4	B	403	J4Q	C8-N3-C6	-5.38	104.36	110.37
3	C	402	HFK	N17-C15-N16	-4.92	109.69	117.96
4	D	401	J4Q	C7-C6-N3	-4.85	107.83	115.13
4	B	403	J4Q	C6-C7-S2	-4.58	104.63	110.56
4	A	403	J4Q	C8-N3-C6	-4.47	105.38	110.37
3	C	402	HFK	C05-C06-N16	-4.24	109.44	115.46
4	A	403	J4Q	C6-C7-S2	-4.03	105.34	110.56
4	B	403	J4Q	C4-C3-N1	-3.84	105.71	110.74
4	D	401	J4Q	C4-C3-N1	-3.82	105.74	110.74
3	A	402	HFK	O22-C21-C23	3.79	134.45	126.49
3	B	402	HFK	O22-C21-C23	3.71	134.30	126.49
3	A	402	HFK	C23-C21-C20	-3.71	119.11	123.62
3	C	402	HFK	N17-C15-N14	-3.66	111.13	117.96
3	C	402	HFK	C15-N16-C06	-3.65	112.34	121.02
3	C	402	HFK	O22-C21-C23	3.64	134.14	126.49
4	A	403	J4Q	C4-C3-N1	-3.56	106.08	110.74
3	C	402	HFK	O22-C18-N19	-3.44	109.39	115.57
3	B	402	HFK	C23-C21-C20	-3.34	119.56	123.62
3	A	402	HFK	C03-C02-C07	-3.25	111.02	117.35
3	B	402	HFK	C15-N16-C06	-3.25	113.31	121.02
3	B	402	HFK	O22-C18-N19	-3.25	109.74	115.57
3	A	402	HFK	O22-C18-N19	-3.18	109.86	115.57
3	A	402	HFK	C15-N16-C06	-3.16	113.52	121.02
3	C	402	HFK	C23-C21-C20	-3.01	119.96	123.62
3	B	402	HFK	C03-C02-C07	-2.98	111.56	117.35
3	B	402	HFK	N17-C15-N14	-2.84	112.66	117.96
3	C	402	HFK	O22-C21-C20	-2.79	105.90	107.80
3	A	402	HFK	N17-C15-N14	-2.66	113.01	117.96
4	B	403	J4Q	S1-C2-N2	2.62	131.25	127.00
4	D	401	J4Q	C6-C7-S2	-2.57	107.24	110.56
3	C	402	HFK	C03-C02-C07	-2.54	112.41	117.35
3	B	402	HFK	O22-C21-C20	-2.42	106.15	107.80
3	A	402	HFK	C21-C20-N19	-2.39	106.38	108.60
3	A	402	HFK	C20-N19-C18	2.29	108.67	104.13
3	B	402	HFK	C09-C10-C11	2.29	114.92	111.35
4	D	401	J4Q	C8-N3-C6	-2.25	107.86	110.37
3	A	402	HFK	N17-C18-N19	-2.19	122.35	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	HFK	C21-C20-N19	-2.15	106.60	108.60
3	B	402	HFK	C20-N19-C18	2.14	108.37	104.13
4	D	401	J4Q	O2-S1-C1	2.11	110.70	108.47

There are no chirality outliers.

All (21) 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
3	C	402	HFK	N14-C15-N17-C18
4	A	403	J4Q	N1-C2-S1-C1
4	B	403	J4Q	N1-C2-S1-C1
4	D	401	J4Q	N1-C2-S1-C1
2	A	401	GAL	O5-C5-C6-O6
2	B	401	GAL	O5-C5-C6-O6
2	B	401	GAL	C4-C5-C6-O6
2	A	401	GAL	C4-C5-C6-O6
2	C	401	GAL	O5-C5-C6-O6
4	B	403	J4Q	N2-C5-C6-N3
3	B	402	HFK	N16-C15-N17-C18
3	C	402	HFK	N16-C15-N17-C18
3	A	402	HFK	N16-C15-N17-C18
4	B	403	J4Q	N1-C2-S1-O1
4	B	403	J4Q	N1-C2-S1-O2
4	A	403	J4Q	N2-C2-S1-O1
4	B	403	J4Q	N2-C2-S1-O1
4	B	403	J4Q	N2-C2-S1-O2
4	A	403	J4Q	C6-C5-N2-C4

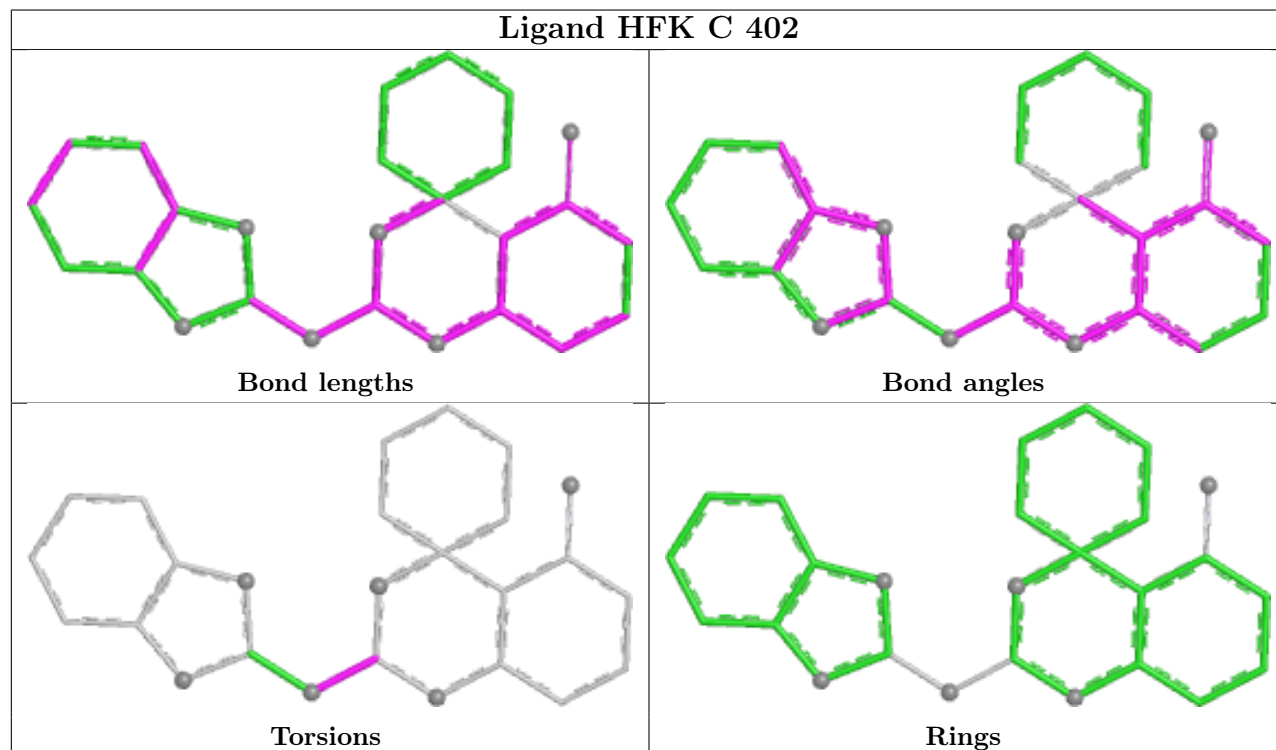
There are no ring outliers.

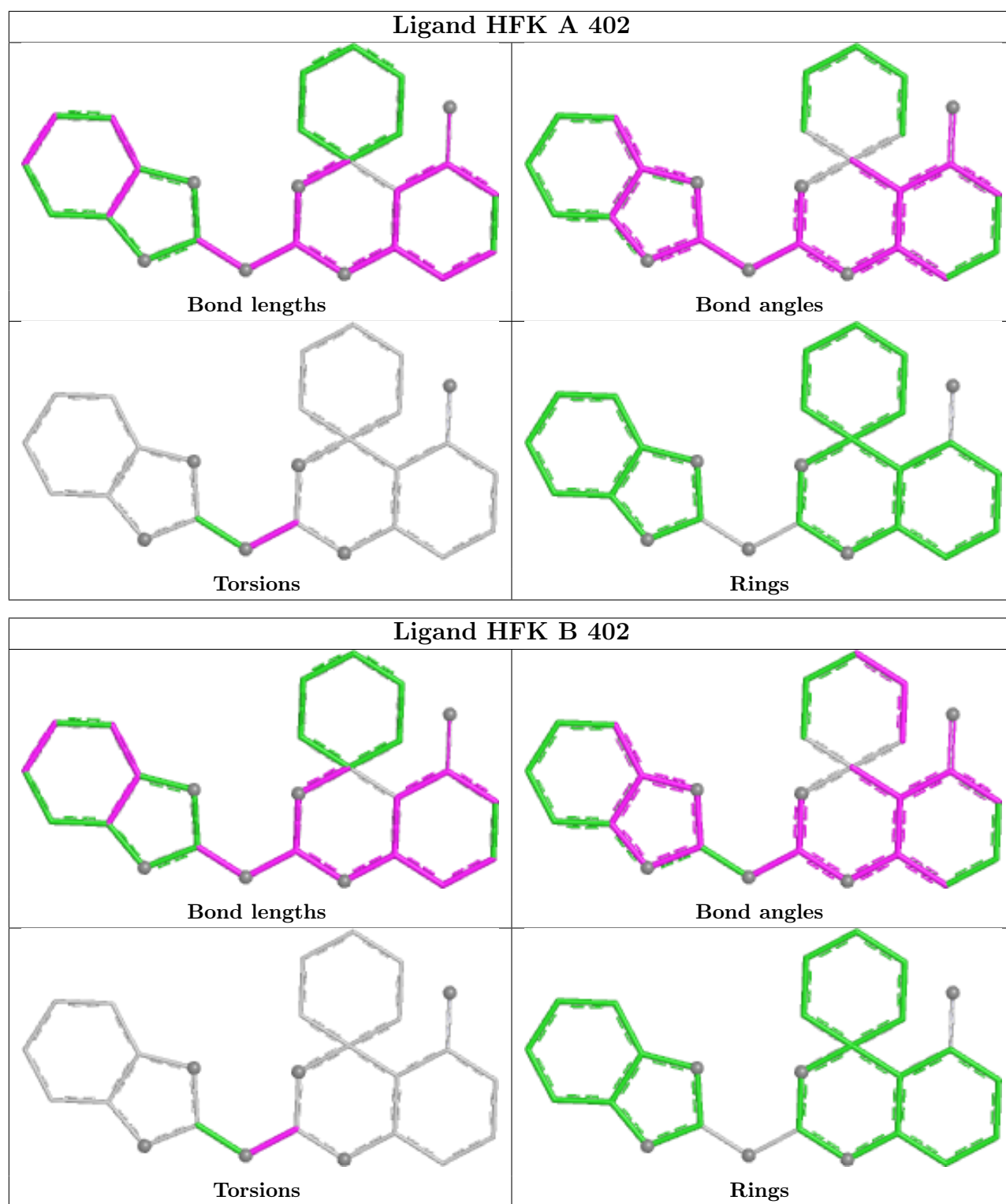
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	J4Q	2	0
3	A	402	HFK	1	0
4	A	403	J4Q	2	0
4	D	401	J4Q	5	0

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

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	390/392 (99%)	0.26	17 (4%) 39 34	31, 47, 73, 89	0
1	B	392/392 (100%)	0.96	65 (16%) 4 3	37, 61, 107, 132	0
1	C	384/392 (97%)	1.00	60 (15%) 5 4	39, 60, 99, 140	0
1	D	352/392 (89%)	1.20	78 (22%) 2 2	33, 62, 111, 140	0
All	All	1518/1568 (96%)	0.85	220 (14%) 6 4	31, 57, 102, 140	0

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	107	ALA	6.7
1	D	318	TYR	6.4
1	D	15	GLU	5.9
1	C	230	SER	5.7
1	D	106	TRP	5.5
1	D	101	PRO	5.4
1	B	265	ALA	5.3
1	B	231	LEU	5.2
1	C	99	LEU	5.1
1	B	266	ALA	5.1
1	D	19	ALA	5.0
1	B	277	ARG	5.0
1	B	370	GLU	4.9
1	B	268	ASP	4.8
1	B	363	HIS	4.8
1	D	185	MET	4.7
1	D	27	GLU	4.6
1	C	234	SER	4.6
1	D	93	PRO	4.5
1	D	6	GLN	4.5
1	C	72	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	270	VAL	4.4
1	D	47	TYR	4.3
1	D	126	SER	4.3
1	C	235	GLU	4.3
1	B	263	LEU	4.3
1	C	236	TYR	4.3
1	B	330	GLU	4.2
1	C	214	SER	4.2
1	C	98	SER	4.2
1	C	97	ARG	4.2
1	C	96	GLN	4.2
1	B	360	ALA	4.0
1	D	70	ASP	4.0
1	C	6	GLN	4.0
1	D	104	PRO	4.0
1	D	21	ARG	4.0
1	B	368	ILE	4.0
1	D	23	GLU	4.0
1	D	116	TYR	3.9
1	C	3	ALA	3.9
1	B	275	PHE	3.9
1	D	43	GLU	3.9
1	B	336	PRO	3.8
1	B	361	ALA	3.7
1	C	84	GLU	3.7
1	B	249	ALA	3.7
1	D	78	THR	3.7
1	B	267	ARG	3.7
1	D	77	THR	3.6
1	D	108	ASN	3.6
1	C	74	SER	3.6
1	B	299	ASP	3.6
1	D	87	ARG	3.6
1	C	26	ALA	3.5
1	B	269	LEU	3.5
1	B	271	SER	3.5
1	C	80	GLU	3.5
1	C	89	GLN	3.4
1	C	100	GLU	3.4
1	D	105	ARG	3.4
1	D	22	GLU	3.4
1	D	174	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	173	ALA	3.4
1	B	259	GLN	3.3
1	C	68	ARG	3.3
1	C	8	GLN	3.3
1	C	259	GLN	3.3
1	C	7	PRO	3.3
1	B	274	GLY	3.3
1	D	177	PHE	3.2
1	C	229	HIS	3.2
1	D	122	LEU	3.2
1	C	238	VAL	3.2
1	D	89	GLN	3.2
1	B	250	LEU	3.2
1	D	159	ASP	3.1
1	D	91	PRO	3.1
1	C	176	SER	3.1
1	D	44	HIS	3.1
1	C	392	LEU	3.1
1	B	339	TYR	3.1
1	B	303	PHE	3.1
1	A	188	PHE	3.1
1	D	90	PHE	3.1
1	D	172	GLN	3.0
1	C	9	VAL	3.0
1	B	260	LEU	3.0
1	D	25	GLY	3.0
1	C	264	GLU	3.0
1	B	188	PHE	3.0
1	D	62	VAL	2.9
1	D	231	LEU	2.9
1	B	245	GLU	2.9
1	B	1	HIS	2.9
1	D	169	VAL	2.9
1	B	80	GLU	2.9
1	C	184	ILE	2.9
1	D	233	SER	2.8
1	D	192	MET	2.8
1	B	273	GLU	2.8
1	B	337	GLY	2.8
1	D	9	VAL	2.8
1	A	4	LEU	2.8
1	C	92	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	72	LEU	2.8
1	A	268	ASP	2.8
1	D	14	ALA	2.8
1	D	7	PRO	2.7
1	B	258	VAL	2.7
1	D	73	VAL	2.7
1	D	92	LEU	2.7
1	B	334	ALA	2.7
1	B	8	GLN	2.7
1	D	102	GLY	2.7
1	D	76	LEU	2.7
1	D	88	LEU	2.7
1	B	4	LEU	2.6
1	B	335	VAL	2.6
1	C	244	GLU	2.6
1	D	74	SER	2.6
1	B	288	THR	2.6
1	D	170	CYS	2.6
1	A	213	LEU	2.6
1	D	72	LEU	2.6
1	B	331	ALA	2.6
1	D	142	SER	2.6
1	D	236	TYR	2.6
1	A	6	GLN	2.6
1	B	366	ARG	2.5
1	D	67	PRO	2.5
1	B	264	GLU	2.5
1	C	188	PHE	2.5
1	D	115	GLN	2.5
1	B	214	SER	2.5
1	C	253	ALA	2.5
1	C	228	ARG	2.5
1	C	107	ALA	2.5
1	C	103	THR	2.5
1	D	75	LEU	2.5
1	B	2	ALA	2.5
1	C	90	PHE	2.5
1	C	5	ARG	2.5
1	D	103	THR	2.5
1	A	269	LEU	2.4
1	B	306	LEU	2.4
1	B	232	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	375	THR	2.4
1	A	218	LEU	2.4
1	D	187	GLN	2.4
1	D	253	ALA	2.4
1	B	317	ASP	2.4
1	D	13	LEU	2.4
1	B	261	GLU	2.4
1	C	248	ARG	2.4
1	A	217	LYS	2.4
1	D	208	THR	2.3
1	B	359	SER	2.3
1	D	160	SER	2.3
1	A	5	ARG	2.3
1	B	229	HIS	2.3
1	D	8	GLN	2.3
1	C	227	VAL	2.3
1	C	300	TYR	2.3
1	B	95	ALA	2.3
1	D	176	SER	2.3
1	B	367	HIS	2.3
1	A	9	VAL	2.3
1	B	290	GLN	2.3
1	B	184	ILE	2.3
1	A	300	TYR	2.3
1	B	252	ALA	2.2
1	C	116	TYR	2.3
1	C	249	ALA	2.2
1	D	175	HIS	2.2
1	B	365	MET	2.2
1	B	381	SER	2.2
1	C	22	GLU	2.2
1	C	348	PHE	2.2
1	B	301	ARG	2.2
1	C	91	PRO	2.2
1	A	3	ALA	2.2
1	C	179	GLY	2.2
1	C	30	LEU	2.2
1	D	12	LEU	2.2
1	B	228	ARG	2.2
1	D	64	VAL	2.2
1	D	129	VAL	2.2
1	C	95	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	94	THR	2.2
1	D	71	GLY	2.2
1	B	364	ALA	2.2
1	D	272	LYS	2.2
1	C	242	GLN	2.2
1	D	168	GLN	2.1
1	C	213	LEU	2.1
1	B	262	GLU	2.1
1	D	271	SER	2.1
1	C	85	PRO	2.1
1	A	389	VAL	2.1
1	C	14	ALA	2.1
1	C	178	ALA	2.1
1	C	88	LEU	2.1
1	B	257	GLU	2.1
1	B	279	ARG	2.1
1	D	33	SER	2.1
1	A	216	PRO	2.1
1	D	171	GLN	2.1
1	A	214	SER	2.1
1	B	286	ARG	2.1
1	B	287	ARG	2.1
1	D	206	LEU	2.1
1	C	78	THR	2.1
1	A	96	GLN	2.0
1	B	253	ALA	2.0
1	C	366	ARG	2.0
1	C	356	LEU	2.0
1	D	130	VAL	2.0
1	D	238	VAL	2.0
1	C	119	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

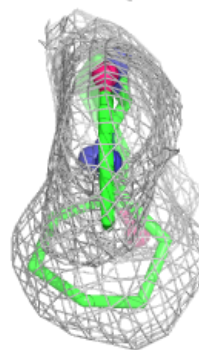
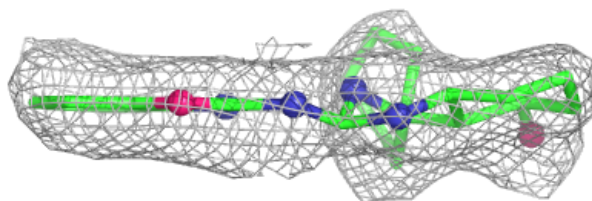
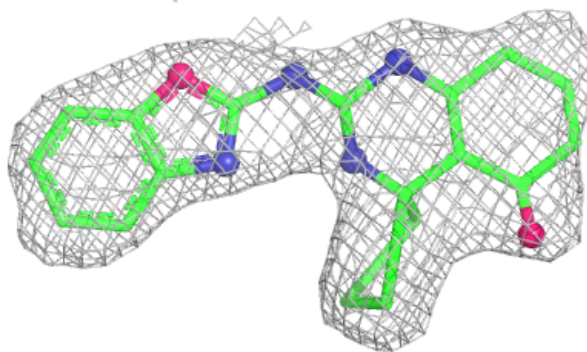
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	J4Q	D	401	15/15	0.66	0.26	55,123,135,135	0
4	J4Q	B	403	15/15	0.68	0.31	52,149,151,151	0
4	J4Q	A	403	15/15	0.72	0.30	85,93,121,153	0
2	GAL	C	401	12/12	0.86	0.12	48,60,64,70	0
5	SO4	C	403	5/5	0.86	0.16	87,88,90,92	0
3	HFK	C	402	26/26	0.87	0.15	62,66,76,79	0
2	GAL	B	401	12/12	0.89	0.10	44,52,55,55	0
3	HFK	B	402	26/26	0.93	0.12	49,54,60,65	0
2	GAL	A	401	12/12	0.93	0.08	32,36,43,53	0
3	HFK	A	402	26/26	0.94	0.10	36,42,53,57	0

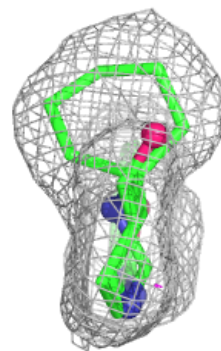
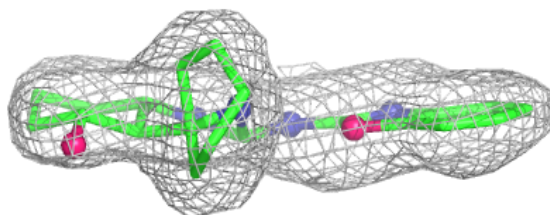
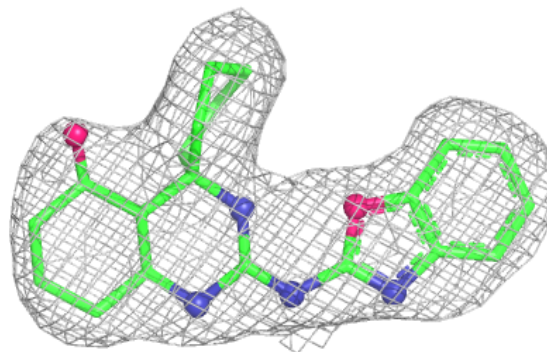
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

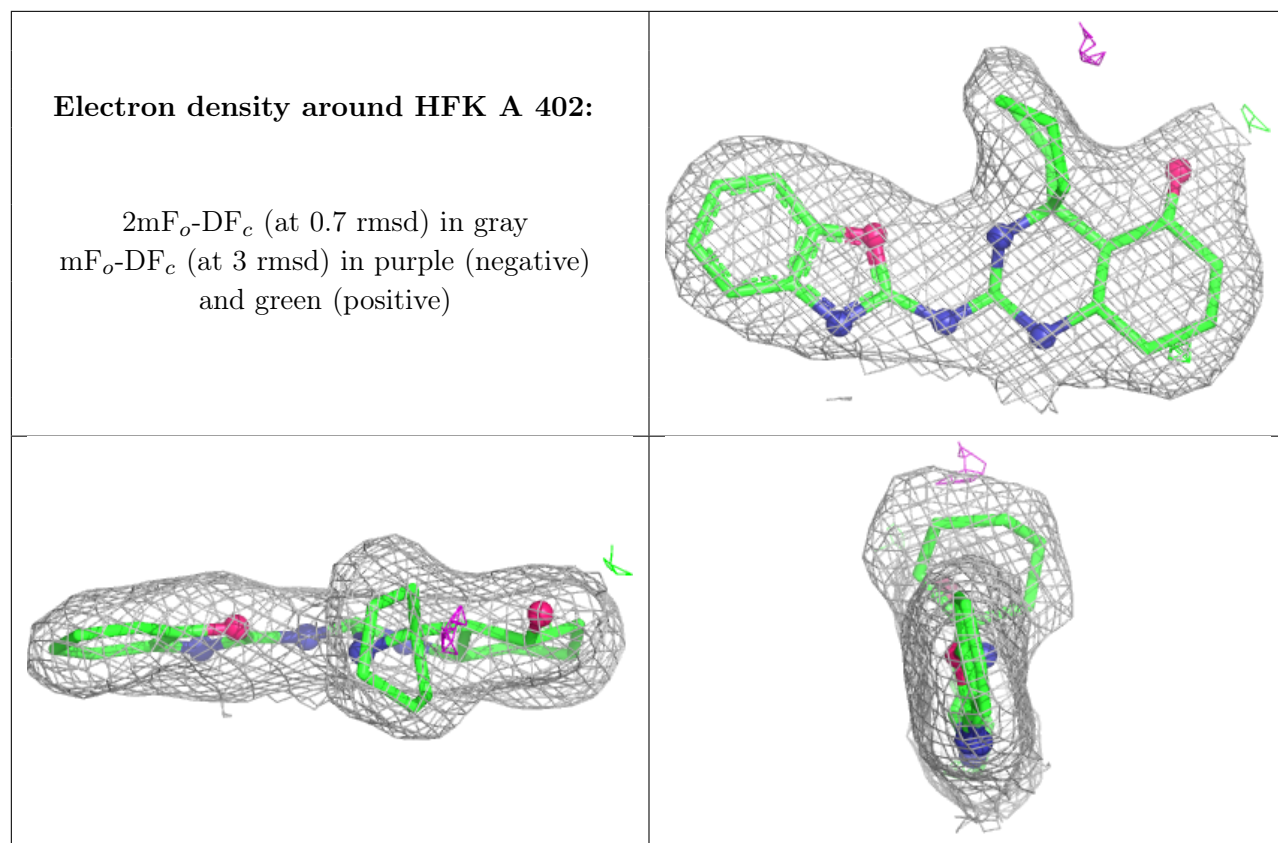
Electron density around HFK C 402:

$2mF_o-DF_c$ (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.