



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:52 PM UTC

PDB ID : 6Q3W / pdb_00006q3w
Title : Structure of human galactokinase 1 bound with Ethyl 1-(2-pyrazinyl)-4-piperidinecarboxylate
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Deposited on : 2018-12-04
Resolution : 1.96 Å(reported)

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

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

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

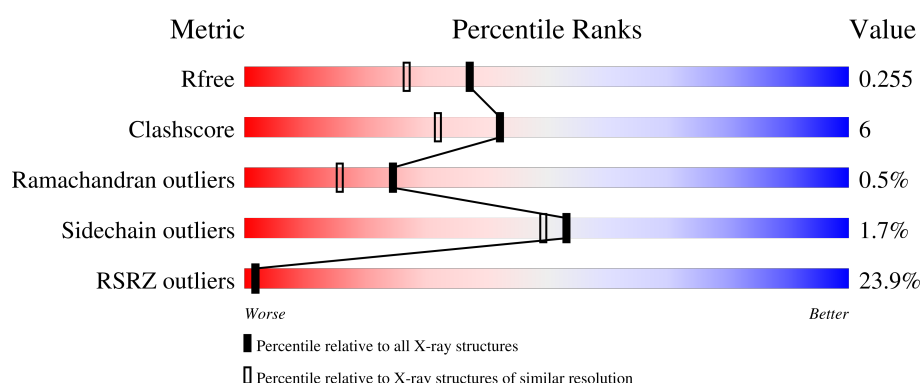
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	391	8% 91% 9% .
1	B	391	18% 87% 10% ..
1	C	391	32% 86% 13% .
1	D	391	35% 79% 11% . 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11460 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

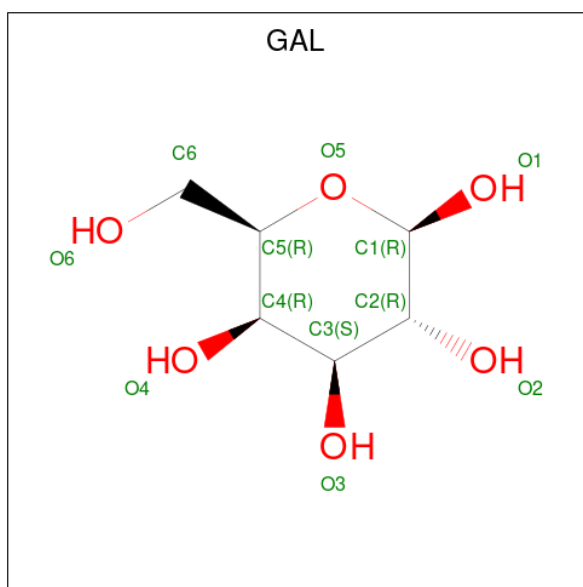
- Molecule 1 is a protein called Galactokinase.

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

There are 8 discrepancies between the modelled and reference sequences:

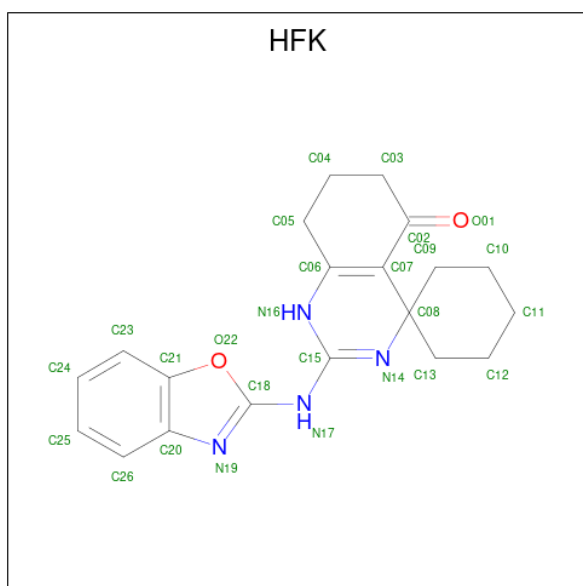
Chain	Residue	Modelled	Actual	Comment	Reference
A	252	ALA	LYS	conflict	UNP P51570
A	253	ALA	GLU	conflict	UNP P51570
B	252	ALA	LYS	conflict	UNP P51570
B	253	ALA	GLU	conflict	UNP P51570
C	252	ALA	LYS	conflict	UNP P51570
C	253	ALA	GLU	conflict	UNP P51570
D	252	ALA	LYS	conflict	UNP P51570
D	253	ALA	GLU	conflict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

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



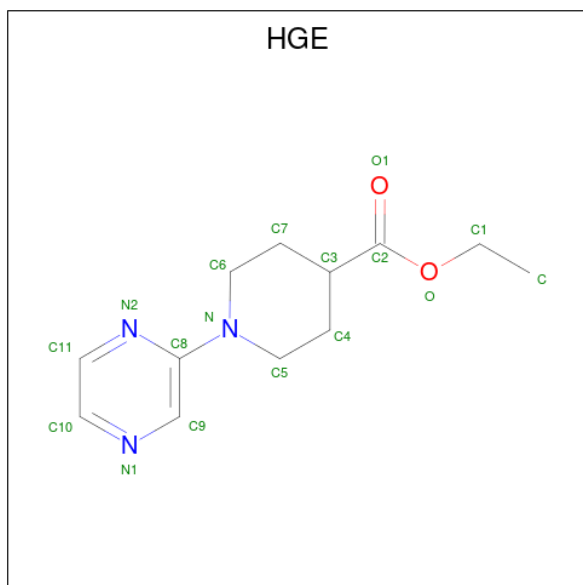
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		

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



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

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



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

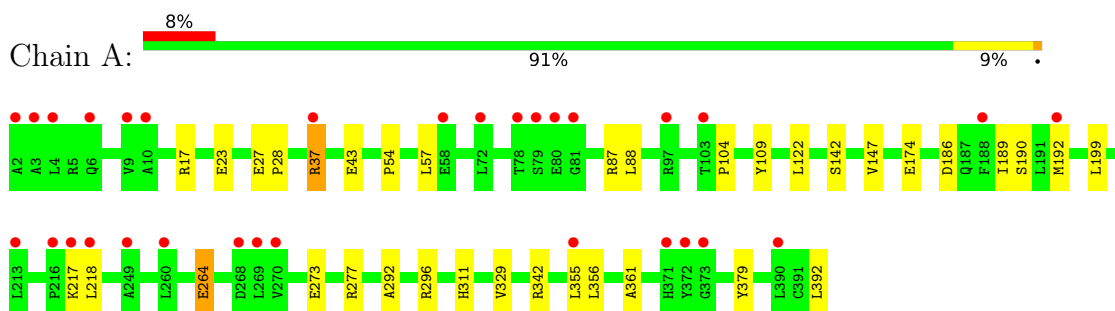
- Molecule 5 is water.

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

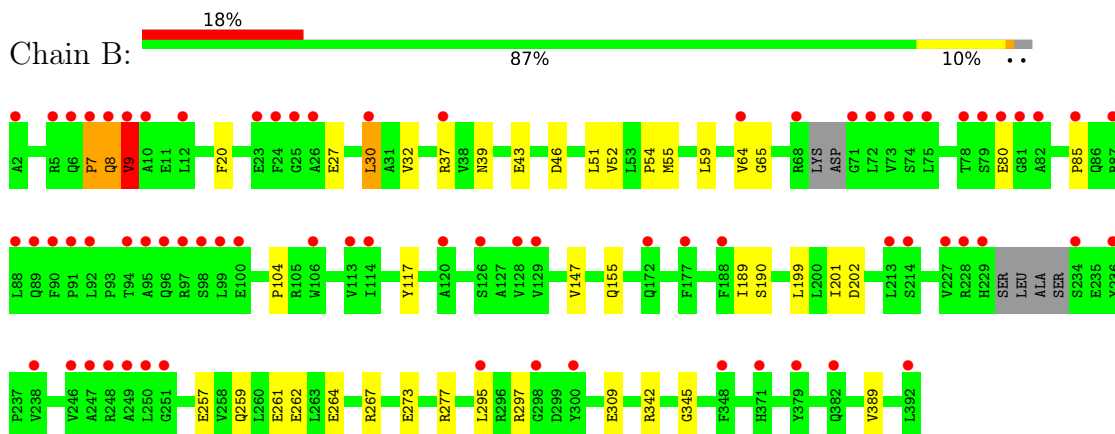
3 Residue-property plots

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.

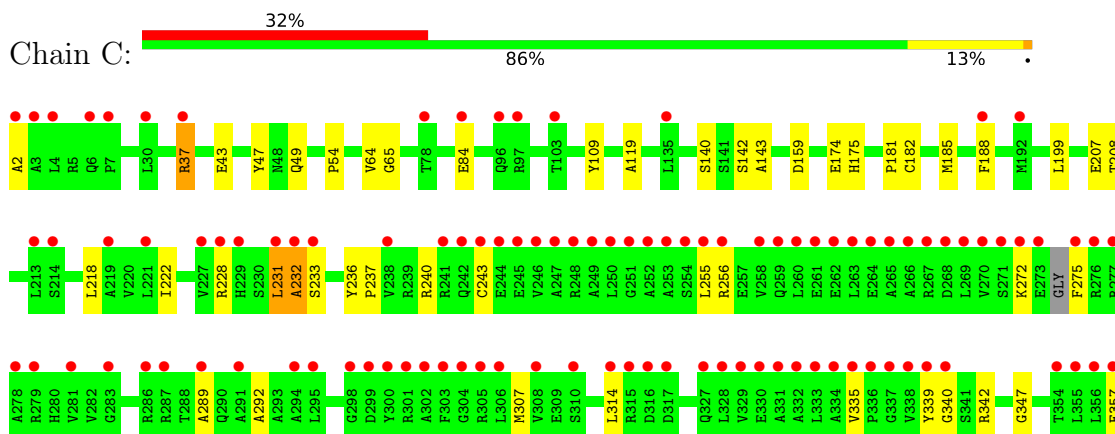
• Molecule 1: Galactokinase



• Molecule 1: Galactokinase

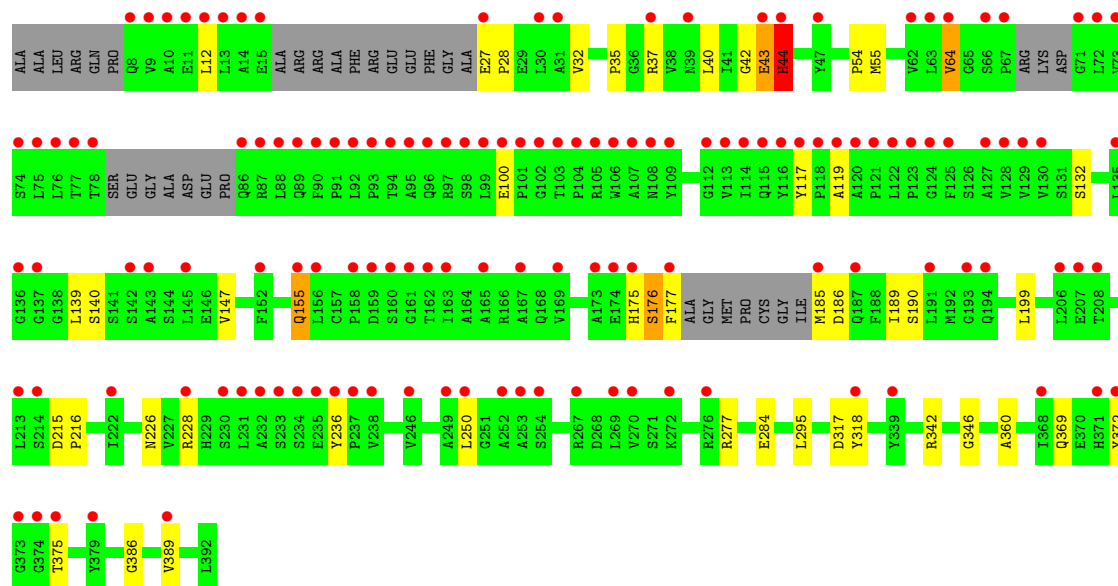
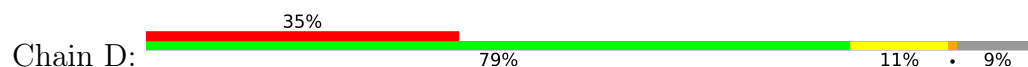


• Molecule 1: Galactokinase





● 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	73.26Å 114.81Å 120.82Å 90.00° 100.49° 90.00°	Depositor
Resolution (Å)	82.56 – 1.96 82.56 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.3 (82.56-1.96) 99.4 (82.56-1.96)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 1.97Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.232 , 0.255 0.234 , 0.255	Depositor DCC
R_{free} test set	7036 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.1	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	11460	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

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

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: GAL, HFK, HGE

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	0.34	0/2851	0.73	0/3889
1	B	0.33	0/2772	0.75	2/3786 (0.1%)
1	C	0.34	0/2761	0.80	3/3775 (0.1%)
1	D	0.37	0/2499	0.85	4/3414 (0.1%)
All	All	0.35	0/10883	0.78	9/14864 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	231	LEU	CA-C-N	7.24	134.73	121.70
1	C	231	LEU	C-N-CA	7.24	134.73	121.70
1	D	44	HIS	N-CA-C	-6.68	101.74	111.30
1	C	65	GLY	N-CA-C	5.51	118.64	110.42
1	D	155	GLN	N-CA-C	-5.10	107.09	113.72
1	B	117	TYR	CA-C-N	5.08	124.78	119.64
1	B	117	TYR	C-N-CA	5.08	124.78	119.64
1	D	100	GLU	CA-C-N	5.05	126.16	119.84
1	D	100	GLU	C-N-CA	5.05	126.16	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2798	0	2683	30	0
1	B	2722	0	2567	25	0
1	C	2710	0	2500	39	0
1	D	2458	0	2245	37	0
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	0	0
3	B	26	0	0	0	0
3	C	26	0	0	0	0
4	C	17	0	0	0	0
5	A	206	0	0	9	0
5	B	154	0	0	6	0
5	C	157	0	0	12	0
5	D	124	0	0	14	0
All	All	11460	0	10031	131	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (131) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:LEU:O	5:A:501:HOH:O	1.83	0.96
1:C:379:TYR:OH	5:C:501:HOH:O	1.87	0.92
1:B:27:GLU:OE1	5:B:501:HOH:O	1.89	0.90
1:D:250:LEU:O	5:D:401:HOH:O	1.91	0.87
1:A:37:ARG:CZ	5:A:504:HOH:O	2.23	0.85
1:A:37:ARG:NH2	5:A:504:HOH:O	2.07	0.85
1:C:243:CYS:SG	5:C:528:HOH:O	2.34	0.84
1:A:37:ARG:HH12	1:A:186:ASP:CG	1.86	0.84
1:C:380:LEU:N	5:C:503:HOH:O	2.01	0.83
1:C:289:ALA:O	5:C:502:HOH:O	1.98	0.81
1:D:228:ARG:NH2	5:D:404:HOH:O	2.14	0.80
1:C:2:ALA:N	5:C:505:HOH:O	2.14	0.80
1:A:122:LEU:O	5:A:502:HOH:O	1.98	0.79
1:D:226:ASN:OD1	5:D:402:HOH:O	2.01	0.78
1:D:185:MET:N	5:D:406:HOH:O	2.17	0.77
1:A:174:GLU:OE2	5:A:503:HOH:O	2.03	0.75
1:A:37:ARG:NH1	1:A:186:ASP:OD1	2.21	0.74
1:D:43:GLU:HG3	1:D:44:HIS:CE1	2.22	0.74
1:B:297:ARG:NH2	5:B:505:HOH:O	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:GLU:OE2	5:A:505:HOH:O	2.08	0.72
1:B:257:GLU:OE2	5:B:502:HOH:O	2.08	0.72
1:D:155:GLN:OE1	1:D:389:VAL:HG11	1.89	0.71
1:D:375:THR:O	5:D:402:HOH:O	2.10	0.69
1:B:309:GLU:OE1	5:B:503:HOH:O	2.12	0.68
1:A:23:GLU:OE2	5:A:506:HOH:O	2.14	0.66
1:C:84:GLU:OE1	5:C:504:HOH:O	2.13	0.66
1:C:37:ARG:HH21	1:C:37:ARG:HG2	1.61	0.66
1:B:7:PRO:HG3	1:B:59:LEU:HD23	1.81	0.63
1:C:37:ARG:NH2	1:C:140:SER:OG	2.31	0.63
1:D:277:ARG:HA	5:D:418:HOH:O	1.99	0.62
1:D:236:TYR:OH	1:D:346:GLY:O	2.12	0.62
1:C:307:MET:SD	5:C:509:HOH:O	2.56	0.61
1:D:43:GLU:HG3	1:D:44:HIS:ND1	2.16	0.61
1:C:339:TYR:OH	1:C:357:GLU:OE2	2.11	0.61
1:A:37:ARG:HA	1:A:57:LEU:HG	1.83	0.60
1:A:37:ARG:HD3	1:A:189:ILE:HG21	1.83	0.59
1:D:185:MET:N	5:D:414:HOH:O	2.35	0.59
1:C:37:ARG:HE	1:C:185:MET:HE3	1.67	0.59
1:D:37:ARG:HD3	1:D:189:ILE:HG21	1.84	0.59
1:D:369:GLN:O	5:D:405:HOH:O	2.16	0.59
1:B:37:ARG:HH22	1:B:345:GLY:HA2	1.69	0.58
1:B:43:GLU:HB2	1:B:342:ARG:NH2	2.19	0.58
1:D:54:PRO:HD2	1:D:199:LEU:O	2.04	0.57
1:D:27:GLU:O	5:D:407:HOH:O	2.17	0.57
1:C:218:LEU:O	5:C:507:HOH:O	2.18	0.57
1:B:262:GLU:OE1	5:B:504:HOH:O	2.18	0.56
1:C:207:GLU:OE1	5:C:508:HOH:O	2.18	0.55
1:A:23:GLU:OE1	1:A:87:ARG:NH2	2.39	0.55
1:C:43:GLU:HB3	1:C:314:LEU:HD21	1.88	0.54
1:D:44:HIS:ND1	1:D:44:HIS:N	2.56	0.54
1:C:140:SER:HB3	1:C:143:ALA:HB3	1.89	0.54
1:A:379:TYR:OH	5:A:507:HOH:O	2.14	0.53
1:C:43:GLU:HB2	1:C:342:ARG:NH2	2.23	0.53
1:A:37:ARG:NH1	1:A:186:ASP:HA	2.24	0.52
1:B:43:GLU:HB2	1:B:342:ARG:HH22	1.75	0.51
1:D:37:ARG:NE	1:D:186:ASP:OD1	2.43	0.51
1:D:32:VAL:HG12	1:D:389:VAL:HG22	1.93	0.51
1:C:272:LYS:C	1:C:275:PHE:H	2.19	0.50
1:B:46:ASP:HB3	1:B:52:VAL:HG11	1.93	0.50
1:B:267:ARG:NH1	5:B:513:HOH:O	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:ASP:C	5:D:418:HOH:O	2.54	0.50
1:B:32:VAL:HG12	1:B:389:VAL:HG22	1.94	0.50
1:D:147:VAL:HG21	1:D:190:SER:HB3	1.93	0.49
1:C:188:PHE:CE2	1:C:208:THR:HG21	2.48	0.49
1:A:43:GLU:HB2	1:A:342:ARG:NH2	2.28	0.49
1:C:49:GLN:O	1:C:256:ARG:HD2	2.13	0.49
1:D:12:LEU:HD21	1:D:132:SER:HB3	1.95	0.49
1:B:39:ASN:HA	1:B:54:PRO:HA	1.96	0.48
1:D:372:TYR:O	5:D:405:HOH:O	2.20	0.48
1:C:340:GLY:O	5:C:509:HOH:O	2.20	0.48
1:A:17:ARG:HH21	1:A:27:GLU:HG3	1.79	0.47
1:D:35:PRO:HG3	1:D:386:GLY:HA2	1.97	0.47
1:B:8:GLN:O	1:B:9:VAL:HG12	2.14	0.47
1:C:366:ARG:O	1:C:370:GLU:N	2.36	0.46
1:A:37:ARG:NE	5:A:504:HOH:O	2.44	0.46
1:A:356:LEU:HD11	1:A:361:ALA:HA	1.97	0.46
1:C:54:PRO:HD2	1:C:199:LEU:O	2.15	0.46
1:B:20:PHE:CE2	1:B:65:GLY:HA2	2.50	0.46
1:C:37:ARG:HG2	1:C:37:ARG:NH2	2.27	0.46
1:B:30:LEU:HD21	1:B:155:GLN:CB	2.46	0.45
1:A:218:LEU:HD11	1:A:355:LEU:HG	1.97	0.45
1:A:273:GLU:O	1:A:277:ARG:HG2	2.17	0.45
1:A:192:MET:HE2	1:A:192:MET:HB3	1.71	0.45
1:A:17:ARG:HH21	1:A:27:GLU:CG	2.29	0.45
1:A:109:TYR:CE1	1:A:142:SER:HB2	2.51	0.45
1:D:318:TYR:HA	5:D:418:HOH:O	2.16	0.45
1:D:386:GLY:HA3	5:D:413:HOH:O	2.17	0.45
1:C:307:MET:HE2	1:C:342:ARG:HG2	1.99	0.44
1:B:54:PRO:HD2	1:B:199:LEU:O	2.17	0.44
1:D:117:TYR:CE2	1:D:119:ALA:HB3	2.53	0.44
1:C:222:ILE:HB	1:C:379:TYR:HB2	1.99	0.44
1:D:37:ARG:HE	1:D:186:ASP:CG	2.26	0.44
1:B:85:PRO:HD2	1:B:104:PRO:HD3	1.99	0.44
1:B:199:LEU:HD23	1:B:201:ILE:HD11	2.00	0.44
1:C:231:LEU:N	1:C:232:ALA:HB2	2.33	0.44
1:C:174:GLU:HG2	1:C:182:CYS:SG	2.58	0.44
1:B:51:LEU:HD23	1:B:202:ASP:HA	1.99	0.43
1:D:215:ASP:HA	1:D:216:PRO:HD3	1.84	0.43
1:D:360:ALA:HA	5:D:423:HOH:O	2.18	0.43
1:A:292:ALA:O	1:A:296:ARG:HG3	2.18	0.43
1:D:176:SER:O	1:D:177:PHE:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ARG:HD3	1:B:189:ILE:HG21	2.00	0.43
1:A:88:LEU:HD22	1:A:104:PRO:HD2	2.00	0.42
1:D:28:PRO:HG3	1:D:64:VAL:HG13	2.01	0.42
1:A:37:ARG:HG2	1:A:37:ARG:HH11	1.84	0.42
1:C:47:TYR:CE1	1:C:240:ARG:HG2	2.54	0.42
1:D:40:LEU:O	1:D:342:ARG:HD3	2.20	0.42
1:C:236:TYR:HB3	1:C:237:PRO:HD3	2.00	0.42
1:B:147:VAL:HG21	1:B:190:SER:HB3	2.02	0.42
1:B:259:GLN:OE1	1:B:261:GLU:HB2	2.20	0.42
1:B:295:LEU:HD12	1:B:295:LEU:HA	1.91	0.42
1:D:295:LEU:HD23	1:D:295:LEU:HA	1.85	0.42
1:A:147:VAL:HG21	1:A:190:SER:HB3	2.00	0.41
1:C:228:ARG:NH1	1:C:228:ARG:HG2	2.35	0.41
1:A:54:PRO:HD2	1:A:199:LEU:O	2.20	0.41
1:C:255:LEU:HD23	1:C:255:LEU:HA	1.89	0.41
1:C:314:LEU:HD11	1:C:342:ARG:HH21	1.86	0.41
1:D:37:ARG:HG2	1:D:37:ARG:HH11	1.86	0.41
1:C:228:ARG:HG2	1:C:228:ARG:HH11	1.85	0.41
1:C:292:ALA:N	5:C:502:HOH:O	2.53	0.41
1:D:42:GLY:HA2	1:D:284:GLU:HG3	2.01	0.41
1:A:311:HIS:CE1	1:A:329:VAL:HG21	2.55	0.41
1:C:109:TYR:CE1	1:C:142:SER:HB2	2.55	0.41
1:A:27:GLU:HG3	1:A:28:PRO:HD2	2.03	0.41
1:D:140:SER:OG	1:D:186:ASP:HB3	2.21	0.41
1:C:43:GLU:HB2	1:C:342:ARG:HH22	1.86	0.41
1:C:175:HIS:CD2	1:C:181:PRO:HA	2.56	0.41
1:D:139:LEU:HD23	1:D:139:LEU:HA	1.84	0.41
1:B:273:GLU:O	1:B:277:ARG:HG2	2.22	0.40
1:C:119:ALA:HB2	1:C:159:ASP:HA	2.02	0.40
1:C:347:GLY:N	5:C:520:HOH:O	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

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	389/391 (100%)	382 (98%)	6 (2%)	1 (0%)	36	28
1	B	379/391 (97%)	367 (97%)	8 (2%)	4 (1%)	11	4
1	C	388/391 (99%)	375 (97%)	12 (3%)	1 (0%)	36	28
1	D	347/391 (89%)	329 (95%)	17 (5%)	1 (0%)	36	28
All	All	1503/1564 (96%)	1453 (97%)	43 (3%)	7 (0%)	24	16

All (7) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/308 (89%)	271 (99%)	2 (1%)	76	76
1	B	260/308 (84%)	255 (98%)	5 (2%)	50	45
1	C	249/308 (81%)	244 (98%)	5 (2%)	48	43
1	D	221/308 (72%)	216 (98%)	5 (2%)	44	38
All	All	1003/1232 (81%)	986 (98%)	17 (2%)	53	49

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG

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Mol	Chain	Res	Type
1	A	264	GLU
1	B	9	VAL
1	B	30	LEU
1	B	55	MET
1	B	64	VAL
1	B	264	GLU
1	C	37	ARG
1	C	64	VAL
1	C	233	SER
1	C	335	VAL
1	C	382	GLN
1	D	43	GLU
1	D	44	HIS
1	D	55	MET
1	D	64	VAL
1	D	176	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	226	ASN
1	C	226	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GAL	B	401	-	12,12,12	0.62	0	17,17,17	0.73	0
4	HGE	C	402	-	18,18,18	1.74	3 (16%)	22,23,23	1.85	6 (27%)
3	HFK	A	402	-	29,30,30	4.30	11 (37%)	32,44,44	4.53	16 (50%)
3	HFK	C	403	-	29,30,30	4.33	11 (37%)	32,44,44	4.56	15 (46%)
3	HFK	B	402	-	29,30,30	4.36	11 (37%)	32,44,44	4.51	17 (53%)
2	GAL	C	401	-	12,12,12	0.51	0	17,17,17	0.79	0
2	GAL	A	401	-	12,12,12	0.74	0	17,17,17	1.01	0

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

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	HFK	C06-C07	13.67	1.54	1.37
3	A	402	HFK	C06-C07	13.56	1.54	1.37
3	B	402	HFK	C06-C07	13.54	1.54	1.37
3	B	402	HFK	C15-N16	10.04	1.52	1.36
3	A	402	HFK	C15-N16	9.70	1.52	1.36
3	C	403	HFK	C15-N16	9.47	1.51	1.36
3	B	402	HFK	C15-N14	8.89	1.53	1.30
3	A	402	HFK	C15-N14	8.84	1.53	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	HFK	C15-N14	8.80	1.53	1.30
3	C	403	HFK	O01-C02	7.57	1.38	1.23
3	B	402	HFK	O01-C02	7.45	1.38	1.23
3	A	402	HFK	O01-C02	7.41	1.38	1.23
3	B	402	HFK	C06-N16	6.05	1.47	1.37
3	A	402	HFK	C06-N16	5.79	1.46	1.37
3	C	403	HFK	C06-N16	5.63	1.46	1.37
3	C	403	HFK	C03-C02	5.21	1.57	1.50
3	A	402	HFK	C03-C02	5.03	1.57	1.50
3	B	402	HFK	C03-C02	4.88	1.57	1.50
4	C	402	HGE	C8-N	4.74	1.48	1.37
3	B	402	HFK	C18-N17	4.25	1.44	1.36
3	C	403	HFK	C18-N17	4.16	1.44	1.36
3	A	402	HFK	C18-N17	4.04	1.44	1.36
4	C	402	HGE	O-C2	3.64	1.41	1.33
3	C	403	HFK	C02-C07	3.51	1.56	1.46
3	A	402	HFK	C02-C07	3.38	1.56	1.46
3	B	402	HFK	C02-C07	3.28	1.56	1.46
3	C	403	HFK	C08-N14	3.00	1.49	1.46
3	B	402	HFK	C05-C06	2.92	1.54	1.49
3	C	403	HFK	C05-C06	2.78	1.54	1.49
3	A	402	HFK	C05-C06	2.70	1.54	1.49
3	A	402	HFK	C08-N14	2.61	1.49	1.46
4	C	402	HGE	O-C1	-2.61	1.38	1.46
3	B	402	HFK	C18-N19	2.33	1.34	1.30
3	C	403	HFK	C18-N19	2.33	1.34	1.30
3	B	402	HFK	C08-N14	2.32	1.48	1.46
3	A	402	HFK	C18-N19	2.20	1.34	1.30

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	HFK	C07-C06-N16	-14.71	110.23	122.11
3	B	402	HFK	C07-C06-N16	-13.74	111.01	122.11
3	C	403	HFK	C07-C06-N16	-12.32	112.16	122.11
3	B	402	HFK	C08-C07-C06	-10.86	109.50	121.75
3	A	402	HFK	C08-C07-C06	-10.30	110.13	121.75
3	C	403	HFK	C08-C07-C06	-9.32	111.24	121.75
3	C	403	HFK	C02-C07-C06	-9.26	110.96	119.18
3	C	403	HFK	O01-C02-C03	-8.36	107.17	120.87
3	C	403	HFK	C05-C06-C07	-7.85	112.04	122.72
3	B	402	HFK	O01-C02-C03	-7.84	108.03	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	HFK	O01-C02-C03	-7.77	108.13	120.87
3	B	402	HFK	O01-C02-C07	-7.09	112.02	121.53
3	A	402	HFK	O01-C02-C07	-6.68	112.58	121.53
3	C	403	HFK	N17-C15-N16	-6.63	106.81	117.96
3	B	402	HFK	C05-C06-C07	-6.45	113.94	122.72
3	A	402	HFK	N17-C15-N16	-6.39	107.21	117.96
3	C	403	HFK	N16-C15-N14	-6.11	112.79	123.63
3	A	402	HFK	C05-C06-C07	-6.08	114.44	122.72
3	B	402	HFK	N17-C15-N16	-5.93	107.98	117.96
3	A	402	HFK	N16-C15-N14	-5.60	113.70	123.63
3	C	403	HFK	O01-C02-C07	-5.46	114.20	121.53
3	B	402	HFK	N16-C15-N14	-5.19	114.44	123.63
3	B	402	HFK	N17-C15-N14	-5.05	108.53	117.96
4	C	402	HGE	O-C2-C3	5.00	120.36	112.00
3	A	402	HFK	N17-C15-N14	-4.68	109.23	117.96
3	B	402	HFK	C02-C07-C06	-4.29	115.37	119.18
3	C	403	HFK	N17-C15-N14	-4.28	109.98	117.96
3	A	402	HFK	C05-C06-N16	-3.91	109.89	115.46
3	B	402	HFK	O22-C21-C23	3.70	134.26	126.49
3	B	402	HFK	C05-C06-N16	-3.69	110.21	115.46
3	A	402	HFK	O22-C21-C23	3.61	134.09	126.49
3	C	403	HFK	C15-N16-C06	-3.61	112.44	121.02
3	C	403	HFK	O22-C21-C23	3.61	134.07	126.49
3	A	402	HFK	C02-C07-C06	-3.56	116.03	119.18
3	C	403	HFK	C05-C06-N16	-3.28	110.80	115.46
3	B	402	HFK	O22-C18-N19	-3.27	109.70	115.57
4	C	402	HGE	C5-C4-C3	3.21	115.62	110.54
3	C	403	HFK	O22-C18-N19	-3.17	109.87	115.57
3	A	402	HFK	C15-N16-C06	-3.16	113.52	121.02
3	B	402	HFK	C23-C21-C20	-3.14	119.81	123.62
3	A	402	HFK	O22-C18-N19	-3.03	110.13	115.57
3	A	402	HFK	C23-C21-C20	-3.02	119.95	123.62
3	C	403	HFK	C23-C21-C20	-3.00	119.97	123.62
3	B	402	HFK	O22-C21-C20	-2.74	105.93	107.80
3	A	402	HFK	O22-C21-C20	-2.70	105.96	107.80
3	C	403	HFK	O22-C21-C20	-2.70	105.96	107.80
3	B	402	HFK	C15-N16-C06	-2.69	114.62	121.02
4	C	402	HGE	C11-N2-C8	2.58	120.56	116.81
4	C	402	HGE	O-C2-O1	-2.44	119.68	124.14
3	B	402	HFK	C03-C02-C07	-2.17	113.12	117.35
3	A	402	HFK	C18-N17-C15	-2.11	120.12	125.27
4	C	402	HGE	N2-C8-N	2.09	119.75	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	402	HGE	C4-C5-N	2.03	115.52	110.92
3	B	402	HFK	C20-N19-C18	2.00	108.10	104.13

There are no chirality outliers.

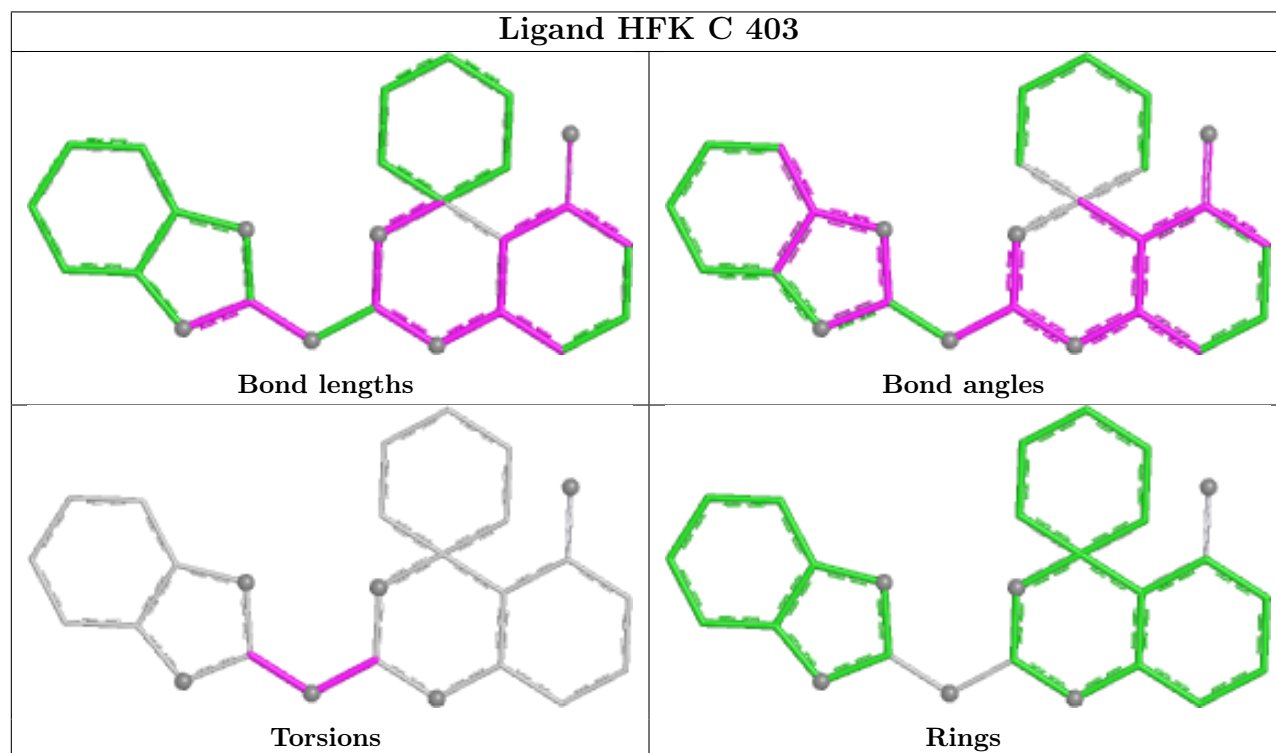
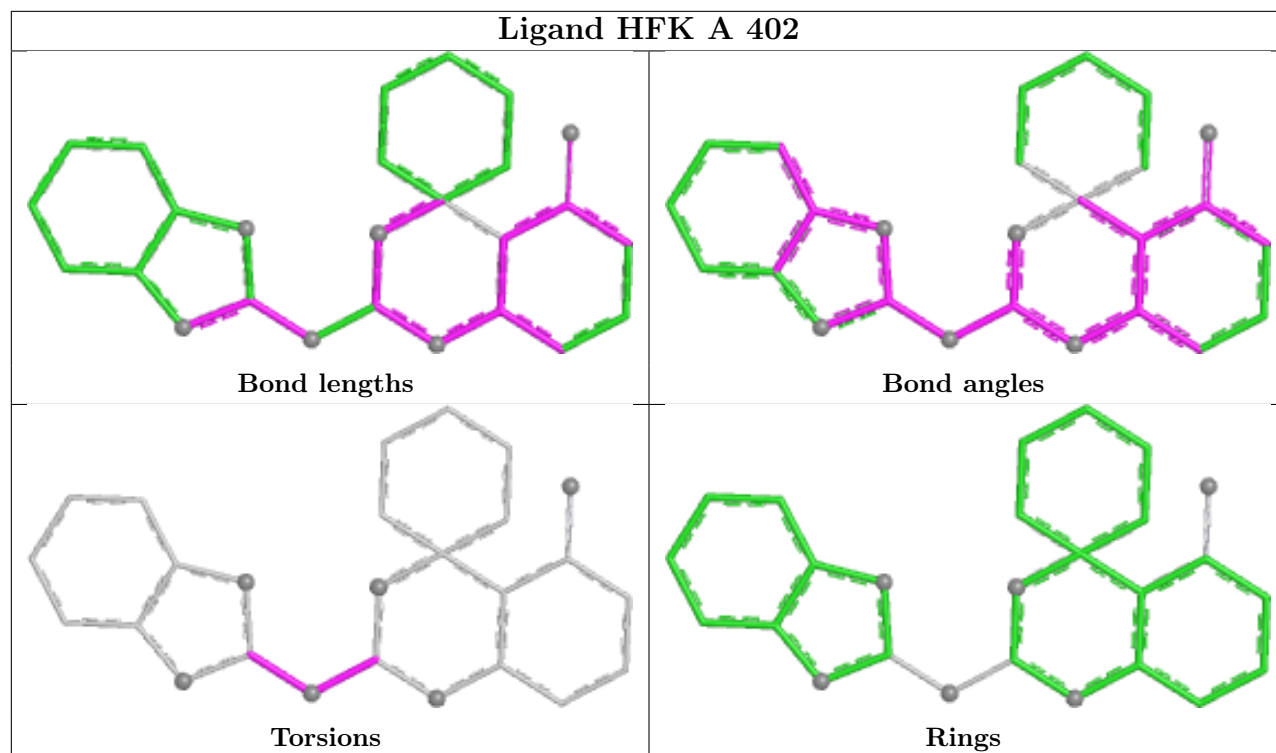
All (18) torsion outliers are listed below:

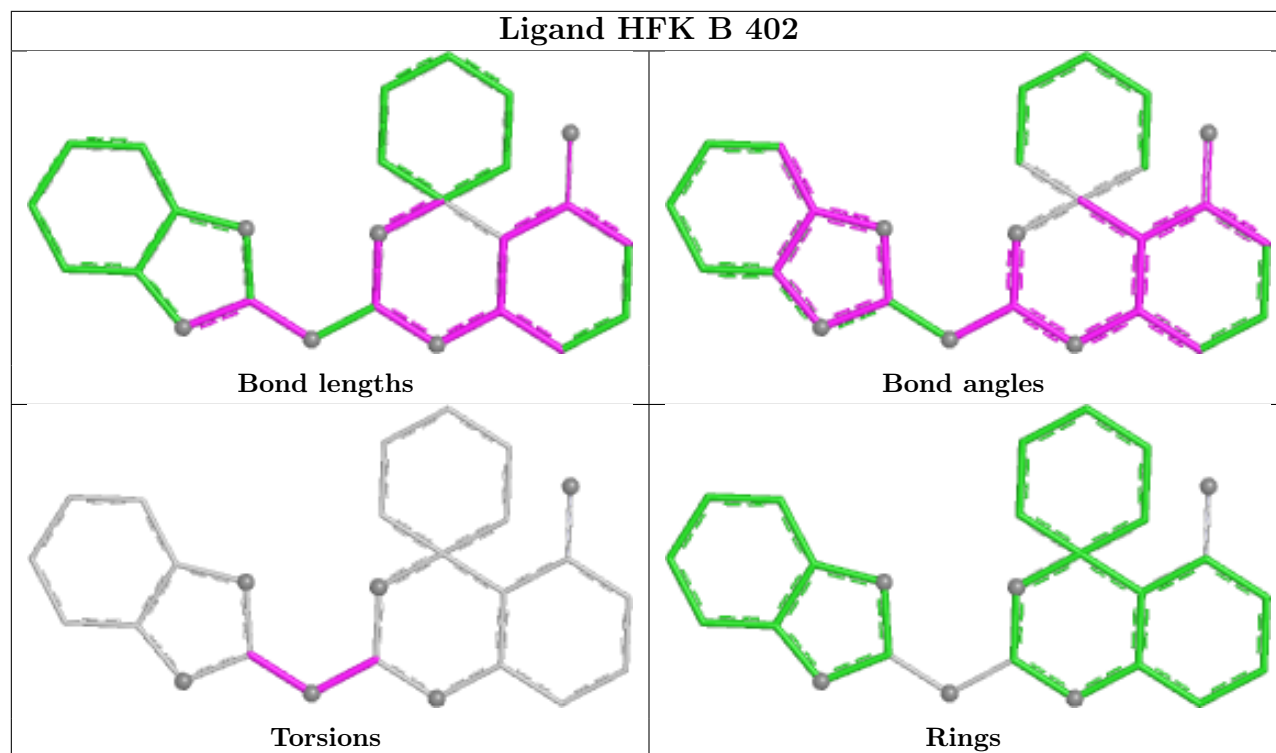
Mol	Chain	Res	Type	Atoms
3	A	402	HFK	N14-C15-N17-C18
3	A	402	HFK	N19-C18-N17-C15
3	B	402	HFK	N14-C15-N17-C18
3	C	403	HFK	N14-C15-N17-C18
3	C	403	HFK	N19-C18-N17-C15
4	C	402	HGE	C9-C8-N-C6
2	B	401	GAL	O5-C5-C6-O6
2	C	401	GAL	O5-C5-C6-O6
4	C	402	HGE	N2-C8-N-C6
2	A	401	GAL	O5-C5-C6-O6
3	A	402	HFK	O22-C18-N17-C15
3	C	403	HFK	O22-C18-N17-C15
3	B	402	HFK	N19-C18-N17-C15
3	A	402	HFK	N16-C15-N17-C18
3	B	402	HFK	N16-C15-N17-C18
2	B	401	GAL	C4-C5-C6-O6
3	C	403	HFK	N16-C15-N17-C18
3	B	402	HFK	O22-C18-N17-C15

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	391/391 (100%)	0.64	31 (7%) 18 21	24, 40, 64, 98	0
1	B	385/391 (98%)	1.15	72 (18%) 3 3	31, 46, 79, 105	0
1	C	390/391 (99%)	1.62	126 (32%) 1 0	28, 49, 100, 125	0
1	D	357/391 (91%)	1.88	135 (37%) 1 0	27, 57, 108, 142	0
All	All	1523/1564 (97%)	1.31	364 (23%) 2 2	24, 47, 93, 142	0

All (364) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	368	ILE	10.2
1	C	275	PHE	9.2
1	C	265	ALA	7.7
1	D	231	LEU	7.6
1	D	120	ALA	6.9
1	D	232	ALA	6.9
1	C	270	VAL	6.7
1	A	372	TYR	6.7
1	D	233	SER	6.5
1	D	71	GLY	6.4
1	C	364	ALA	6.3
1	D	106	TRP	6.3
1	C	365	MET	6.3
1	B	7	PRO	6.1
1	C	367	HIS	6.1
1	D	119	ALA	5.9
1	C	188	PHE	5.8
1	C	246	VAL	5.7
1	D	122	LEU	5.7
1	D	99	LEU	5.6
1	B	80	GLU	5.6

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Mol	Chain	Res	Type	RSRZ
1	D	44	HIS	5.5
1	D	373	GLY	5.5
1	C	263	LEU	5.4
1	D	88	LEU	5.4
1	C	329	VAL	5.4
1	D	47	TYR	5.4
1	D	15	GLU	5.3
1	D	230	SER	5.2
1	C	271	SER	5.2
1	C	266	ALA	5.2
1	D	64	VAL	5.0
1	D	75	LEU	5.0
1	C	360	ALA	4.9
1	C	269	LEU	4.9
1	D	43	GLU	4.8
1	C	369	GLN	4.8
1	D	236	TYR	4.8
1	B	9	VAL	4.8
1	D	128	VAL	4.8
1	D	169	VAL	4.7
1	D	101	PRO	4.7
1	D	234	SER	4.7
1	D	374	GLY	4.7
1	C	250	LEU	4.7
1	D	118	PRO	4.6
1	C	2	ALA	4.6
1	C	4	LEU	4.6
1	A	268	ASP	4.6
1	D	318	TYR	4.6
1	D	72	LEU	4.6
1	C	361	ALA	4.5
1	A	2	ALA	4.5
1	C	249	ALA	4.5
1	A	4	LEU	4.5
1	D	90	PHE	4.4
1	C	268	ASP	4.4
1	C	331	ALA	4.4
1	B	37	ARG	4.4
1	D	86	GLN	4.4
1	D	92	LEU	4.4
1	D	121	PRO	4.4
1	C	232	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	235	GLU	4.4
1	A	9	VAL	4.3
1	B	99	LEU	4.3
1	D	135	LEU	4.3
1	B	79	SER	4.3
1	C	260	LEU	4.3
1	D	161	GLY	4.3
1	C	362	PRO	4.3
1	D	78	THR	4.3
1	B	97	ARG	4.3
1	D	98	SER	4.3
1	C	231	LEU	4.2
1	C	356	LEU	4.2
1	D	30	LEU	4.2
1	C	363	HIS	4.2
1	C	261	GLU	4.2
1	B	6	GLN	4.1
1	B	64	VAL	4.1
1	C	366	ARG	4.1
1	D	163	ILE	4.1
1	C	332	ALA	4.1
1	C	334	ALA	4.1
1	D	107	ALA	4.1
1	C	330	GLU	4.1
1	B	92	LEU	4.1
1	D	123	PRO	4.1
1	B	72	LEU	4.1
1	B	88	LEU	4.1
1	D	76	LEU	4.1
1	B	10	ALA	4.0
1	C	3	ALA	4.0
1	C	302	ALA	4.0
1	B	68	ARG	4.0
1	D	95	ALA	3.9
1	D	375	THR	3.9
1	C	370	GLU	3.9
1	A	103	THR	3.9
1	C	337	GLY	3.9
1	C	300	TYR	3.9
1	D	213	LEU	3.9
1	D	253	ALA	3.9
1	D	9	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	277	ARG	3.8
1	A	80	GLU	3.8
1	B	71	GLY	3.8
1	B	234	SER	3.8
1	D	13	LEU	3.8
1	D	177	PHE	3.8
1	C	229	HIS	3.7
1	A	216	PRO	3.7
1	B	2	ALA	3.7
1	C	252	ALA	3.7
1	C	253	ALA	3.7
1	C	338	VAL	3.7
1	D	10	ALA	3.7
1	D	94	THR	3.7
1	D	103	THR	3.7
1	D	8	GLN	3.6
1	C	333	LEU	3.6
1	D	108	ASN	3.6
1	D	174	GLU	3.6
1	C	317	ASP	3.6
1	D	173	ALA	3.6
1	A	37	ARG	3.6
1	B	247	ALA	3.5
1	D	269	LEU	3.6
1	C	304	GLY	3.5
1	D	12	LEU	3.5
1	D	74	SER	3.5
1	D	77	THR	3.5
1	B	8	GLN	3.4
1	D	67	PRO	3.4
1	C	238	VAL	3.4
1	D	73	VAL	3.4
1	C	233	SER	3.4
1	C	276	ARG	3.4
1	B	73	VAL	3.4
1	D	89	GLN	3.4
1	D	191	LEU	3.4
1	D	114	ILE	3.4
1	C	335	VAL	3.4
1	C	306	LEU	3.4
1	C	262	GLU	3.3
1	D	254	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	249	ALA	3.3
1	D	104	PRO	3.3
1	B	128	VAL	3.3
1	C	258	VAL	3.3
1	D	130	VAL	3.3
1	B	98	SER	3.3
1	D	214	SER	3.3
1	C	213	LEU	3.3
1	C	355	LEU	3.3
1	B	188	PHE	3.3
1	C	308	VAL	3.2
1	D	87	ARG	3.2
1	B	106	TRP	3.2
1	C	259	GLN	3.2
1	D	194	GLN	3.2
1	B	74	SER	3.2
1	D	136	GLY	3.2
1	B	96	GLN	3.2
1	C	242	GLN	3.2
1	C	243	CYS	3.2
1	D	159	ASP	3.2
1	A	3	ALA	3.2
1	B	26	ALA	3.2
1	D	93	PRO	3.2
1	D	62	VAL	3.2
1	A	213	LEU	3.2
1	C	228	ARG	3.2
1	C	358	ALA	3.1
1	C	340	GLY	3.1
1	D	124	GLY	3.1
1	A	373	GLY	3.1
1	D	379	TYR	3.0
1	C	245	GLU	3.0
1	D	160	SER	3.0
1	D	102	GLY	3.0
1	C	273	GLU	3.0
1	D	91	PRO	3.0
1	D	167	ALA	3.0
1	C	281	VAL	3.0
1	D	175	HIS	3.0
1	C	336	PRO	3.0
1	D	97	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	143	ALA	3.0
1	B	229	HIS	2.9
1	C	267	ARG	2.9
1	C	264	GLU	2.9
1	C	291	ALA	2.9
1	B	246	VAL	2.9
1	D	27	GLU	2.9
1	D	152	PHE	2.9
1	C	214	SER	2.9
1	B	100	GLU	2.9
1	C	227	VAL	2.9
1	C	303	PHE	2.9
1	C	37	ARG	2.9
1	C	279	ARG	2.9
1	C	254	SER	2.9
1	B	250	LEU	2.9
1	B	227	VAL	2.8
1	C	305	ARG	2.8
1	A	249	ALA	2.8
1	C	278	ALA	2.8
1	A	72	LEU	2.8
1	D	155	GLN	2.8
1	B	371	HIS	2.8
1	A	269	LEU	2.8
1	C	241	ARG	2.8
1	C	286	ARG	2.8
1	D	105	ARG	2.8
1	B	238	VAL	2.8
1	B	81	GLY	2.8
1	D	372	TYR	2.7
1	C	357	GLU	2.7
1	C	328	LEU	2.7
1	D	156	LEU	2.7
1	C	96	GLN	2.7
1	D	270	VAL	2.7
1	C	372	TYR	2.7
1	D	339	TYR	2.7
1	C	373	GLY	2.7
1	C	316	ASP	2.7
1	D	185	MET	2.7
1	A	218	LEU	2.7
1	C	272	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	192	MET	2.7
1	D	368	ILE	2.7
1	C	371	HIS	2.7
1	D	31	ALA	2.6
1	D	252	ALA	2.6
1	B	248	ARG	2.6
1	D	276	ARG	2.6
1	B	30	LEU	2.6
1	D	113	VAL	2.6
1	D	249	ALA	2.6
1	C	289	ALA	2.6
1	B	90	PHE	2.6
1	D	222	ILE	2.6
1	B	91	PRO	2.5
1	D	158	PRO	2.5
1	B	348	PHE	2.5
1	C	6	GLN	2.5
1	D	115	GLN	2.5
1	D	11	GLU	2.5
1	B	95	ALA	2.5
1	A	371	HIS	2.5
1	D	129	VAL	2.5
1	D	238	VAL	2.5
1	B	94	THR	2.5
1	A	6	GLN	2.5
1	B	300	TYR	2.5
1	A	217	LYS	2.5
1	C	30	LEU	2.5
1	D	250	LEU	2.5
1	C	283	GLY	2.5
1	C	301	ARG	2.5
1	C	359	SER	2.5
1	A	10	ALA	2.5
1	D	100	GLU	2.5
1	D	246	VAL	2.5
1	D	117	TYR	2.5
1	C	314	LEU	2.5
1	D	96	GLN	2.5
1	C	299	ASP	2.5
1	D	237	PRO	2.5
1	B	87	ARG	2.4
1	C	248	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	188	PHE	2.4
1	D	206	LEU	2.4
1	D	272	LYS	2.4
1	B	228	ARG	2.4
1	D	137	GLY	2.4
1	B	172	GLN	2.4
1	C	135	LEU	2.4
1	C	255	LEU	2.4
1	C	339	TYR	2.4
1	D	116	TYR	2.4
1	D	165	ALA	2.4
1	A	81	GLY	2.4
1	B	295	LEU	2.4
1	D	63	LEU	2.4
1	D	14	ALA	2.4
1	D	127	ALA	2.4
1	D	66	SER	2.4
1	D	142	SER	2.4
1	C	78	THR	2.3
1	B	85	PRO	2.3
1	C	315	ARG	2.3
1	B	75	LEU	2.3
1	B	382	GLN	2.3
1	D	145	LEU	2.3
1	D	109	TYR	2.3
1	B	114	ILE	2.3
1	D	228	ARG	2.3
1	B	392	LEU	2.3
1	C	380	LEU	2.3
1	A	192	MET	2.3
1	D	125	PHE	2.3
1	C	287	ARG	2.3
1	A	270	VAL	2.3
1	B	129	VAL	2.3
1	C	103	THR	2.3
1	B	379	TYR	2.2
1	C	244	GLU	2.2
1	C	294	ALA	2.2
1	A	79	SER	2.2
1	A	355	LEU	2.2
1	A	390	LEU	2.2
1	B	213	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	295	LEU	2.2
1	C	327	GLN	2.2
1	D	193	GLY	2.2
1	D	371	HIS	2.2
1	C	221	LEU	2.2
1	B	298	GLY	2.2
1	C	219	ALA	2.2
1	B	177	PHE	2.2
1	D	208	THR	2.2
1	B	126	SER	2.2
1	D	112	GLY	2.2
1	D	37	ARG	2.2
1	D	267	ARG	2.2
1	B	24	PHE	2.1
1	C	378	PHE	2.1
1	C	382	GLN	2.1
1	C	354	THR	2.1
1	D	162	THR	2.1
1	C	310	SER	2.1
1	B	25	GLY	2.1
1	B	5	ARG	2.1
1	B	12	LEU	2.1
1	C	256	ARG	2.1
1	B	120	ALA	2.1
1	D	39	ASN	2.1
1	A	78	THR	2.1
1	B	78	THR	2.1
1	C	251	GLY	2.1
1	C	84	GLU	2.1
1	B	82	ALA	2.1
1	B	236	TYR	2.1
1	B	251	GLY	2.1
1	D	389	VAL	2.1
1	C	7	PRO	2.1
1	A	260	LEU	2.1
1	A	97	ARG	2.1
1	A	58	GLU	2.0
1	B	23	GLU	2.0
1	B	214	SER	2.0
1	C	375	THR	2.0
1	B	89	GLN	2.0
1	D	187	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	113	VAL	2.0
1	C	97	ARG	2.0
1	C	247	ALA	2.0
1	D	207	GLU	2.0
1	C	381	SER	2.0
1	C	298	GLY	2.0
1	C	374	GLY	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](#)

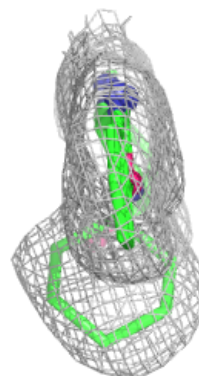
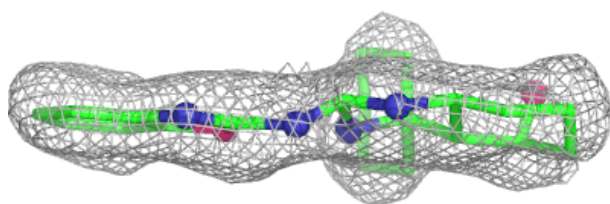
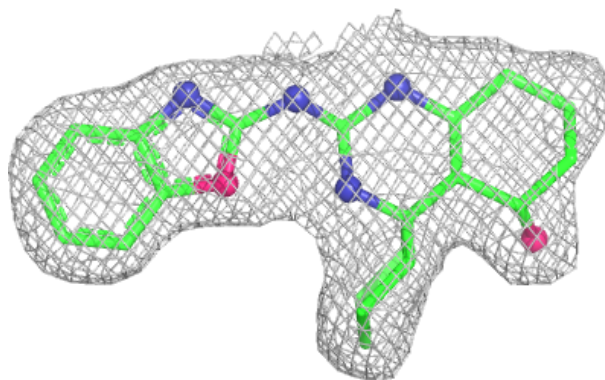
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	HGE	C	402	17/17	0.70	0.27	87,88,102,102	0
2	GAL	C	401	12/12	0.87	0.10	31,37,39,41	0
3	HFK	B	402	26/26	0.89	0.14	49,54,58,80	0
3	HFK	C	403	26/26	0.90	0.14	47,49,61,68	0
2	GAL	B	401	12/12	0.91	0.10	32,37,43,45	0
3	HFK	A	402	26/26	0.92	0.11	35,38,47,54	0
2	GAL	A	401	12/12	0.92	0.08	23,27,32,40	0

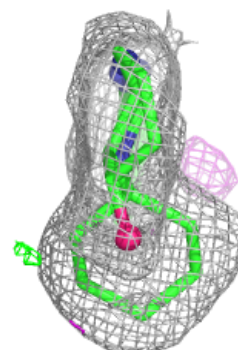
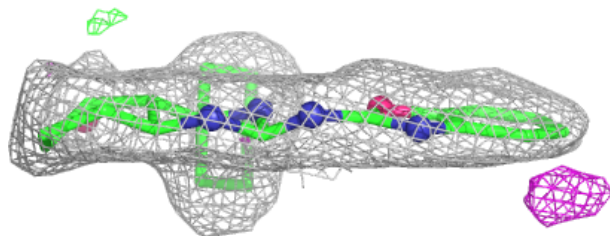
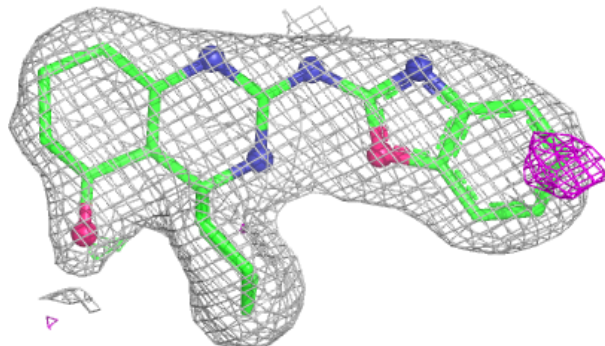
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

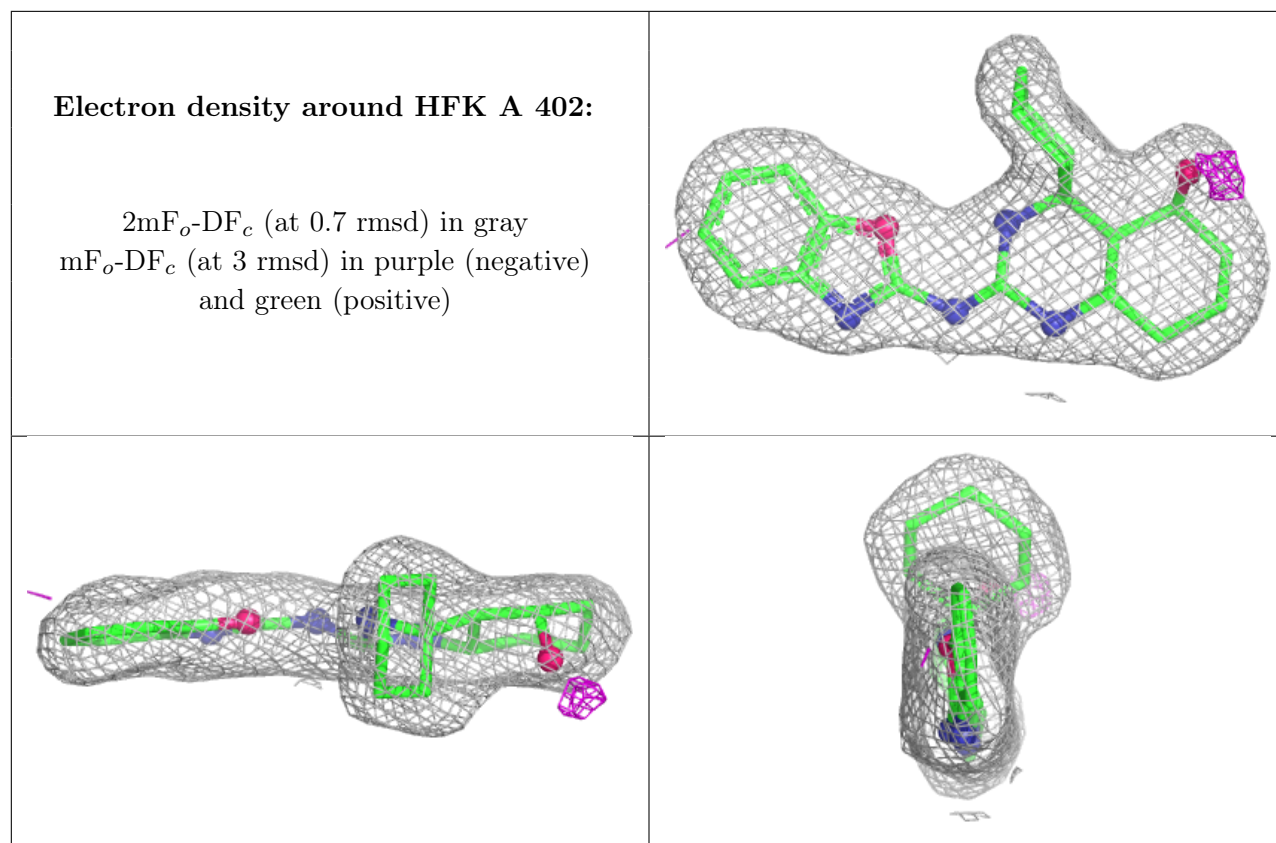
Electron density around HFK B 402:

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

**Electron density around HFK C 403:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.