



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:58 PM EDT

PDB ID : 6Q91 / pdb_00006q91
Title : Structure of human galactokinase 1 bound with 5-Chloro-N-isobutyl-2-methoxybenzamide
Authors : Mackinnon, S.R.; Bezerra, G.A.; Zhang, M.; Foster, W.; Krojer, T.; Brandao-Neto, J.; Douangamath, A.; Arrowsmith, C.; Edwards, A.; Bountra, C.; Brennan, P.; Lai, K.; Yue, W.W.
Deposited on : 2018-12-17
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:

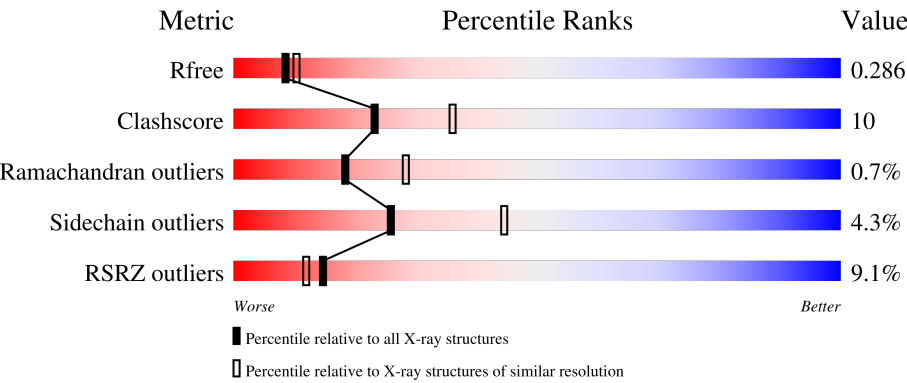
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

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	% 83%16%•
1	B	392	4% 83%15%•
1	C	392	16% 70%26%•
1	D	392	16% 72%18%8%•

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11516 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.

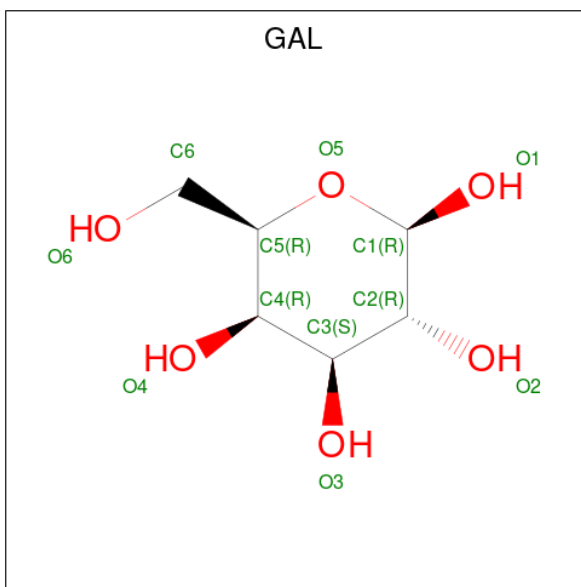
- Molecule 1 is a protein called Galactokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	5	1	0
			2879	1804	508	550	17			
1	B	392	Total	C	N	O	S	2	1	0
			2851	1780	505	551	15			
1	C	392	Total	C	N	O	S	0	0	0
			2791	1749	494	532	16			
1	D	360	Total	C	N	O	S	0	0	0
			2492	1558	441	480	13			

There are 12 discrepancies between the modelled and reference sequences:

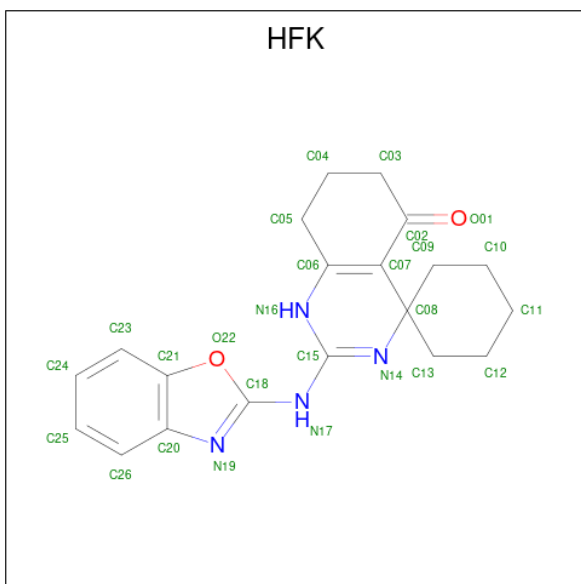
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	expression tag	UNP P51570
A	252	ALA	LYS	engineered mutation	UNP P51570
A	253	ALA	GLU	engineered mutation	UNP P51570
B	1	HIS	-	expression tag	UNP P51570
B	252	ALA	LYS	engineered mutation	UNP P51570
B	253	ALA	GLU	engineered mutation	UNP P51570
C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



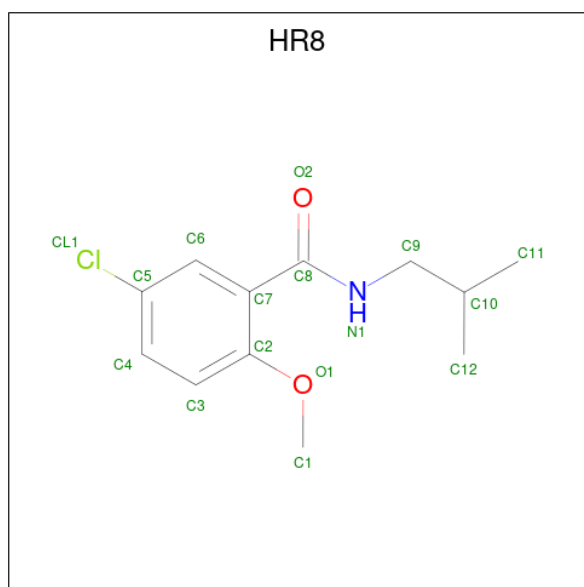
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		

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



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 5-chloranyl-2-methoxy- {N}-(2-methylpropyl)benzamide (CCD ID: HR8) (formula: C₁₂H₁₆ClNO₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			16	12	1	1	2		
4	B	1	Total	C	Cl	N	O	0	0
			16	12	1	1	2		
4	C	1	Total	C	Cl	N	O	0	0
			16	12	1	1	2		
4	D	1	Total	C	Cl	N	O	0	0
			16	12	1	1	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	115	Total	O	0	0
			115	115		
5	B	87	Total	O	0	0
			87	87		

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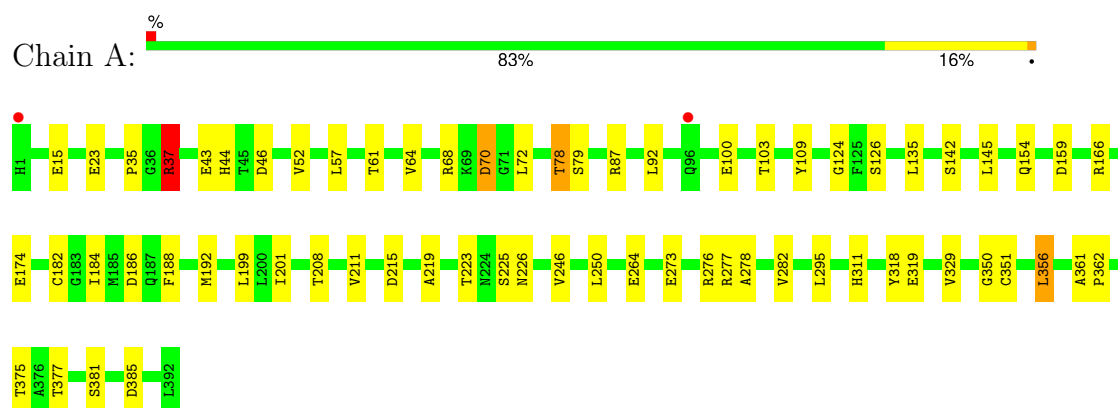
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	71	Total 71	O 71	0	0
5	D	52	Total 52	O 52	0	0

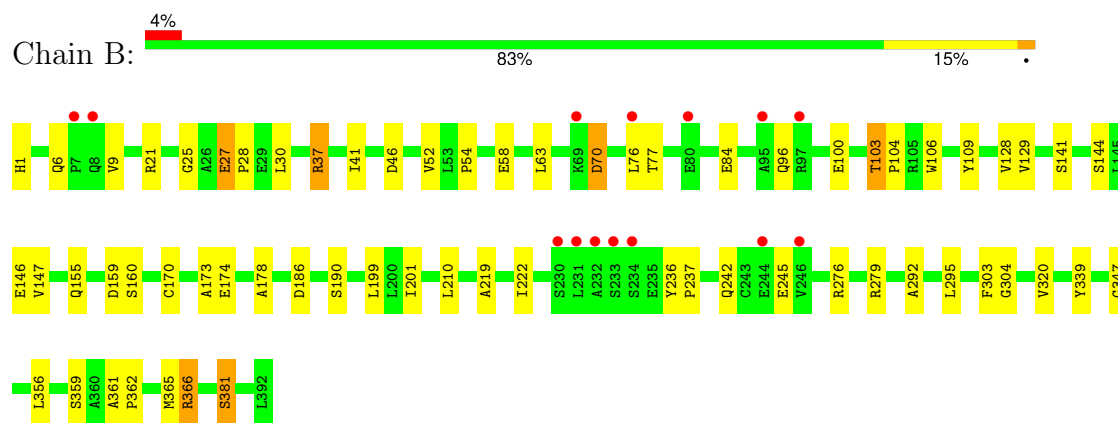
3 Residue-property plots [i](#)

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.

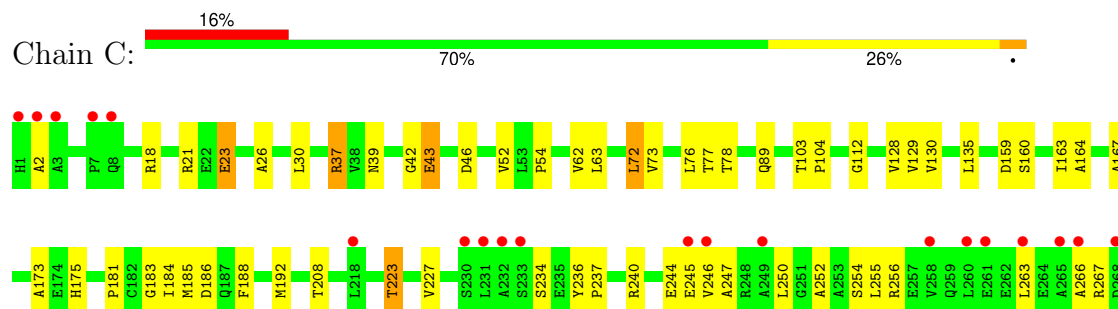
• Molecule 1: Galactokinase

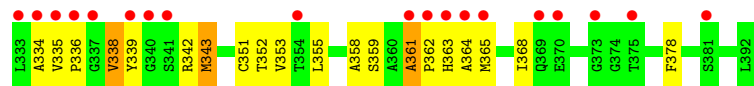
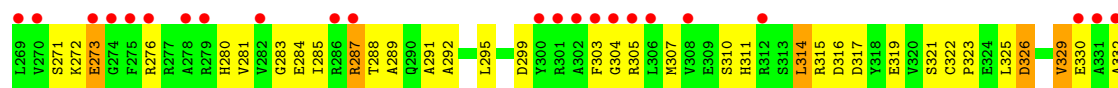


• Molecule 1: Galactokinase

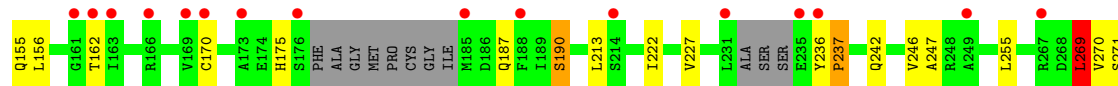
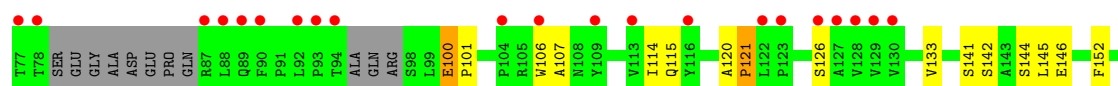


• Molecule 1: Galactokinase





● 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	73.32Å 114.96Å 120.92Å 90.00° 100.79° 90.00°	Depositor
Resolution (Å)	82.74 – 2.40 82.74 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (82.74-2.40) 99.5 (82.74-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.216 , 0.285 0.220 , 0.286	Depositor DCC
R_{free} test set	4499 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11516	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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, GAL, HR8

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	1.12	0/2937	1.50	5/3997 (0.1%)
1	B	1.12	0/2908	1.54	10/3962 (0.3%)
1	C	1.18	1/2842 (0.0%)	1.59	17/3875 (0.4%)
1	D	1.15	0/2530	1.63	6/3450 (0.2%)
All	All	1.14	1/11217 (0.0%)	1.56	38/15284 (0.2%)

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	2
1	C	0	1
1	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	183	GLY	C-O	5.26	1.28	1.23

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	ASP	CA-CB-CG	6.85	119.45	112.60
1	B	41	ILE	CA-C-O	-6.84	116.08	120.66
1	C	288	THR	N-CA-C	-6.83	103.45	111.03
1	C	23	GLU	CB-CA-C	-6.64	99.56	110.85
1	B	103	THR	CB-CA-C	6.52	118.67	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	GLN	CB-CA-C	6.52	118.59	108.61
1	B	159	ASP	CA-CB-CG	6.48	119.08	112.60
1	D	237	PRO	N-CA-C	6.32	121.84	113.57
1	B	303	PHE	N-CA-C	-5.87	104.79	111.07
1	C	314	LEU	CA-C-N	5.83	128.35	120.65
1	C	314	LEU	C-N-CA	5.83	128.35	120.65
1	C	359	SER	CA-C-N	5.73	128.75	120.79
1	C	359	SER	C-N-CA	5.73	128.75	120.79
1	D	247	ALA	CA-C-N	5.57	128.06	120.54
1	D	247	ALA	C-N-CA	5.57	128.06	120.54
1	B	1	HIS	CA-C-N	5.53	127.69	120.28
1	B	1	HIS	C-N-CA	5.53	127.69	120.28
1	A	70	ASP	CA-CB-CG	5.52	118.12	112.60
1	B	366	ARG	N-CA-C	-5.48	104.34	111.02
1	C	273	GLU	CA-C-N	5.38	127.13	120.34
1	C	273	GLU	C-N-CA	5.38	127.13	120.34
1	C	104	PRO	CA-C-N	5.37	127.42	120.44
1	C	104	PRO	C-N-CA	5.37	127.42	120.44
1	A	375	THR	CA-CB-OG1	-5.34	101.59	109.60
1	C	46	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	57	LEU	CA-C-N	5.28	128.34	120.31
1	A	57	LEU	C-N-CA	5.28	128.34	120.31
1	C	77	THR	CA-CB-OG1	-5.24	101.74	109.60
1	C	256	ARG	CA-C-N	5.23	129.44	120.71
1	C	256	ARG	C-N-CA	5.23	129.44	120.71
1	C	325	LEU	CA-C-N	5.21	127.98	120.38
1	C	325	LEU	C-N-CA	5.21	127.98	120.38
1	D	274	GLY	CA-C-N	5.17	127.51	120.54
1	D	274	GLY	C-N-CA	5.17	127.51	120.54
1	B	46	ASP	CA-CB-CG	5.10	117.70	112.60
1	B	279	ARG	N-CA-C	-5.05	105.85	111.36
1	C	159	ASP	CA-CB-CG	5.04	117.64	112.60
1	D	340	GLY	CA-C-O	-5.01	116.13	121.29

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	37	ARG	Peptide
1	A	381	SER	Peptide
1	C	363	HIS	Peptide
1	D	269	LEU	Peptide

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	2879	0	2795	40	0
1	B	2851	0	2735	39	0
1	C	2791	0	2668	101	0
1	D	2492	0	2308	45	0
2	A	12	0	11	0	0
2	B	12	0	12	0	0
2	C	12	0	12	1	0
3	A	26	0	0	0	0
3	B	26	0	0	0	0
3	C	26	0	0	0	0
4	A	16	0	0	0	0
4	B	16	0	0	0	0
4	C	16	0	0	1	0
4	D	16	0	0	0	0
5	A	115	0	0	1	0
5	B	87	0	0	4	0
5	C	71	0	0	10	0
5	D	52	0	0	5	0
All	All	11516	0	10541	224	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 (224) 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:C:273:GLU:CB	5:C:569:HOH:O	1.83	1.25
1:B:96:GLN:CB	5:B:572:HOH:O	1.86	1.22
1:C:307:MET:SD	5:C:537:HOH:O	2.12	1.04
1:C:361:ALA:HB1	1:C:362:PRO:HD3	1.40	0.98
1:A:37:ARG:HH11	1:A:37:ARG:HG2	1.28	0.95
1:D:43:GLU:OE2	1:D:345:GLY:N	2.01	0.93
1:D:39:ASN:HB2	5:D:545:HOH:O	1.71	0.91
1:B:58:GLU:OE1	1:B:381:SER:OG	1.95	0.85
1:C:63:LEU:HD11	1:C:129:VAL:HG22	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ARG:HG2	1:B:37:ARG:HH21	1.43	0.80
1:C:78:THR:HG22	1:C:130:VAL:HG12	1.64	0.80
1:A:276:ARG:NH2	1:A:319:GLU:OE1	2.18	0.75
1:C:307:MET:CE	5:C:537:HOH:O	2.31	0.75
1:C:307:MET:HE1	5:C:537:HOH:O	1.85	0.74
1:C:361:ALA:CB	1:C:362:PRO:CD	2.67	0.73
1:C:304:GLY:HA3	1:C:339:TYR:O	1.88	0.73
1:D:30:LEU:HD21	1:D:155:GLN:HB3	1.71	0.73
1:C:223:THR:O	1:C:351:CYS:HA	1.90	0.72
1:C:54:PRO:HB3	1:C:185:MET:CE	2.20	0.72
1:C:361:ALA:HB1	1:C:362:PRO:CD	2.16	0.71
1:C:39:ASN:CG	1:C:185:MET:HE1	2.15	0.71
1:C:361:ALA:CB	1:C:362:PRO:HD3	2.17	0.71
1:B:37:ARG:HG2	1:B:37:ARG:NH2	2.04	0.71
1:B:219:ALA:HB3	1:B:356:LEU:CD1	2.21	0.71
1:B:210:LEU:HD12	1:C:192:MET:HE1	1.72	0.70
1:D:30:LEU:HD21	1:D:155:GLN:CB	2.22	0.70
1:C:335:VAL:HG12	1:C:336:PRO:HD2	1.74	0.69
1:C:283:GLY:C	1:C:287:ARG:HE	2.00	0.68
1:C:39:ASN:CB	1:C:185:MET:HE1	2.23	0.67
1:C:311:HIS:CE1	1:C:329:VAL:HG21	2.29	0.67
1:D:335:VAL:HG21	1:D:364:ALA:HA	1.77	0.67
1:D:74:SER:O	1:D:126:SER:HA	1.95	0.66
1:C:72:LEU:C	1:C:72:LEU:HD12	2.21	0.66
1:C:78:THR:CG2	1:C:130:VAL:HG12	2.27	0.64
1:C:314:LEU:O	1:C:319:GLU:N	2.31	0.63
1:D:43:GLU:OE2	1:D:344:THR:HA	1.98	0.63
1:C:314:LEU:HB3	1:C:343:MET:HE1	1.81	0.63
1:C:332:ALA:HA	1:C:335:VAL:HG21	1.81	0.63
1:C:355:LEU:CB	5:C:537:HOH:O	2.46	0.63
1:D:61:THR:HG21	1:D:145:LEU:HA	1.80	0.63
1:C:314:LEU:HD13	1:C:343:MET:HE3	1.81	0.62
1:C:332:ALA:HB2	1:C:368:ILE:HD12	1.79	0.62
1:D:43:GLU:HB3	1:D:44:HIS:ND1	2.15	0.62
1:C:355:LEU:HB2	5:C:537:HOH:O	2.00	0.61
1:B:30:LEU:HD21	1:B:155:GLN:HB3	1.83	0.61
1:C:358:ALA:O	1:C:361:ALA:HB2	2.00	0.61
1:D:34:ALA:HB3	1:D:144:SER:O	2.00	0.60
1:C:263:LEU:O	1:C:266:ALA:N	2.35	0.59
1:C:39:ASN:HB2	1:C:185:MET:HE1	1.83	0.59
1:D:242:GLN:O	1:D:246:VAL:HG13	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:GLU:OE1	1:D:170:CYS:O	2.21	0.58
1:C:240:ARG:O	1:C:244:GLU:HG3	2.04	0.58
1:D:269:LEU:HD12	5:D:505:HOH:O	2.02	0.58
1:C:311:HIS:ND1	1:C:329:VAL:HG21	2.19	0.57
1:D:242:GLN:NE2	1:D:273:GLU:OE2	2.35	0.57
1:A:109:TYR:HB2	1:A:145:LEU:HD23	1.87	0.56
1:C:37:ARG:NE	1:C:186:ASP:OD1	2.38	0.56
1:C:291:ALA:HB1	1:C:303:PHE:CE1	2.39	0.56
1:A:72:LEU:C	1:A:72:LEU:HD12	2.30	0.56
1:B:30:LEU:HD21	1:B:155:GLN:CB	2.35	0.56
1:C:326:ASP:OD1	1:C:326:ASP:N	2.39	0.56
1:B:84:GLU:O	5:B:501:HOH:O	2.18	0.55
1:C:175:HIS:CD2	1:C:181:PRO:HA	2.41	0.55
1:B:63:LEU:HD11	1:B:129:VAL:HG22	1.88	0.55
1:C:37:ARG:HG2	1:C:37:ARG:HH21	1.70	0.55
1:A:15:GLU:OE2	1:A:78:THR:HG21	2.07	0.55
1:C:284:GLU:OE1	1:C:284:GLU:HA	2.07	0.55
1:C:223:THR:OG1	1:C:352:THR:OG1	2.23	0.55
1:C:283:GLY:O	1:C:287:ARG:HG3	2.06	0.55
1:B:37:ARG:HH21	1:B:37:ARG:CG	2.16	0.54
1:B:236:TYR:HB3	1:B:237:PRO:HD3	1.89	0.54
1:D:276:ARG:O	1:D:317:ASP:HB3	2.07	0.54
1:C:335:VAL:HG12	1:C:336:PRO:CD	2.38	0.54
1:C:321:SER:OG	1:C:326:ASP:OD1	2.26	0.54
1:C:164:ALA:HA	1:C:188:PHE:HE1	1.73	0.54
1:D:246:VAL:CG2	1:D:255:LEU:HD21	2.37	0.53
1:B:219:ALA:HB3	1:B:356:LEU:HD11	1.89	0.53
1:A:100:GLU:HB3	5:A:543:HOH:O	2.07	0.53
1:B:37:ARG:HE	1:B:186:ASP:CG	2.16	0.53
1:A:361:ALA:HB3	1:A:362:PRO:HD3	1.91	0.53
1:C:63:LEU:CD1	1:C:129:VAL:HG22	2.37	0.53
1:C:332:ALA:O	1:C:338:VAL:HG11	2.08	0.53
1:A:311:HIS:CE1	1:A:329:VAL:HG21	2.44	0.52
1:C:236:TYR:HB3	1:C:237:PRO:HD3	1.91	0.52
1:D:42:GLY:O	1:D:52:VAL:HG12	2.10	0.52
1:C:364:ALA:O	1:C:368:ILE:HG22	2.10	0.52
1:A:92:LEU:HD11	1:A:124:GLY:N	2.25	0.51
1:C:54:PRO:HB3	1:C:185:MET:HE2	1.90	0.51
1:C:271:SER:OG	1:C:272:LYS:N	2.41	0.51
1:C:335:VAL:CG1	1:C:336:PRO:HD2	2.40	0.51
1:B:70:ASP:HB3	5:B:554:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:VAL:O	1:C:89:GLN:HA	2.10	0.51
1:D:31:ALA:HB2	1:D:64:VAL:HG12	1.93	0.51
1:C:54:PRO:HB3	1:C:185:MET:HE3	1.93	0.50
1:C:280:HIS:O	1:C:284:GLU:HB2	2.12	0.50
1:B:52:VAL:HG22	1:B:201:ILE:HB	1.94	0.50
1:A:46:ASP:HB3	1:A:52:VAL:HG11	1.94	0.50
1:B:219:ALA:HB3	1:B:356:LEU:HD12	1.92	0.50
1:C:283:GLY:O	1:C:287:ARG:CG	2.60	0.49
1:A:37:ARG:HG2	1:A:37:ARG:NH1	2.07	0.49
1:D:320:VAL:O	1:D:347:GLY:HA3	2.11	0.49
1:C:247:ALA:HB1	1:C:252:ALA:O	2.11	0.49
1:B:141:SER:O	1:B:144:SER:OG	2.26	0.49
1:B:276:ARG:HD2	5:B:514:HOH:O	2.12	0.49
1:D:305:ARG:O	1:D:309:GLU:HG3	2.12	0.49
1:A:219:ALA:HB3	1:A:356:LEU:CD1	2.42	0.49
1:B:76:LEU:O	1:B:128:VAL:HA	2.13	0.49
1:C:314:LEU:HB3	1:C:343:MET:CE	2.43	0.49
1:C:332:ALA:HB2	1:C:368:ILE:CD1	2.43	0.49
1:A:174:GLU:HG2	1:A:182:CYS:SG	2.53	0.49
1:D:236:TYR:N	1:D:237:PRO:CD	2.76	0.49
1:C:62:VAL:O	1:C:63:LEU:HD12	2.13	0.48
1:D:272:LYS:O	5:D:501:HOH:O	2.19	0.48
1:D:187:GLN:CB	5:D:541:HOH:O	2.61	0.48
1:A:109:TYR:CE1	1:A:142:SER:HB2	2.47	0.48
1:C:43:GLU:OE2	2:C:401:GAL:O6	2.27	0.48
1:A:211:VAL:HG11	1:A:295:LEU:HD23	1.95	0.48
1:C:276:ARG:C	1:C:317:ASP:OD1	2.57	0.48
1:C:188:PHE:HE2	1:C:208:THR:HG21	1.79	0.47
1:D:213:LEU:HD12	1:D:295:LEU:HD11	1.95	0.47
1:C:43:GLU:HB2	1:C:342:ARG:NH2	2.28	0.47
1:C:314:LEU:CD1	1:C:343:MET:HE3	2.44	0.47
1:D:361:ALA:N	1:D:362:PRO:HD2	2.30	0.47
1:D:142:SER:O	1:D:146:GLU:HG3	2.14	0.47
1:B:242:GLN:O	1:B:245:GLU:HB2	2.14	0.47
1:C:280:HIS:C	1:C:280:HIS:CD2	2.87	0.47
1:A:44:HIS:CG	1:A:318:TYR:CE2	3.03	0.47
1:A:52:VAL:CG2	1:A:201:ILE:HB	2.44	0.47
1:A:356:LEU:HD12	1:A:356:LEU:O	2.15	0.47
1:A:246:VAL:HG11	1:A:278:ALA:HB2	1.97	0.46
1:C:52:VAL:HG21	1:C:185:MET:HG3	1.97	0.46
1:C:322:CYS:O	1:C:323:PRO:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ARG:NE	1:A:186:ASP:OD1	2.48	0.46
1:A:68:ARG:CZ	1:A:72:LEU:HD11	2.45	0.46
1:D:31:ALA:CB	1:D:64:VAL:HG12	2.45	0.46
1:C:335:VAL:CG1	1:C:336:PRO:CD	2.94	0.46
1:B:54:PRO:HD2	1:B:199:LEU:O	2.15	0.46
1:B:37:ARG:NE	1:B:186:ASP:OD1	2.42	0.46
1:A:199:LEU:HD11	1:A:208:THR:HB	1.98	0.46
1:D:16:ALA:HB1	1:D:64:VAL:HG22	1.98	0.46
1:D:133:VAL:HG11	1:D:141:SER:HA	1.98	0.46
1:C:112:GLY:HA3	1:C:173:ALA:HB1	1.98	0.46
1:C:295:LEU:HD13	4:C:403:HR8:C4	2.46	0.46
1:D:33:SER:HA	1:D:61:THR:O	2.16	0.45
1:D:100:GLU:N	1:D:101:PRO:CD	2.80	0.45
1:C:192:MET:HE2	1:C:192:MET:HB3	1.83	0.45
1:C:299:ASP:CB	5:C:502:HOH:O	2.64	0.45
1:C:304:GLY:O	1:C:305:ARG:C	2.60	0.45
1:C:280:HIS:CE1	1:C:314:LEU:HG	2.52	0.45
1:A:246:VAL:O	1:A:250:LEU:HD13	2.17	0.44
1:A:273:GLU:O	1:A:277:ARG:HG2	2.17	0.44
1:C:315:ARG:NE	1:C:316:ASP:OD1	2.50	0.44
1:D:35:PRO:O	1:D:190:SER:OG	2.36	0.44
1:D:213:LEU:HD13	1:D:295:LEU:HD21	1.99	0.44
1:D:56:ALA:HB3	1:D:384:ALA:O	2.17	0.44
1:B:146:GLU:OE2	1:B:174:GLU:OE1	2.35	0.44
1:B:292:ALA:O	1:B:295:LEU:HB3	2.18	0.44
1:A:37:ARG:HH11	1:A:37:ARG:CG	2.15	0.44
1:C:245:GLU:CB	5:C:529:HOH:O	2.66	0.44
1:A:184:ILE:HG13	1:A:188:PHE:HD2	1.82	0.44
1:C:355:LEU:HB3	5:C:537:HOH:O	2.16	0.44
1:D:152:PHE:CE1	1:D:156:LEU:HD11	2.53	0.44
1:C:281:VAL:O	1:C:284:GLU:N	2.51	0.44
1:C:21:ARG:HA	1:C:26:ALA:O	2.18	0.43
1:A:215:ASP:OD1	1:A:215:ASP:C	2.61	0.43
1:C:289:ALA:O	1:C:292:ALA:HB3	2.19	0.43
1:C:167:ALA:HB1	1:C:184:ILE:HD11	1.99	0.43
1:B:109:TYR:CE1	1:B:178:ALA:HB2	2.53	0.43
1:C:329:VAL:O	1:C:330:GLU:C	2.61	0.43
1:D:162:THR:OG1	5:D:502:HOH:O	2.21	0.43
1:D:213:LEU:CD1	1:D:295:LEU:HD21	2.49	0.43
1:B:77:THR:HA	1:B:129:VAL:O	2.19	0.43
1:C:43:GLU:OE2	1:C:43:GLU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:LEU:CB	1:C:343:MET:CE	2.97	0.43
1:C:332:ALA:HA	1:C:335:VAL:CG2	2.47	0.43
1:D:33:SER:O	1:D:387:ALA:HA	2.19	0.43
1:C:307:MET:O	1:C:310:SER:N	2.51	0.43
1:C:23:GLU:CG	1:C:76:LEU:HD22	2.48	0.43
1:D:114:ILE:O	1:D:115:GLN:C	2.61	0.43
1:A:52:VAL:HG22	1:A:201:ILE:HB	2.00	0.42
1:A:184:ILE:O	1:A:188:PHE:HB2	2.19	0.42
1:A:226:ASN:OD1	1:A:377:THR:OG1	2.37	0.42
1:C:42:GLY:O	1:C:52:VAL:HG12	2.19	0.42
1:A:225:SER:OG	1:A:350:GLY:O	2.33	0.42
1:C:163:ILE:HG21	1:C:192:MET:CG	2.48	0.42
1:A:61:THR:HG21	1:A:145:LEU:HA	2.00	0.42
1:C:362:PRO:HA	1:C:365:MET:HB2	2.00	0.42
1:C:311:HIS:C	1:C:311:HIS:CD2	2.97	0.42
1:C:353:VAL:HG13	1:C:353:VAL:O	2.19	0.42
1:B:104:PRO:HB2	1:B:106:TRP:CD1	2.55	0.42
1:A:154:GLN:HE22	1:A:166:ARG:CZ	2.32	0.42
1:A:68:ARG:HD2	1:A:126:SER:OG	2.20	0.42
1:B:27:GLU:OE1	1:B:28:PRO:HD2	2.20	0.42
1:B:320:VAL:O	1:B:347:GLY:HA3	2.20	0.42
1:D:246:VAL:HG21	1:D:278:ALA:CB	2.50	0.42
1:A:109:TYR:CB	1:A:145:LEU:HD23	2.48	0.41
1:B:63:LEU:CD1	1:B:129:VAL:HG22	2.50	0.41
1:C:246:VAL:O	1:C:250:LEU:HD13	2.19	0.41
1:C:365:MET:HA	1:C:378:PHE:CZ	2.54	0.41
1:D:106:TRP:CE3	1:D:107:ALA:N	2.88	0.41
1:D:23:GLU:O	1:D:24:PHE:CB	2.68	0.41
1:C:314:LEU:CB	1:C:343:MET:HE1	2.50	0.41
1:D:120:ALA:HA	1:D:121:PRO:HA	1.86	0.41
1:B:304:GLY:HA3	1:B:339:TYR:O	2.19	0.41
1:A:70:ASP:OD1	1:A:72:LEU:HG	2.20	0.41
1:A:223:THR:O	1:A:351:CYS:HA	2.20	0.41
1:A:35:PRO:HG3	1:A:385:ASP:O	2.21	0.41
1:B:21:ARG:O	1:B:25:GLY:N	2.40	0.41
1:B:361:ALA:N	1:B:362:PRO:CD	2.84	0.41
1:C:184:ILE:HA	1:C:184:ILE:HD12	1.78	0.41
1:A:192:MET:HE3	1:A:192:MET:HB3	1.86	0.41
1:B:147:VAL:HG21	1:B:190:SER:HB3	2.02	0.41
1:B:170:CYS:O	1:B:173:ALA:HB3	2.21	0.41
1:B:365:MET:O	1:B:366:ARG:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ILE:HD12	1:B:222:ILE:N	2.36	0.40
1:C:163:ILE:HG21	1:C:192:MET:HG3	2.02	0.40
1:D:43:GLU:HB3	1:D:44:HIS:CE1	2.56	0.40
1:C:18:ARG:HD2	5:C:506:HOH:O	2.21	0.40
1:A:23:GLU:CD	1:A:87:ARG:HE	2.29	0.40
1:C:37:ARG:HG2	1:C:37:ARG:NH2	2.35	0.40
1:C:54:PRO:CB	1:C:185:MET:HE3	2.51	0.40
1:C:76:LEU:O	1:C:128:VAL:HA	2.21	0.40
1:B:359:SER:O	1:B:362:PRO:HD2	2.21	0.40
1:D:246:VAL:HG21	1:D:278:ALA:HB2	2.02	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	391/392 (100%)	379 (97%)	12 (3%)	0	100	100
1	B	391/392 (100%)	376 (96%)	15 (4%)	0	100	100
1	C	390/392 (100%)	336 (86%)	48 (12%)	6 (2%)	8	12
1	D	346/392 (88%)	316 (91%)	25 (7%)	5 (1%)	9	13
All	All	1518/1568 (97%)	1407 (93%)	100 (7%)	11 (1%)	18	28

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2	ALA
1	C	334	ALA
1	C	361	ALA
1	D	24	PHE
1	D	100	GLU

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Mol	Chain	Res	Type
1	D	175	HIS
1	D	22	GLU
1	C	329	VAL
1	C	267	ARG
1	C	285	ILE
1	D	121	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	289/309 (94%)	279 (96%)	10 (4%)	32	53
1	B	283/309 (92%)	275 (97%)	8 (3%)	38	60
1	C	268/309 (87%)	252 (94%)	16 (6%)	17	31
1	D	230/309 (74%)	218 (95%)	12 (5%)	21	36
All	All	1070/1236 (87%)	1024 (96%)	46 (4%)	26	44

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	43	GLU
1	A	64	VAL
1	A	78	THR
1	A	79	SER
1	A	103	THR
1	A	135	LEU
1	A	264	GLU
1	A	282	VAL
1	A	356	LEU
1	B	9	VAL
1	B	27	GLU
1	B	37	ARG
1	B	70	ASP
1	B	100	GLU

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Mol	Chain	Res	Type
1	B	103	THR
1	B	160	SER
1	B	381	SER
1	C	30	LEU
1	C	37	ARG
1	C	43	GLU
1	C	72	LEU
1	C	103	THR
1	C	135	LEU
1	C	160	SER
1	C	223	THR
1	C	227	VAL
1	C	234	SER
1	C	254	SER
1	C	255	LEU
1	C	287	ARG
1	C	326	ASP
1	C	338	VAL
1	C	343	MET
1	D	43	GLU
1	D	63	LEU
1	D	66	SER
1	D	190	SER
1	D	222	ILE
1	D	227	VAL
1	D	269	LEU
1	D	270	VAL
1	D	271	SER
1	D	295	LEU
1	D	356	LEU
1	D	375	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	371	HIS
1	C	96	GLN
1	C	226	ASN
1	C	280	HIS
1	D	39	ASN
1	D	48	ASN
1	D	154	GLN

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Mol	Chain	Res	Type
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	$\# Z > 2$
4	HR8	B	403	-	16,16,16	0.42	0	21,21,21	0.80	0
2	GAL	C	401	-	12,12,12	0.57	0	17,17,17	2.17	6 (35%)
4	HR8	A	403	-	16,16,16	0.39	0	21,21,21	0.58	0
2	GAL	A	401	-	12,12,12	0.78	0	17,17,17	2.52	5 (29%)
3	HFK	C	402	-	29,30,30	4.18	11 (37%)	32,44,44	4.81	16 (50%)
3	HFK	B	402	-	29,30,30	4.24	11 (37%)	32,44,44	4.35	15 (46%)
2	GAL	B	401	-	12,12,12	0.78	0	17,17,17	2.16	6 (35%)
3	HFK	A	402	-	29,30,30	4.19	13 (44%)	32,44,44	4.96	20 (62%)
4	HR8	D	401	-	16,16,16	0.36	0	21,21,21	0.62	0
4	HR8	C	403	-	16,16,16	0.39	0	21,21,21	0.76	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
4	HR8	B	403	-	-	4/11/11/11	0/1/1/1
2	GAL	C	401	-	-	2/2/22/22	0/1/1/1
4	HR8	A	403	-	-	2/11/11/11	0/1/1/1
2	GAL	A	401	-	-	2/2/22/22	0/1/1/1
3	HFK	C	402	-	-	2/4/43/43	0/5/5/5
3	HFK	B	402	-	-	2/4/43/43	0/5/5/5
2	GAL	B	401	-	-	1/2/22/22	0/1/1/1
3	HFK	A	402	-	-	2/4/43/43	0/5/5/5
4	HR8	D	401	-	-	2/11/11/11	0/1/1/1
4	HR8	C	403	-	-	0/11/11/11	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	HFK	C06-C07	15.28	1.56	1.37
3	A	402	HFK	C06-C07	14.41	1.55	1.37
3	C	402	HFK	C06-C07	13.75	1.54	1.37
3	C	402	HFK	C06-N16	7.68	1.49	1.37
3	A	402	HFK	C15-N16	7.61	1.48	1.36
3	A	402	HFK	C06-N16	7.58	1.49	1.37
3	B	402	HFK	C15-N14	7.55	1.49	1.30
3	B	402	HFK	C21-C20	7.55	1.47	1.38
3	C	402	HFK	C21-C20	7.54	1.47	1.38
3	C	402	HFK	C15-N16	7.54	1.48	1.36
3	C	402	HFK	C15-N14	7.33	1.49	1.30
3	B	402	HFK	C06-N16	7.30	1.49	1.37
3	A	402	HFK	C21-C20	7.18	1.47	1.38
3	B	402	HFK	C15-N16	7.10	1.48	1.36
3	A	402	HFK	C15-N14	6.59	1.47	1.30
3	C	402	HFK	O22-C21	-4.87	1.30	1.38
3	C	402	HFK	C08-N14	4.72	1.51	1.46
3	A	402	HFK	C15-N17	4.16	1.46	1.37
3	B	402	HFK	C15-N17	4.09	1.46	1.37
3	A	402	HFK	C18-N19	3.97	1.37	1.30
3	A	402	HFK	C08-N14	3.80	1.50	1.46
3	B	402	HFK	O22-C21	-3.65	1.32	1.38
3	B	402	HFK	C08-N14	3.51	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	HFK	C18-N19	3.49	1.36	1.30
3	C	402	HFK	C15-N17	3.46	1.45	1.37
3	B	402	HFK	C18-N19	3.38	1.36	1.30
3	A	402	HFK	O22-C21	-3.29	1.33	1.38
3	A	402	HFK	C02-C07	2.62	1.54	1.46
3	B	402	HFK	C05-C06	2.58	1.54	1.49
3	A	402	HFK	C05-C06	2.54	1.53	1.49
3	C	402	HFK	C05-C06	2.47	1.53	1.49
3	A	402	HFK	C20-N19	-2.42	1.35	1.39
3	A	402	HFK	C03-C02	2.32	1.53	1.50
3	C	402	HFK	C02-C07	2.28	1.53	1.46
3	B	402	HFK	C02-C07	2.22	1.53	1.46

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	HFK	C02-C07-C06	-15.02	105.85	119.18
3	A	402	HFK	C07-C06-N16	-15.01	109.98	122.11
3	C	402	HFK	C07-C06-N16	-12.41	112.09	122.11
3	B	402	HFK	C02-C07-C06	-11.67	108.83	119.18
3	B	402	HFK	C07-C06-N16	-11.54	112.79	122.11
3	A	402	HFK	C02-C07-C06	-11.29	109.17	119.18
3	C	402	HFK	C05-C06-C07	-10.00	109.11	122.72
3	A	402	HFK	C05-C06-C07	-9.79	109.40	122.72
3	B	402	HFK	N16-C15-N14	-8.93	107.80	123.63
3	C	402	HFK	N16-C15-N14	-8.26	108.99	123.63
3	A	402	HFK	N16-C15-N14	-7.63	110.10	123.63
3	B	402	HFK	C05-C06-C07	-7.61	112.36	122.72
3	A	402	HFK	C08-C07-C06	-7.42	113.37	121.75
3	B	402	HFK	C15-N16-C06	-6.88	104.67	121.02
2	A	401	GAL	C1-O5-C5	-6.55	100.98	113.65
3	C	402	HFK	N17-C15-N16	-6.04	107.80	117.96
3	A	402	HFK	O22-C21-C20	5.96	111.85	107.80
3	A	402	HFK	C21-C20-N19	-5.83	103.20	108.60
3	B	402	HFK	C08-C07-C06	-5.75	115.26	121.75
3	C	402	HFK	C08-C07-C06	-5.73	115.29	121.75
2	B	401	GAL	C1-O5-C5	-5.49	103.03	113.65
3	A	402	HFK	C15-N16-C06	-5.05	109.04	121.02
3	B	402	HFK	C05-C06-N16	-4.73	108.74	115.46
2	A	401	GAL	C1-C2-C3	-4.60	100.97	110.36
3	C	402	HFK	C15-N16-C06	-4.56	110.20	121.02
2	C	401	GAL	O2-C2-C1	4.31	119.20	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	HFK	N17-C15-N14	-4.29	109.95	117.96
3	A	402	HFK	N17-C15-N16	-4.23	110.84	117.96
3	A	402	HFK	C09-C10-C11	4.20	117.89	111.35
3	B	402	HFK	C21-C20-N19	-4.19	104.72	108.60
3	B	402	HFK	O22-C21-C20	3.87	110.43	107.80
3	B	402	HFK	N17-C15-N16	-3.80	111.57	117.96
2	C	401	GAL	C1-O5-C5	-3.69	106.52	113.65
2	C	401	GAL	O5-C1-C2	-3.56	104.05	110.30
2	B	401	GAL	C1-C2-C3	-3.49	103.23	110.36
2	C	401	GAL	O1-C1-C2	3.46	119.03	108.98
3	B	402	HFK	C26-C20-N19	3.35	137.72	128.21
3	C	402	HFK	C26-C20-N19	3.33	137.66	128.21
3	A	402	HFK	C23-C21-C20	-3.28	119.63	123.62
3	A	402	HFK	O01-C02-C03	-3.25	115.54	120.87
3	C	402	HFK	C03-C02-C07	3.22	123.61	117.35
2	A	401	GAL	O1-C1-C2	3.21	118.29	108.98
3	A	402	HFK	C26-C20-N19	3.21	137.31	128.21
3	A	402	HFK	N17-C15-N14	-3.17	112.05	117.96
3	C	402	HFK	C21-C20-N19	-3.11	105.71	108.60
3	A	402	HFK	C13-C12-C11	3.03	116.07	111.35
3	C	402	HFK	C05-C06-N16	-2.99	111.21	115.46
3	C	402	HFK	C26-C20-C21	-2.91	116.61	120.31
2	A	401	GAL	O3-C3-C4	2.84	117.06	110.38
3	A	402	HFK	C05-C06-N16	-2.83	111.43	115.46
3	C	402	HFK	C13-C12-C11	2.76	115.65	111.35
2	C	401	GAL	C1-C2-C3	-2.75	104.75	110.36
3	A	402	HFK	N17-C18-N19	-2.68	120.97	128.58
3	C	402	HFK	O22-C21-C20	2.58	109.55	107.80
3	A	402	HFK	C03-C02-C07	2.55	122.31	117.35
3	C	402	HFK	O01-C02-C03	-2.55	116.69	120.87
2	B	401	GAL	O5-C5-C6	2.44	112.50	106.44
3	B	402	HFK	N17-C15-N14	-2.34	113.60	117.96
2	B	401	GAL	O5-C1-C2	-2.32	106.21	110.30
3	B	402	HFK	C23-C21-C20	-2.30	120.82	123.62
2	A	401	GAL	O1-C1-O5	-2.30	103.59	110.41
2	B	401	GAL	O4-C4-C3	2.29	115.78	110.38
3	B	402	HFK	O01-C02-C07	2.25	124.54	121.53
3	A	402	HFK	C18-N17-C15	2.25	130.76	125.27
2	C	401	GAL	C3-C4-C5	2.24	114.29	110.23
3	B	402	HFK	C26-C20-C21	-2.16	117.56	120.31
2	B	401	GAL	O1-C1-C2	2.13	115.15	108.98
3	A	402	HFK	C20-N19-C18	2.08	108.26	104.13

There are no chirality outliers.

All (19) torsion outliers are listed below:

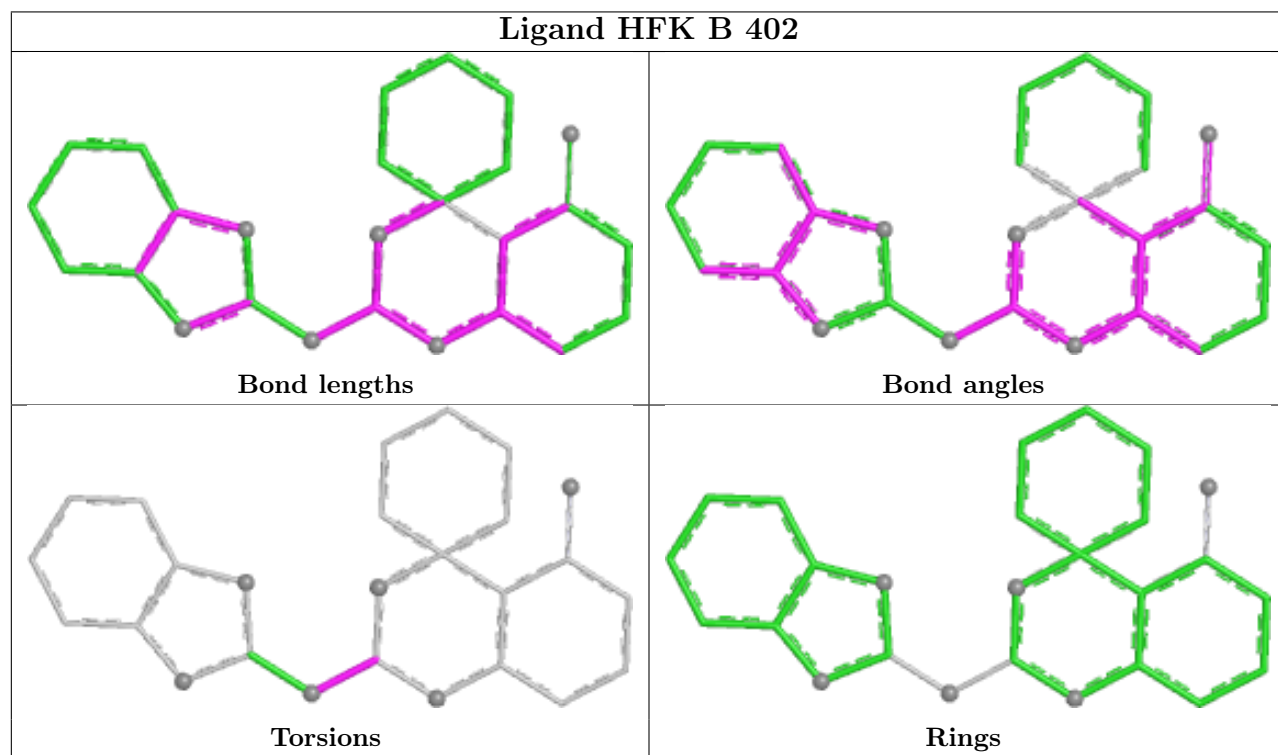
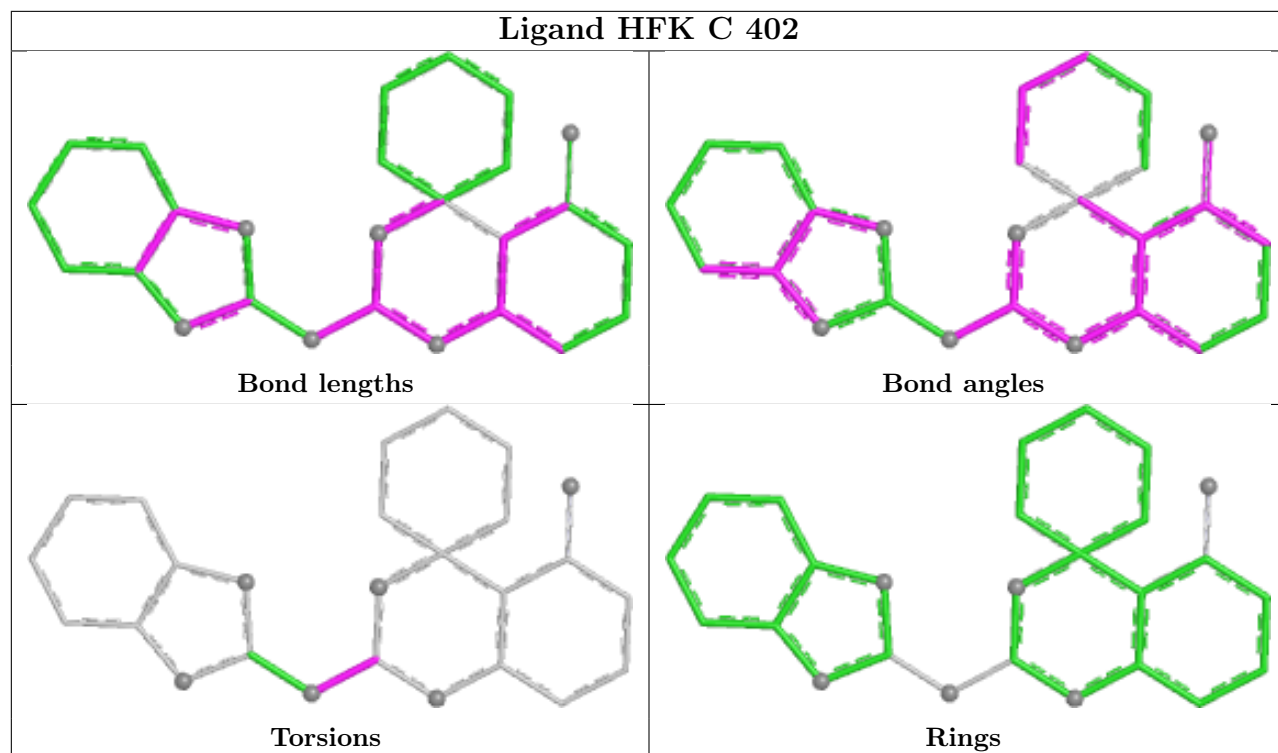
Mol	Chain	Res	Type	Atoms
3	A	402	HFK	N14-C15-N17-C18
3	A	402	HFK	N16-C15-N17-C18
3	B	402	HFK	N14-C15-N17-C18
3	C	402	HFK	N14-C15-N17-C18
3	C	402	HFK	N16-C15-N17-C18
4	B	403	HR8	C7-C8-N1-C9
4	B	403	HR8	C12-C10-C9-N1
4	B	403	HR8	O2-C8-N1-C9
2	C	401	GAL	O5-C5-C6-O6
2	A	401	GAL	O5-C5-C6-O6
2	C	401	GAL	C4-C5-C6-O6
4	A	403	HR8	C11-C10-C9-N1
4	D	401	HR8	C11-C10-C9-N1
2	B	401	GAL	O5-C5-C6-O6
2	A	401	GAL	C4-C5-C6-O6
4	B	403	HR8	C11-C10-C9-N1
3	B	402	HFK	N16-C15-N17-C18
4	D	401	HR8	C12-C10-C9-N1
4	A	403	HR8	C12-C10-C9-N1

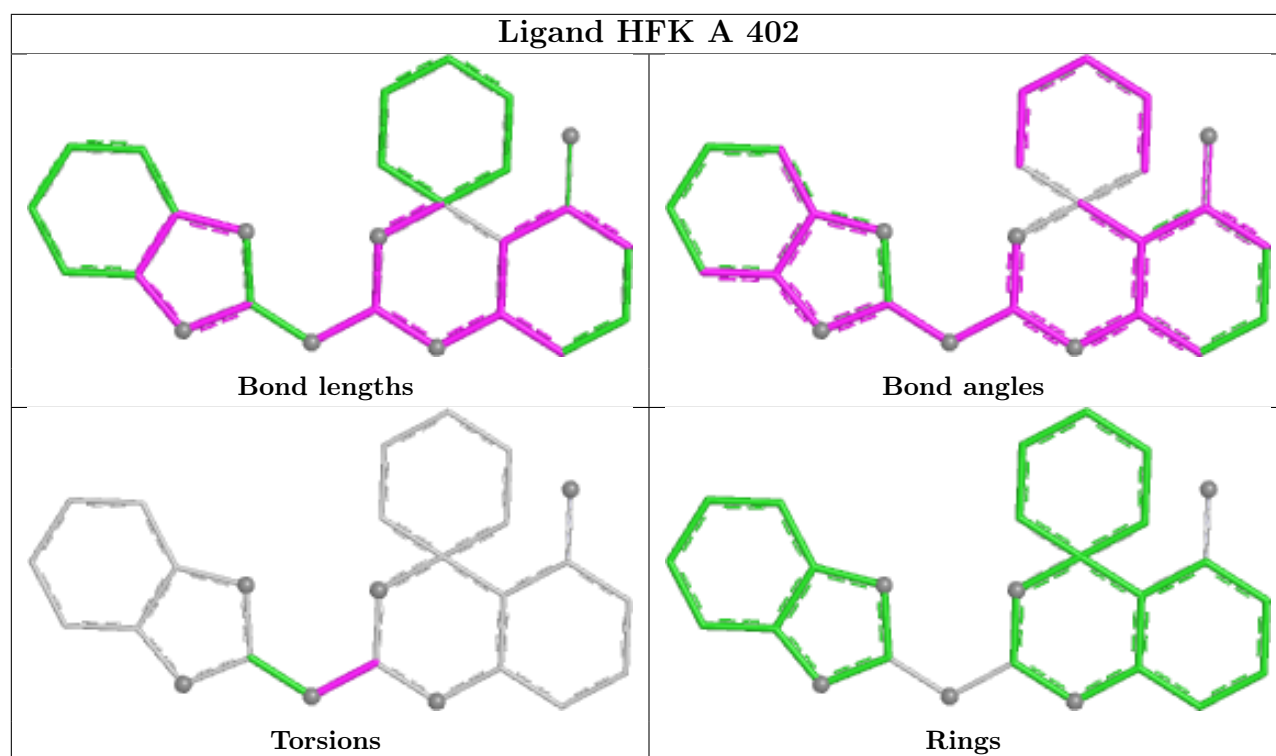
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	GAL	1	0
4	C	403	HR8	1	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 [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	392/392 (100%)	-0.13	2 (0%) 87 85	25, 40, 63, 97	1 (0%)
1	B	392/392 (100%)	0.21	14 (3%) 46 42	27, 45, 77, 107	1 (0%)
1	C	392/392 (100%)	0.76	62 (15%) 5 4	25, 49, 88, 115	0
1	D	360/392 (91%)	0.87	62 (17%) 4 3	26, 56, 99, 123	0
All	All	1536/1568 (97%)	0.42	140 (9%) 15 12	25, 47, 88, 123	2 (0%)

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	340	GLY	5.1
1	D	104	PRO	5.0
1	C	233	SER	4.9
1	C	332	ALA	4.8
1	C	2	ALA	4.8
1	C	305	ARG	4.6
1	C	1	HIS	4.5
1	D	129	VAL	4.5
1	C	339	TYR	4.4
1	D	106	TRP	4.3
1	D	169	VAL	4.3
1	D	236	TYR	4.1
1	C	231	LEU	4.0
1	C	275	PHE	3.9
1	B	232	ALA	3.9
1	D	109	TYR	3.9
1	C	269	LEU	3.8
1	D	23	GLU	3.8
1	C	334	ALA	3.8
1	C	230	SER	3.7
1	D	123	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	63	LEU	3.7
1	C	363	HIS	3.6
1	D	128	VAL	3.6
1	D	130	VAL	3.6
1	D	176	SER	3.5
1	C	306	LEU	3.5
1	C	337	GLY	3.5
1	D	70	ASP	3.5
1	D	77	THR	3.5
1	D	94	THR	3.5
1	D	8	GLN	3.4
1	D	126	SER	3.4
1	D	163	ILE	3.4
1	B	97	ARG	3.4
1	C	370	GLU	3.4
1	C	303	PHE	3.3
1	B	230	SER	3.3
1	C	270	VAL	3.3
1	C	302	ALA	3.3
1	C	364	ALA	3.3
1	D	26	ALA	3.3
1	D	231	LEU	3.2
1	D	188	PHE	3.2
1	C	333	LEU	3.2
1	C	362	PRO	3.2
1	D	173	ALA	3.1
1	A	1	HIS	3.1
1	C	273	GLU	3.1
1	C	278	ALA	3.1
1	D	9	VAL	3.1
1	D	73	VAL	3.1
1	C	336	PRO	3.0
1	C	274	GLY	3.0
1	D	21	ARG	3.0
1	C	263	LEU	3.0
1	D	185	MET	2.9
1	D	16	ALA	2.9
1	D	12	LEU	2.9
1	C	261	GLU	2.9
1	D	87	ARG	2.9
1	D	89	GLN	2.9
1	D	88	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	76	LEU	2.8
1	C	249	ALA	2.8
1	D	122	LEU	2.7
1	B	231	LEU	2.7
1	C	268	ASP	2.7
1	D	10	ALA	2.7
1	D	90	PHE	2.6
1	B	233	SER	2.6
1	C	279	ARG	2.6
1	C	265	ALA	2.6
1	D	93	PRO	2.6
1	B	7	PRO	2.5
1	C	300	TYR	2.5
1	C	260	LEU	2.5
1	C	308	VAL	2.5
1	C	232	ALA	2.5
1	D	18	ARG	2.5
1	D	127	ALA	2.5
1	D	22	GLU	2.5
1	D	92	LEU	2.5
1	D	19	ALA	2.5
1	D	25	GLY	2.4
1	D	235	GLU	2.4
1	D	13	LEU	2.4
1	D	113	VAL	2.4
1	D	11	GLU	2.4
1	B	234	SER	2.4
1	C	8	GLN	2.4
1	C	276	ARG	2.4
1	D	267	ARG	2.4
1	C	246	VAL	2.4
1	C	266	ALA	2.4
1	D	214	SER	2.4
1	B	69	LYS	2.3
1	B	76	LEU	2.3
1	B	95	ALA	2.3
1	C	354	THR	2.3
1	C	331	ALA	2.3
1	A	96	GLN	2.3
1	D	75	LEU	2.3
1	C	245	GLU	2.3
1	D	249	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	375	THR	2.2
1	C	218	LEU	2.2
1	D	15	GLU	2.2
1	C	335	VAL	2.2
1	D	67	PRO	2.2
1	C	3	ALA	2.2
1	D	170	CYS	2.2
1	C	381	SER	2.2
1	C	330	GLU	2.2
1	D	78	THR	2.2
1	C	304	GLY	2.2
1	C	286	ARG	2.2
1	D	166	ARG	2.2
1	C	282	VAL	2.2
1	D	64	VAL	2.2
1	B	244	GLU	2.2
1	B	246	VAL	2.1
1	C	373	GLY	2.1
1	D	72	LEU	2.1
1	B	8	GLN	2.1
1	B	80	GLU	2.1
1	C	7	PRO	2.1
1	D	162	THR	2.1
1	C	301	ARG	2.1
1	D	116	TYR	2.1
1	C	369	GLN	2.1
1	C	258	VAL	2.1
1	D	24	PHE	2.1
1	C	312	ARG	2.1
1	D	161	GLY	2.1
1	C	341	SER	2.1
1	C	287	ARG	2.0
1	D	14	ALA	2.0
1	C	361	ALA	2.0
1	C	365	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

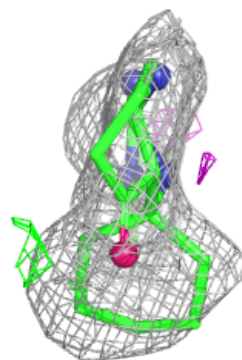
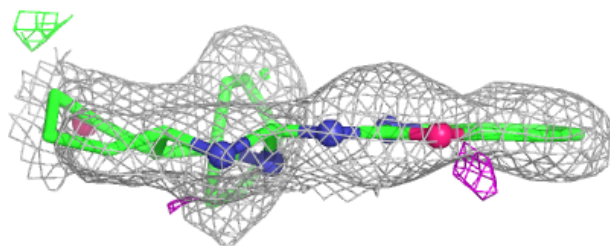
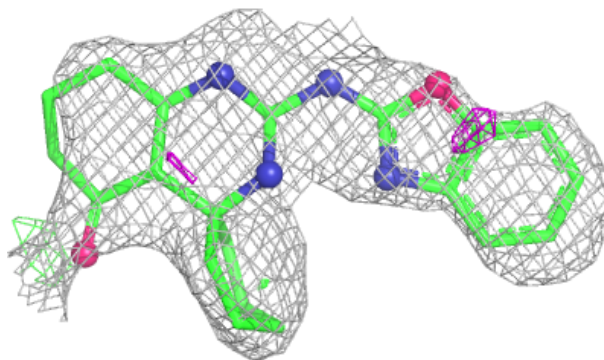
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HFK	B	402	26/26	0.83	0.21	60,79,97,106	0
4	HR8	D	401	16/16	0.86	0.16	55,64,80,81	0
4	HR8	C	403	16/16	0.87	0.15	51,70,79,82	0
3	HFK	C	402	26/26	0.90	0.14	47,70,80,83	0
4	HR8	A	403	16/16	0.90	0.14	56,63,68,73	0
3	HFK	A	402	26/26	0.92	0.10	39,48,55,61	0
2	GAL	C	401	12/12	0.92	0.08	37,42,49,51	0
4	HR8	B	403	16/16	0.94	0.10	44,47,53,59	0
2	GAL	B	401	12/12	0.95	0.08	32,40,47,54	0
2	GAL	A	401	12/12	0.96	0.05	23,28,33,38	0

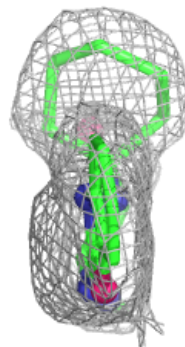
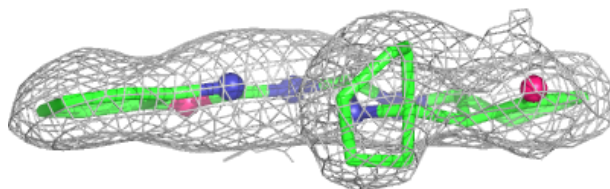
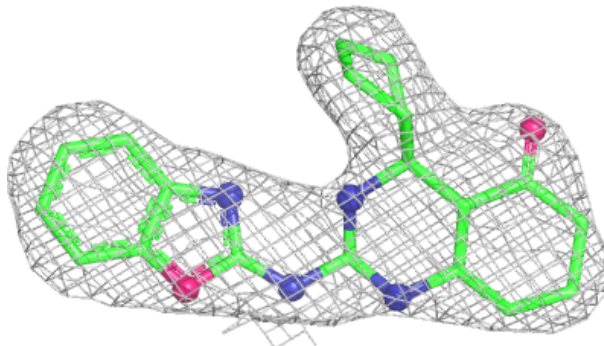
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

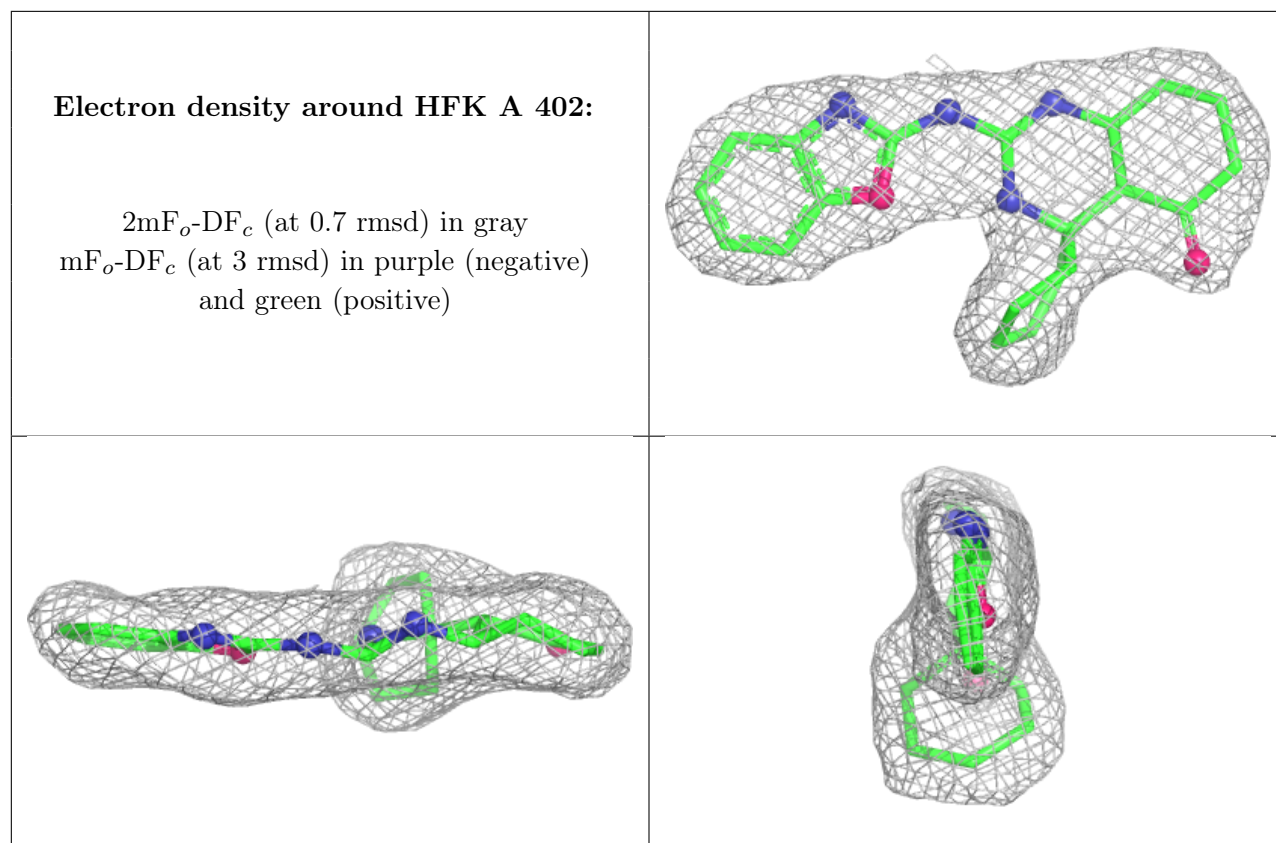
Electron density around HFK B 402:

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

**Electron density around HFK C 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.