



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:47 PM UTC

PDB ID : 6ZGW / pdb_00006zgw
Title : Structure of human galactokinase 1 bound with (4-chlorophenyl)methyl pyridine-3-carboxylate
Authors : Mackinnon, S.R.; Bezerra, G.A.; Zhang, M.; Foster, W.; Krojer, T.; Brandao-Neto, J.; Douangamath, A.; Arrowsmith, C.; Edwards, A.; Bountra, C.; Brennan, P.; Lai, K.; Yue, W.W.
Deposited on : 2020-06-20
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

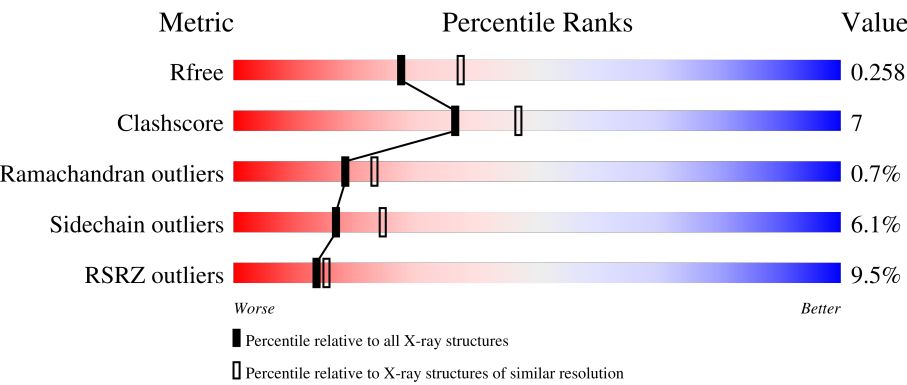
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	399	14% 75% 19% • • •
1	B	399	8% 80% 15% • •
1	D	399	12% 70% 20% • 7%
1	E	399	3% 85% 13% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11522 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
			2747	1719	486	526	16			
1	B	390	Total	C	N	O	S	0	1	0
			2772	1744	482	531	15			
1	E	391	Total	C	N	O	S	0	0	0
			2823	1773	493	541	16			
1	D	371	Total	C	N	O	S	0	0	0
			2569	1611	451	493	14			

There are 40 discrepancies between the modelled and reference sequences:

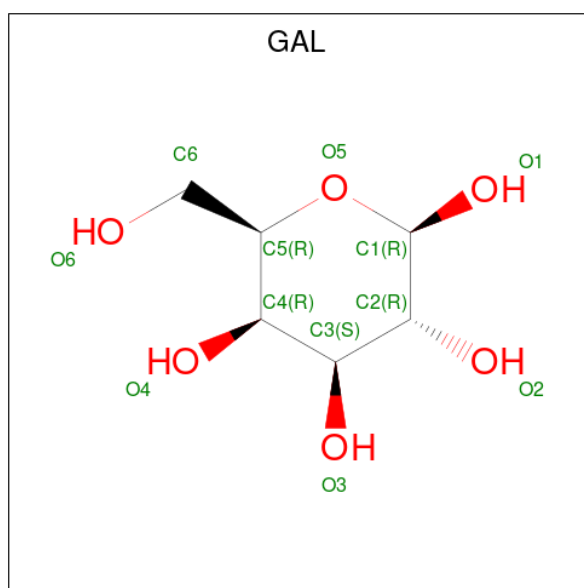
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP P51570
A	-5	ALA	-	expression tag	UNP P51570
A	-4	HIS	-	expression tag	UNP P51570
A	-3	HIS	-	expression tag	UNP P51570
A	-2	HIS	-	expression tag	UNP P51570
A	-1	HIS	-	expression tag	UNP P51570
A	0	HIS	-	expression tag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

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

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



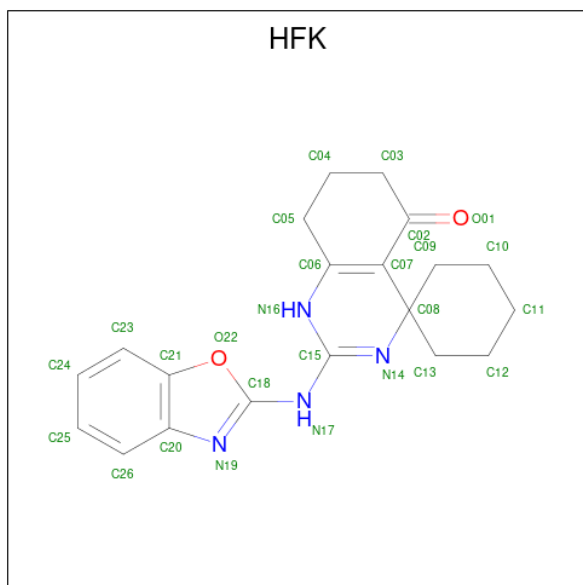
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

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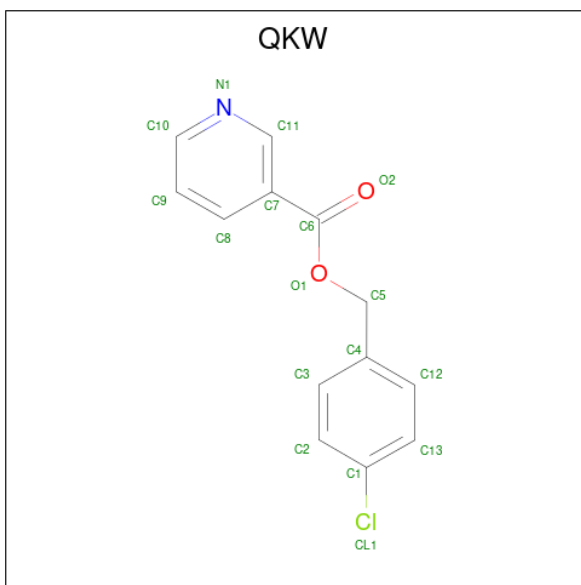
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			12	6	6		

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



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

- Molecule 4 is (4-chlorophenyl)methyl pyridine-3-carboxylate (CCD ID: QKW) (formula: $C_{13}H_{10}ClNO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	Cl	N	O	0	0
			17	13	1	1	2		

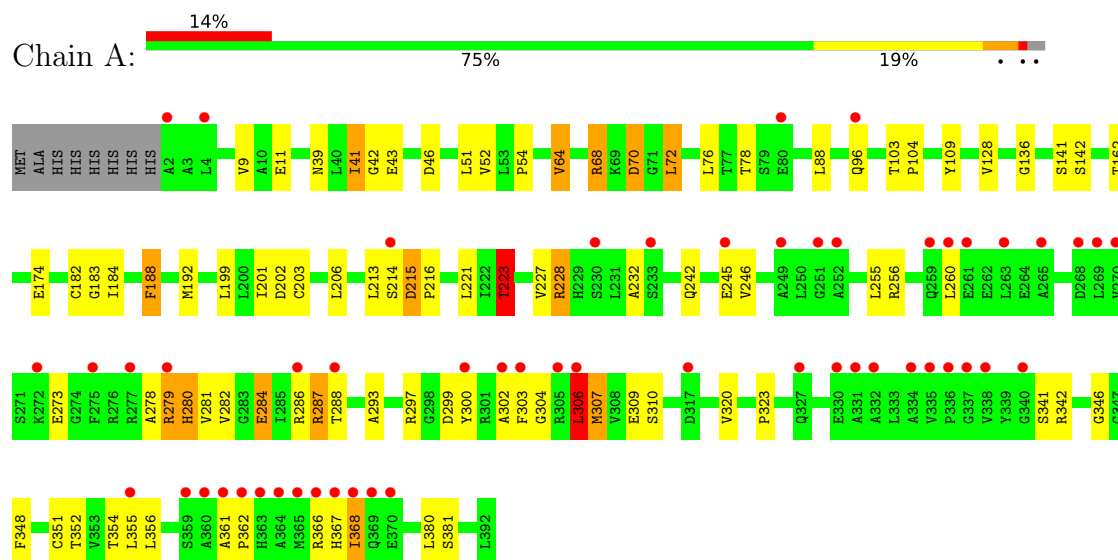
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total	O	0	0
			108	108		
5	B	114	Total	O	0	0
			114	114		
5	E	160	Total	O	0	0
			160	160		
5	D	98	Total	O	0	0
			98	98		

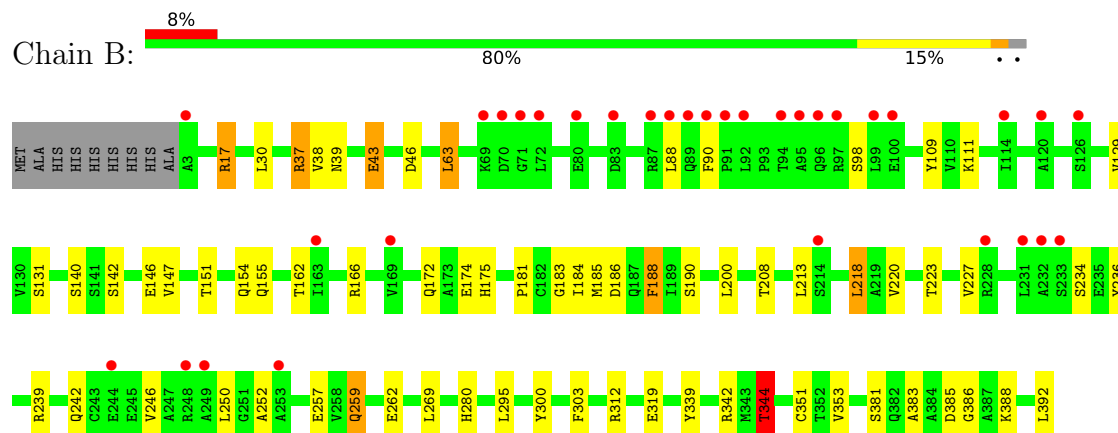
3 Residue-property plots [i](#)

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.

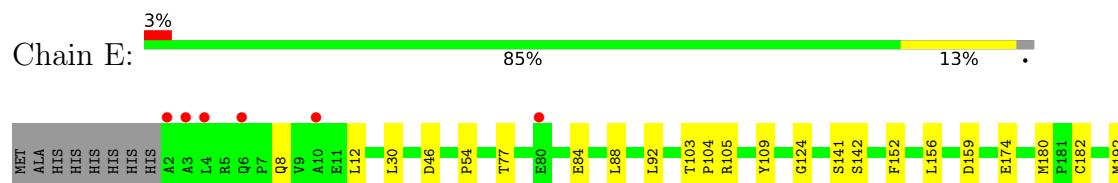
• Molecule 1: Galactokinase



• Molecule 1: Galactokinase

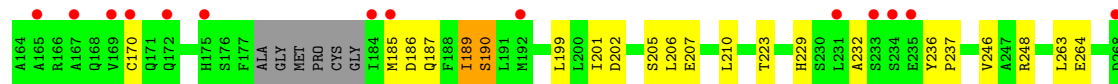
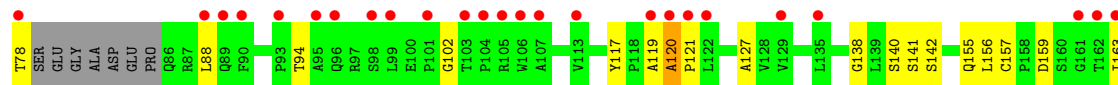
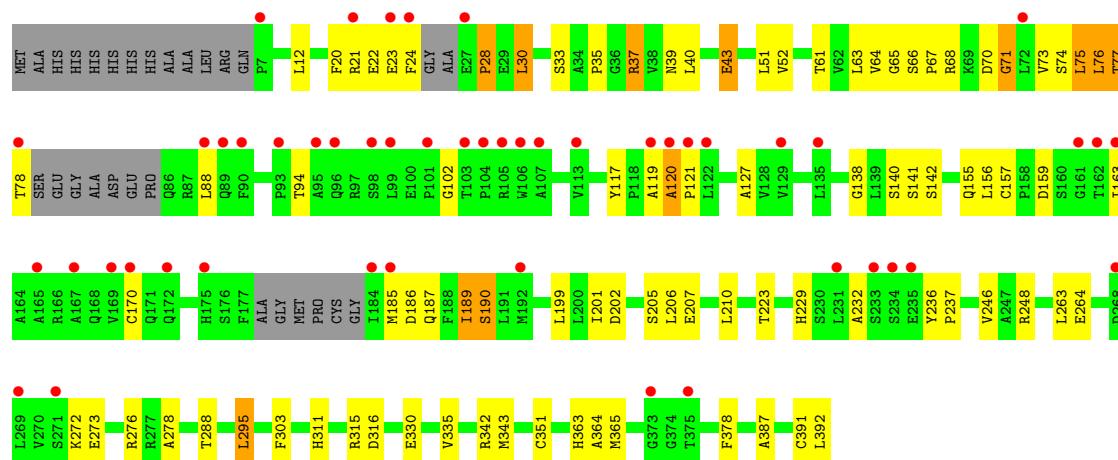


• Molecule 1: Galactokinase





● 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	73.67Å 114.56Å 120.93Å 90.00° 100.49° 90.00°	Depositor
Resolution (Å)	118.91 – 2.30 118.91 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (118.91-2.30) 99.9 (118.91-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.209 , 0.255 0.213 , 0.258	Depositor DCC
R_{free} test set	5376 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11522	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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: GAL, HFK, QKW

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	1.27	8/2799 (0.3%)	1.61	21/3822 (0.5%)
1	B	1.20	3/2829 (0.1%)	1.58	10/3864 (0.3%)
1	D	1.29	8/2612 (0.3%)	1.65	17/3566 (0.5%)
1	E	1.20	0/2876	1.54	11/3921 (0.3%)
All	All	1.24	19/11116 (0.2%)	1.59	59/15173 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	GLU	C-O	9.92	1.35	1.24
1	D	24	PHE	C-O	8.78	1.41	1.23
1	D	28	PRO	C-O	8.44	1.33	1.23
1	A	183	GLY	C-O	6.63	1.29	1.23
1	A	68	ARG	C-O	6.51	1.32	1.23
1	D	28	PRO	CA-C	6.48	1.60	1.52
1	D	22	GLU	CD-OE1	6.43	1.37	1.25
1	A	299	ASP	C-O	6.37	1.31	1.24
1	D	229	HIS	CE1-NE2	6.16	1.38	1.32
1	D	71	GLY	CA-C	5.68	1.60	1.51
1	A	286	ARG	C-O	5.67	1.32	1.24
1	A	188	PHE	C-O	5.65	1.30	1.24
1	D	71	GLY	C-N	5.58	1.41	1.33
1	A	299	ASP	CB-CG	5.54	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	71	GLY	C-O	5.50	1.31	1.24
1	B	386	GLY	C-O	5.49	1.29	1.23
1	B	183	GLY	C-O	5.10	1.28	1.23
1	B	200	LEU	C-O	-5.09	1.17	1.24
1	A	323	PRO	C-O	-5.02	1.17	1.24

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	43	GLU	CB-CA-C	-10.88	92.18	110.68
1	B	280	HIS	CA-CB-CG	-7.79	106.01	113.80
1	B	46	ASP	CA-CB-CG	7.73	120.33	112.60
1	A	288	THR	N-CA-C	-7.06	103.51	111.14
1	A	306	LEU	CA-C-N	6.86	129.96	120.63
1	A	306	LEU	C-N-CA	6.86	129.96	120.63
1	A	223	THR	CB-CA-C	6.75	121.36	110.16
1	D	37	ARG	CG-CD-NE	-6.40	97.93	112.00
1	E	103	THR	CA-CB-OG1	-6.36	100.06	109.60
1	E	374	GLY	CA-C-O	-6.24	117.82	122.37
1	A	280	HIS	CA-CB-CG	-6.12	107.68	113.80
1	D	276	ARG	CB-CA-C	6.07	120.53	110.81
1	A	279	ARG	N-CA-C	-6.05	104.01	111.33
1	E	311	HIS	CA-CB-CG	-5.88	107.92	113.80
1	A	282	VAL	O-C-N	5.86	127.55	121.87
1	D	70	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	46	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	70	ASP	CA-CB-CG	5.51	118.11	112.60
1	D	102	GLY	CA-C-N	5.51	127.64	120.26
1	D	102	GLY	C-N-CA	5.51	127.64	120.26
1	B	344	THR	CB-CA-C	-5.51	98.97	109.66
1	A	366	ARG	CA-C-N	5.49	128.43	120.79
1	A	366	ARG	C-N-CA	5.49	128.43	120.79
1	E	77	THR	CA-CB-OG1	-5.47	101.39	109.60
1	A	288	THR	CB-CA-C	5.45	119.50	110.90
1	A	64	VAL	CB-CA-C	5.38	118.19	110.33
1	E	301	ARG	N-CA-C	-5.33	105.47	111.28
1	D	24	PHE	CA-C-O	-5.33	111.74	120.80
1	D	273	GLU	N-CA-C	-5.32	105.48	111.28
1	B	312	ARG	N-CA-C	-5.32	105.48	111.28
1	B	172	GLN	CA-C-N	5.30	127.33	120.44
1	B	172	GLN	C-N-CA	5.30	127.33	120.44
1	B	303	PHE	CA-C-N	5.30	125.82	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	303	PHE	C-N-CA	5.30	125.82	119.94
1	D	232	ALA	CA-C-N	5.28	127.61	120.38
1	D	232	ALA	C-N-CA	5.28	127.61	120.38
1	E	312	ARG	N-CA-C	-5.24	105.57	111.28
1	A	281	VAL	O-C-N	5.24	127.54	121.94
1	A	162	THR	CA-CB-OG1	-5.21	101.78	109.60
1	A	281	VAL	CA-C-N	5.20	127.59	120.46
1	A	281	VAL	C-N-CA	5.20	127.59	120.46
1	B	43	GLU	CA-C-N	5.19	129.50	122.19
1	B	43	GLU	C-N-CA	5.19	129.50	122.19
1	D	288	THR	CA-CB-OG1	-5.19	101.82	109.60
1	E	159	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	256	ARG	CA-C-N	5.16	127.20	120.28
1	A	256	ARG	C-N-CA	5.16	127.20	120.28
1	D	21	ARG	CA-C-N	5.13	127.67	120.28
1	D	21	ARG	C-N-CA	5.13	127.67	120.28
1	E	84	GLU	CB-CG-CD	5.12	121.31	112.60
1	D	248	ARG	CA-C-N	5.12	127.86	120.38
1	D	248	ARG	C-N-CA	5.12	127.86	120.38
1	E	235	GLU	CB-CG-CD	5.12	121.31	112.60
1	E	46	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	368	ILE	CA-C-O	-5.06	116.01	121.27
1	E	103	THR	CB-CA-C	5.04	116.44	108.88
1	A	52	VAL	CA-C-O	-5.01	116.41	121.67
1	D	141	SER	CA-C-N	5.00	126.94	120.44
1	D	141	SER	C-N-CA	5.00	126.94	120.44

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	71	GLY	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2747	0	2570	46	0
1	B	2772	0	2630	38	0
1	D	2569	0	2378	49	0
1	E	2823	0	2730	23	0
2	A	12	0	10	0	0
2	B	12	0	12	1	0
2	E	12	0	11	0	0
3	A	26	0	0	1	0
3	B	26	0	0	0	0
3	E	26	0	0	1	0
4	D	17	0	0	2	0
5	A	108	0	0	4	0
5	B	114	0	0	1	0
5	D	98	0	0	0	0
5	E	160	0	0	2	0
All	All	11522	0	10341	153	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (153) 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:B:37:ARG:NH1	1:B:186:ASP:OD1	2.00	0.94
1:D:40:LEU:HD13	4:D:401:QKW:CL1	2.22	0.77
1:B:242:GLN:OE1	5:B:501:HOH:O	2.02	0.76
1:A:72:LEU:C	1:A:72:LEU:HD12	2.11	0.75
1:B:43:GLU:HB2	1:B:342:ARG:NH2	2.07	0.70
1:A:287:ARG:HB3	1:A:306:LEU:HD12	1.74	0.69
1:E:8:GLN:CB	5:E:643:HOH:O	2.40	0.68
1:B:147:VAL:HG21	1:B:190:SER:HB3	1.75	0.67
1:A:320:VAL:HG13	1:A:348:PHE:CE2	2.29	0.67
1:B:109:TYR:CE1	1:B:142:SER:HB2	2.32	0.65
1:A:367:HIS:CE1	5:A:504:HOH:O	2.50	0.64
1:D:75:LEU:HD12	1:D:75:LEU:N	2.13	0.63
1:D:342:ARG:HG3	1:D:343:MET:O	1.99	0.62
1:E:276:ARG:HG2	1:E:317:ASP:HA	1.82	0.61
1:D:335:VAL:HG21	1:D:364:ALA:HA	1.83	0.61
1:B:37:ARG:NH1	1:B:186:ASP:CG	2.58	0.61
1:B:43:GLU:HB2	1:B:342:ARG:HH22	1.64	0.61
1:B:218:LEU:HD11	1:B:339:TYR:HE2	1.64	0.60
1:A:199:LEU:HD23	1:A:201:ILE:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ALA:HB3	1:D:121:PRO:HD3	1.84	0.60
1:B:213:LEU:HD12	1:B:383:ALA:HB2	1.84	0.59
1:B:259:GLN:HE21	1:B:262:GLU:CD	2.10	0.59
1:D:73:VAL:HG12	1:D:75:LEU:HD11	1.83	0.59
1:D:40:LEU:CD1	4:D:401:QKW:CL1	2.87	0.59
1:A:361:ALA:HB1	1:A:380:LEU:HD11	1.85	0.58
1:A:223:THR:HG23	1:A:352:THR:OG1	2.04	0.58
1:D:39:ASN:CB	1:D:43:GLU:HG3	2.33	0.58
1:A:287:ARG:HB3	1:A:306:LEU:CD1	2.35	0.57
1:A:68:ARG:CZ	1:A:72:LEU:HD11	2.35	0.56
1:B:38:VAL:CG2	1:B:344:THR:HG21	2.36	0.56
1:B:385:ASP:OD2	1:B:388:LYS:NZ	2.39	0.55
1:D:37:ARG:NH1	1:D:186:ASP:OD1	2.37	0.55
1:D:159:ASP:OD1	1:D:159:ASP:C	2.49	0.55
1:D:75:LEU:N	1:D:75:LEU:CD1	2.69	0.55
1:D:20:PHE:CE2	1:D:65:GLY:HA2	2.42	0.55
1:E:174:GLU:HG2	1:E:182:CYS:SG	2.47	0.55
1:A:306:LEU:HD11	5:A:608:HOH:O	2.07	0.54
1:B:39:ASN:O	1:B:344:THR:HG22	2.07	0.54
1:B:37:ARG:NH1	1:B:185:MET:HE3	2.23	0.53
1:E:180:MET:SD	5:E:619:HOH:O	2.59	0.53
1:A:341:SER:O	5:A:501:HOH:O	2.19	0.53
1:B:17:ARG:HD3	1:B:392:LEU:HD13	1.90	0.53
1:A:320:VAL:HG12	1:A:320:VAL:O	2.08	0.52
1:A:184:ILE:HD12	1:A:184:ILE:C	2.34	0.52
1:D:39:ASN:HB3	1:D:43:GLU:HG3	1.91	0.52
1:A:51:LEU:HD23	1:A:202:ASP:HA	1.90	0.52
1:A:287:ARG:HH12	1:A:310:SER:HA	1.74	0.52
1:B:175:HIS:CD2	1:B:181:PRO:HA	2.44	0.52
1:A:70:ASP:OD1	1:A:72:LEU:HG	2.10	0.51
1:D:76:LEU:C	1:D:76:LEU:HD12	2.35	0.51
1:A:280:HIS:O	1:A:284:GLU:N	2.44	0.51
1:B:38:VAL:HG23	1:B:344:THR:HG21	1.92	0.51
1:D:295:LEU:HD13	1:D:303:PHE:CD2	2.46	0.51
1:D:185:MET:O	1:D:189:ILE:HG22	2.11	0.50
1:B:252:ALA:HB1	1:B:257:GLU:HB2	1.92	0.50
1:D:365:MET:HE3	1:D:378:PHE:HB3	1.92	0.50
1:E:218:LEU:HD11	1:E:355:LEU:HG	1.92	0.50
1:A:136:GLY:O	1:A:228:ARG:HD2	2.12	0.50
1:B:162:THR:O	1:B:166:ARG:HG3	2.12	0.50
1:D:121:PRO:HD2	1:D:157:CYS:SG	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ASN:O	1:B:344:THR:CG2	2.60	0.49
1:E:180:MET:HA	1:E:180:MET:HE2	1.94	0.49
1:D:365:MET:HG2	1:D:378:PHE:CG	2.47	0.49
1:D:75:LEU:HA	1:D:127:ALA:O	2.13	0.49
1:A:109:TYR:CE1	1:A:142:SER:HB2	2.48	0.49
1:D:33:SER:HA	1:D:61:THR:O	2.13	0.48
1:A:54:PRO:HD2	1:A:199:LEU:O	2.13	0.48
1:E:109:TYR:CE1	1:E:142:SER:HB2	2.48	0.48
1:B:218:LEU:HD11	1:B:339:TYR:CE2	2.45	0.48
1:D:67:PRO:HB3	1:D:156:LEU:HD22	1.94	0.48
1:D:23:GLU:OE2	1:D:76:LEU:HD22	2.13	0.48
1:A:141:SER:HB2	3:A:402:HFK:N19	2.28	0.48
1:D:30:LEU:HD13	1:D:155:GLN:HG3	1.94	0.48
1:D:365:MET:HE2	1:D:378:PHE:HB2	1.94	0.48
1:E:30:LEU:CD2	1:D:391:CYS:HB2	2.44	0.48
1:E:263:LEU:HG	1:E:275:PHE:CE1	2.48	0.48
1:B:30:LEU:CD2	1:B:155:GLN:HB3	2.44	0.47
1:D:223:THR:O	1:D:351:CYS:HA	2.14	0.47
1:A:320:VAL:CG1	1:A:346:GLY:O	2.63	0.47
1:D:76:LEU:HD12	1:D:77:THR:O	2.15	0.47
1:E:217:LYS:O	1:E:357:GLU:HA	2.15	0.46
1:D:170:CYS:HB2	1:D:187:GLN:HG2	1.97	0.46
1:E:320:VAL:HA	1:E:348:PHE:CZ	2.50	0.46
1:D:51:LEU:HD23	1:D:202:ASP:HA	1.97	0.46
1:A:72:LEU:C	1:A:72:LEU:CD1	2.85	0.46
1:B:295:LEU:HD12	1:B:295:LEU:HA	1.77	0.46
1:A:43:GLU:HB2	1:A:342:ARG:NH2	2.29	0.46
1:E:192:MET:HE1	1:D:210:LEU:HD12	1.96	0.46
1:E:246:VAL:HG11	1:E:278:ALA:HB2	1.98	0.46
1:D:37:ARG:NH2	1:D:138:GLY:O	2.47	0.46
1:A:280:HIS:O	1:A:284:GLU:HB2	2.16	0.46
1:A:278:ALA:O	1:A:279:ARG:C	2.58	0.46
1:A:246:VAL:HG12	1:A:255:LEU:HD21	1.97	0.46
1:B:188:PHE:CE1	1:B:208:THR:HG21	2.51	0.45
1:A:309:GLU:CB	5:A:603:HOH:O	2.63	0.45
1:D:335:VAL:HG13	1:D:363:HIS:CD2	2.51	0.45
1:D:52:VAL:CG2	1:D:201:ILE:HB	2.47	0.45
1:E:250:LEU:HD22	1:E:266:ALA:HB1	1.99	0.45
1:A:307:MET:O	1:A:310:SER:HB3	2.15	0.45
1:A:174:GLU:HG2	1:A:182:CYS:SG	2.57	0.45
1:E:88:LEU:HD22	1:E:104:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:ARG:HD2	1:D:316:ASP:OD1	2.16	0.45
1:A:221:LEU:HB3	1:A:354:THR:HB	1.98	0.45
1:E:152:PHE:CE2	1:E:156:LEU:HD11	2.51	0.44
1:B:218:LEU:HD22	1:B:300:TYR:CE2	2.52	0.44
1:A:192:MET:HE2	1:A:192:MET:HB3	1.89	0.44
1:E:54:PRO:HD2	1:E:199:LEU:O	2.17	0.44
1:B:63:LEU:CD2	1:B:129:VAL:HG22	2.48	0.44
1:B:174:GLU:HA	1:B:174:GLU:OE1	2.17	0.44
1:E:105:ARG:NH1	3:E:402:HFK:O01	2.51	0.44
1:B:63:LEU:HD22	1:B:129:VAL:HG22	1.99	0.44
1:D:39:ASN:CG	1:D:43:GLU:HG3	2.43	0.43
1:A:76:LEU:O	1:A:128:VAL:HA	2.18	0.43
1:B:146:GLU:OE2	1:B:174:GLU:OE1	2.36	0.43
1:D:35:PRO:O	1:D:190:SER:OG	2.37	0.43
1:D:311:HIS:HB2	1:D:342:ARG:HB2	2.00	0.43
1:A:242:GLN:NE2	1:A:273:GLU:OE1	2.52	0.43
1:B:184:ILE:O	1:B:185:MET:C	2.61	0.43
1:E:92:LEU:HD11	1:E:124:GLY:N	2.34	0.43
1:E:361:ALA:HB3	1:E:362:PRO:HD3	2.01	0.43
1:D:246:VAL:HG11	1:D:278:ALA:CB	2.49	0.43
1:B:30:LEU:HD21	1:B:155:GLN:HB3	2.01	0.43
1:A:303:PHE:O	1:A:307:MET:N	2.50	0.42
1:D:205:SER:O	1:D:206:LEU:HB2	2.18	0.42
1:D:74:SER:C	1:D:75:LEU:HD12	2.43	0.42
1:A:78:THR:O	1:A:78:THR:HG22	2.20	0.42
1:B:239:ARG:NH2	1:B:319:GLU:O	2.52	0.42
1:A:202:ASP:O	1:A:206:LEU:N	2.47	0.42
1:D:39:ASN:CB	1:D:43:GLU:CG	2.97	0.42
1:A:184:ILE:HD11	1:A:203:CYS:SG	2.60	0.42
1:B:236:TYR:HH	2:B:401:GAL:HO4	1.66	0.42
1:B:246:VAL:O	1:B:250:LEU:HG	2.20	0.42
1:E:276:ARG:O	1:E:317:ASP:HB3	2.20	0.42
1:D:33:SER:O	1:D:387:ALA:HA	2.19	0.42
1:B:151:THR:O	1:B:154:GLN:HB2	2.19	0.41
1:B:220:VAL:CG1	1:B:353:VAL:HG23	2.50	0.41
1:E:296:ARG:HE	1:D:207:GLU:CD	2.29	0.41
1:A:68:ARG:HD3	1:A:72:LEU:O	2.20	0.41
1:D:117:TYR:CE2	1:D:119:ALA:HB3	2.56	0.41
1:A:361:ALA:HB3	1:A:362:PRO:HD3	2.03	0.41
1:D:159:ASP:OD1	1:D:159:ASP:O	2.38	0.41
1:D:311:HIS:HB2	1:D:342:ARG:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ILE:HG13	1:A:42:GLY:N	2.36	0.41
1:A:215:ASP:HA	1:A:216:PRO:HD3	1.92	0.41
1:A:223:THR:O	1:A:351:CYS:HA	2.20	0.41
1:D:28:PRO:HG2	1:D:392:LEU:CD1	2.51	0.41
1:B:223:THR:O	1:B:351:CYS:HA	2.20	0.41
1:D:236:TYR:N	1:D:237:PRO:HD2	2.36	0.40
1:A:293:ALA:O	1:A:297:ARG:HG3	2.22	0.40
1:E:12:LEU:HD23	1:E:12:LEU:HA	1.85	0.40
1:A:39:ASN:HA	1:A:54:PRO:HA	2.04	0.40
1:A:88:LEU:HD22	1:A:104:PRO:HD2	2.03	0.40
1:B:90:PHE:CE2	1:B:111:LYS:HG2	2.56	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	389/399 (98%)	365 (94%)	17 (4%)	7 (2%)	6	6
1	B	389/399 (98%)	365 (94%)	24 (6%)	0	100	100
1	D	363/399 (91%)	335 (92%)	25 (7%)	3 (1%)	16	20
1	E	389/399 (98%)	379 (97%)	10 (3%)	0	100	100
All	All	1530/1596 (96%)	1444 (94%)	76 (5%)	10 (1%)	18	23

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	ALA
1	D	68	ARG
1	A	300	TYR
1	A	304	GLY

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Mol	Chain	Res	Type
1	A	214	SER
1	A	232	ALA
1	D	88	LEU
1	A	96	GLN
1	A	215	ASP
1	D	120	ALA

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	257/315 (82%)	237 (92%)	20 (8%)	11	16
1	B	268/315 (85%)	252 (94%)	16 (6%)	17	25
1	D	236/315 (75%)	215 (91%)	21 (9%)	9	12
1	E	281/315 (89%)	274 (98%)	7 (2%)	42	60
All	All	1042/1260 (83%)	978 (94%)	64 (6%)	17	24

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	11	GLU
1	A	41	ILE
1	A	64	VAL
1	A	72	LEU
1	A	103	THR
1	A	188	PHE
1	A	213	LEU
1	A	223	THR
1	A	227	VAL
1	A	228	ARG
1	A	245	GLU
1	A	260	LEU
1	A	287	ARG
1	A	306	LEU

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Mol	Chain	Res	Type
1	A	307	MET
1	A	355	LEU
1	A	356	LEU
1	A	368	ILE
1	A	381	SER
1	B	17	ARG
1	B	37	ARG
1	B	63	LEU
1	B	88	LEU
1	B	98	SER
1	B	131[A]	SER
1	B	131[B]	SER
1	B	140	SER
1	B	188	PHE
1	B	218	LEU
1	B	227	VAL
1	B	234	SER
1	B	259	GLN
1	B	269	LEU
1	B	344	THR
1	B	381	SER
1	E	141	SER
1	E	213	LEU
1	E	262	GLU
1	E	264	GLU
1	E	282	VAL
1	E	359	SER
1	E	381	SER
1	D	12	LEU
1	D	30	LEU
1	D	63	LEU
1	D	64	VAL
1	D	66	SER
1	D	75	LEU
1	D	76	LEU
1	D	77	THR
1	D	78	THR
1	D	94	THR
1	D	140	SER
1	D	142	SER
1	D	163	ILE
1	D	189	ILE

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Mol	Chain	Res	Type
1	D	190	SER
1	D	199	LEU
1	D	263	LEU
1	D	264	GLU
1	D	272	LYS
1	D	295	LEU
1	D	330	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	A	226	ASN
1	B	172	GLN
1	B	259	GLN
1	B	371	HIS
1	E	367	HIS
1	D	39	ASN
1	D	48	ASN
1	D	154	GLN
1	D	363	HIS

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	E	401	-	12,12,12	1.15	2 (16%)	17,17,17	3.57	8 (47%)
2	GAL	B	401	-	12,12,12	0.82	0	17,17,17	1.98	4 (23%)
3	HFK	E	402	-	29,30,30	2.65	11 (37%)	32,44,44	2.20	12 (37%)
4	QKW	D	401	-	18,18,18	0.68	1 (5%)	23,23,23	0.71	1 (4%)
3	HFK	B	402	-	29,30,30	2.65	8 (27%)	32,44,44	1.84	10 (31%)
3	HFK	A	402	-	29,30,30	3.10	11 (37%)	32,44,44	1.92	10 (31%)
2	GAL	A	401	-	12,12,12	0.91	0	17,17,17	2.70	7 (41%)

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	E	401	-	-	1/2/22/22	0/1/1/1
2	GAL	B	401	-	-	2/2/22/22	0/1/1/1
3	HFK	E	402	-	-	2/4/43/43	0/5/5/5
4	QKW	D	401	-	-	0/9/9/9	0/2/2/2
3	HFK	B	402	-	-	2/4/43/43	0/5/5/5
3	HFK	A	402	-	-	2/4/43/43	0/5/5/5
2	GAL	A	401	-	-	2/2/22/22	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	HFK	C06-C07	10.97	1.51	1.37
3	B	402	HFK	C06-C07	9.83	1.49	1.37
3	E	402	HFK	C06-C07	8.86	1.48	1.37
3	A	402	HFK	C15-N14	6.56	1.47	1.30
3	B	402	HFK	C15-N14	5.67	1.45	1.30
3	E	402	HFK	C15-N14	5.17	1.43	1.30
3	B	402	HFK	C05-C06	4.19	1.56	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	HFK	C08-N14	3.96	1.50	1.46
3	A	402	HFK	C18-N17	3.89	1.43	1.36
3	E	402	HFK	C15-N16	3.64	1.42	1.36
3	A	402	HFK	C18-N19	3.50	1.36	1.30
3	A	402	HFK	C15-N17	3.28	1.44	1.37
3	A	402	HFK	C15-N16	3.15	1.41	1.36
3	B	402	HFK	C15-N16	3.15	1.41	1.36
3	E	402	HFK	C15-N17	3.11	1.44	1.37
3	E	402	HFK	C03-C02	3.10	1.55	1.50
3	E	402	HFK	C18-N19	3.09	1.35	1.30
3	B	402	HFK	C18-N17	3.02	1.42	1.36
3	B	402	HFK	C15-N17	3.01	1.44	1.37
3	E	402	HFK	C05-C06	2.88	1.54	1.49
3	B	402	HFK	C18-N19	2.84	1.35	1.30
3	A	402	HFK	C23-C21	2.83	1.45	1.39
3	E	402	HFK	C18-N17	2.78	1.41	1.36
3	A	402	HFK	C26-C20	2.73	1.44	1.40
3	E	402	HFK	C20-N19	-2.66	1.34	1.39
3	E	402	HFK	C13-C08	2.60	1.58	1.54
3	A	402	HFK	O22-C21	2.42	1.42	1.38
3	A	402	HFK	C25-C26	2.31	1.42	1.38
2	E	401	GAL	C4-C3	2.22	1.58	1.52
2	E	401	GAL	O2-C2	-2.16	1.37	1.43
4	D	401	QKW	C3-C2	2.15	1.42	1.38
3	B	402	HFK	C06-N16	2.15	1.41	1.37
3	E	402	HFK	C08-N14	2.13	1.48	1.46

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	GAL	C1-O5-C5	-9.91	94.48	113.65
2	A	401	GAL	C1-O5-C5	-6.95	100.20	113.65
3	E	402	HFK	C07-C06-N16	-6.85	116.58	122.11
2	E	401	GAL	C1-C2-C3	-6.62	96.86	110.36
2	A	401	GAL	C1-C2-C3	-6.10	97.92	110.36
2	B	401	GAL	C1-O5-C5	-5.22	103.55	113.65
3	B	402	HFK	C07-C06-N16	-5.03	118.05	122.11
3	E	402	HFK	C23-C21-C20	-4.51	118.14	123.62
2	E	401	GAL	C3-C4-C5	4.12	117.70	110.23
3	A	402	HFK	C23-C21-C20	-4.08	118.66	123.62
3	B	402	HFK	C23-C21-C20	-3.67	119.15	123.62
2	E	401	GAL	O4-C4-C5	-3.67	100.29	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	HFK	O22-C18-N19	-3.52	109.24	115.57
3	E	402	HFK	C05-C06-N16	3.49	120.43	115.46
3	B	402	HFK	O22-C21-C23	3.49	133.82	126.49
3	A	402	HFK	O22-C21-C23	3.44	133.72	126.49
3	A	402	HFK	C05-C06-C07	-3.38	118.12	122.72
2	E	401	GAL	O1-C1-C2	3.27	118.48	108.98
2	B	401	GAL	C1-C2-C3	-3.18	103.86	110.36
2	E	401	GAL	O3-C3-C4	3.12	117.72	110.38
3	E	402	HFK	O22-C21-C23	2.99	132.78	126.49
2	B	401	GAL	O5-C5-C6	2.99	113.85	106.44
3	A	402	HFK	C20-N19-C18	2.99	110.06	104.13
3	E	402	HFK	C09-C10-C11	2.99	116.00	111.35
3	A	402	HFK	C05-C06-N16	2.92	119.62	115.46
3	E	402	HFK	O01-C02-C07	-2.84	117.72	121.53
2	E	401	GAL	O6-C6-C5	-2.83	101.71	111.33
2	A	401	GAL	O5-C5-C4	-2.81	104.64	109.70
3	E	402	HFK	N17-C18-N19	-2.79	120.66	128.58
3	B	402	HFK	O22-C18-N19	-2.78	110.57	115.57
3	A	402	HFK	N17-C15-N14	2.67	122.95	117.96
2	A	401	GAL	C6-C5-C4	2.63	119.49	113.02
4	D	401	QKW	C5-O1-C6	2.62	120.90	115.91
3	E	402	HFK	N17-C15-N14	2.62	122.85	117.96
3	B	402	HFK	N17-C15-N14	2.60	122.83	117.96
3	B	402	HFK	N17-C18-N19	-2.60	121.20	128.58
2	A	401	GAL	O5-C5-C6	2.60	112.87	106.44
3	B	402	HFK	C13-C12-C11	2.41	115.10	111.35
3	E	402	HFK	C02-C07-C06	-2.39	117.06	119.18
2	A	401	GAL	O1-C1-C2	2.30	115.64	108.98
3	E	402	HFK	O22-C18-N19	-2.27	111.49	115.57
3	A	402	HFK	C13-C12-C11	2.24	114.84	111.35
2	B	401	GAL	C3-C4-C5	-2.22	106.21	110.23
3	B	402	HFK	C05-C06-N16	2.20	118.59	115.46
3	A	402	HFK	C21-C20-N19	-2.18	106.58	108.60
2	E	401	GAL	C4-C3-C2	-2.15	107.05	110.83
2	A	401	GAL	O2-C2-C1	2.11	114.11	109.25
3	A	402	HFK	C07-C06-N16	-2.11	120.41	122.11
3	E	402	HFK	N17-C15-N16	-2.11	114.42	117.96
3	E	402	HFK	C20-N19-C18	2.06	108.21	104.13
3	B	402	HFK	C02-C07-C06	-2.06	117.36	119.18
3	B	402	HFK	C09-C10-C11	-2.04	108.17	111.35

There are no chirality outliers.

All (11) torsion outliers are listed below:

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

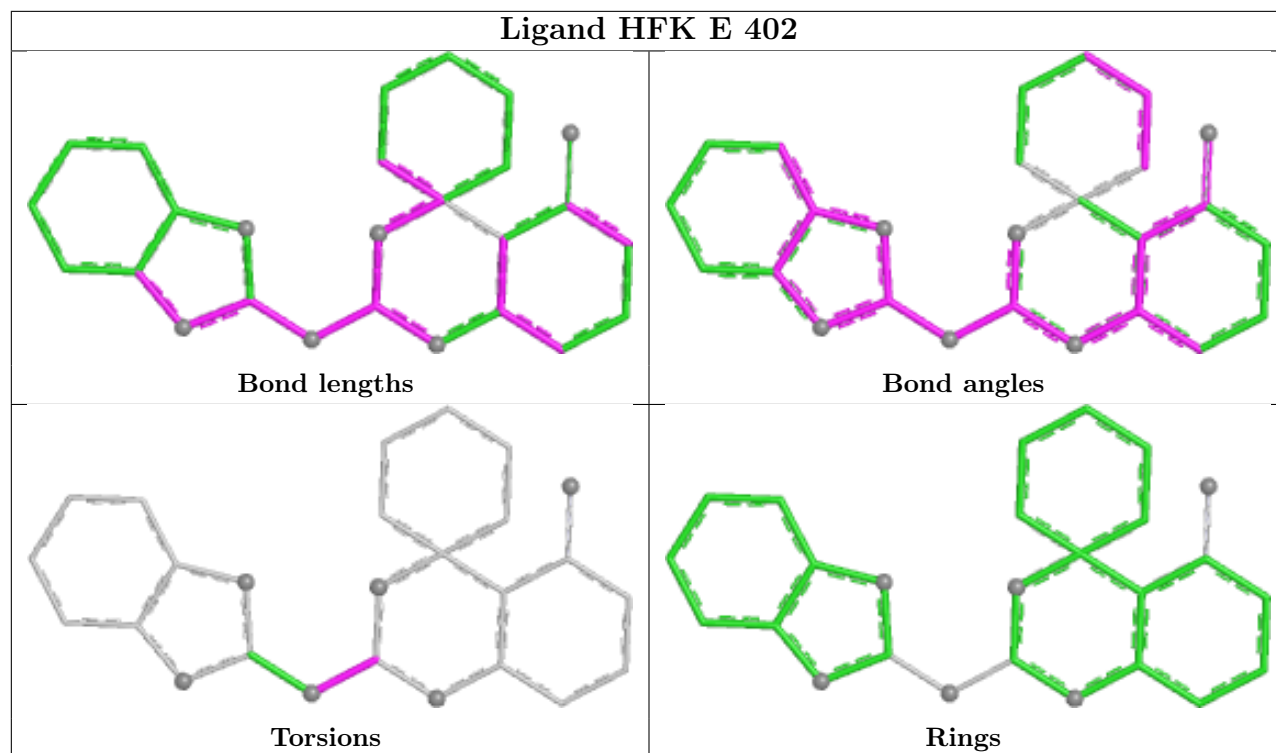
There are no ring outliers.

4 monomers are involved in 5 short contacts:

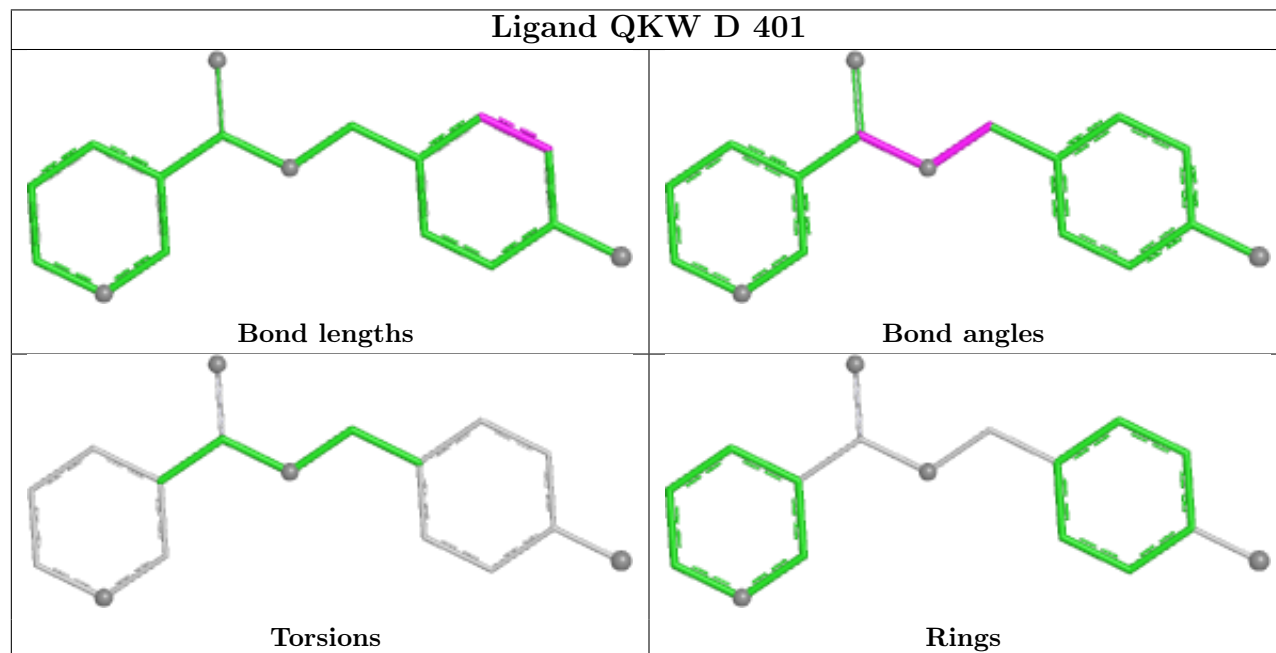
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	GAL	1	0
3	E	402	HFK	1	0
4	D	401	QKW	2	0
3	A	402	HFK	1	0

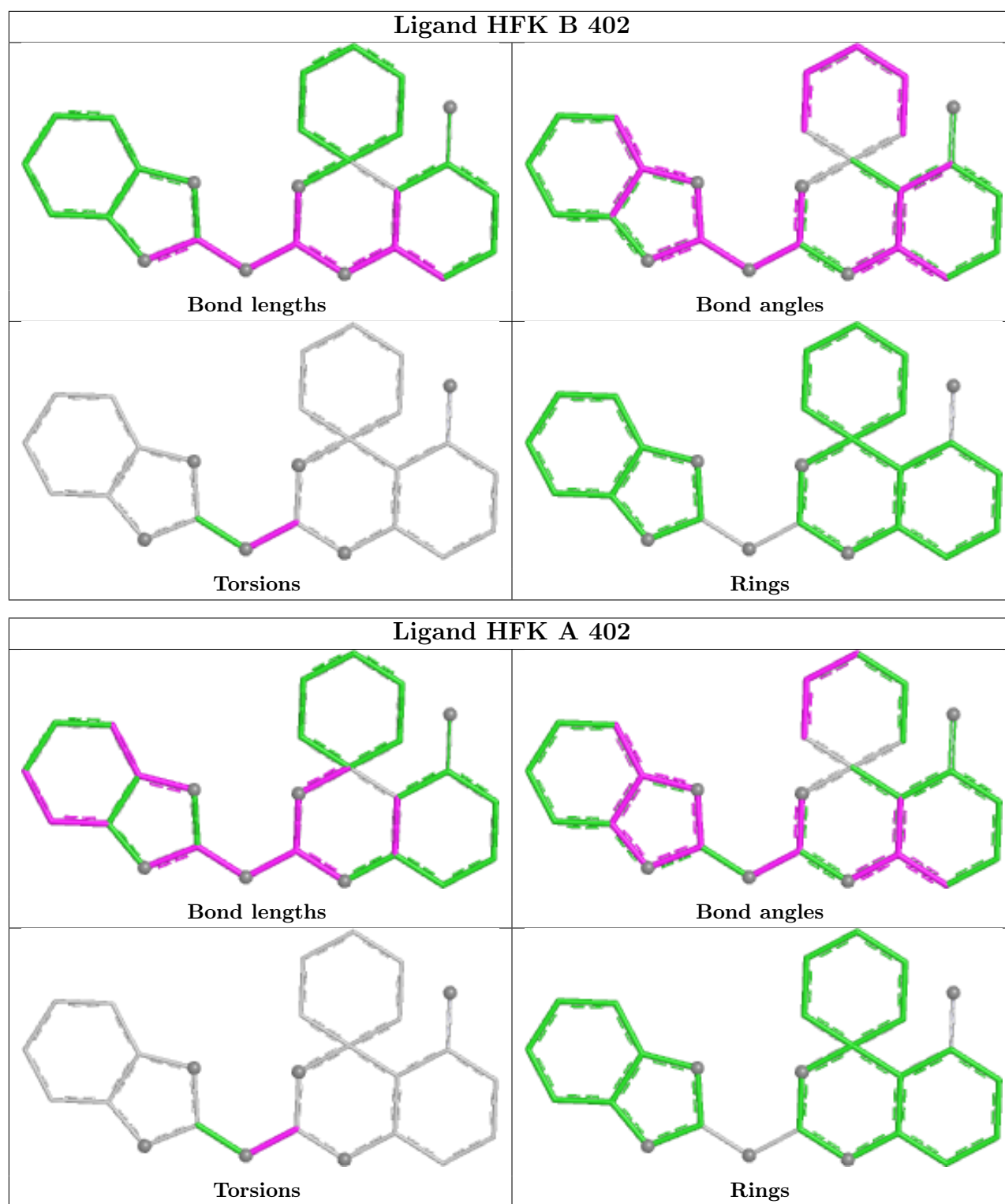
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand HFK E 402



Ligand QKW D 401





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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	391/399 (97%)	0.68	54 (13%) 6 7	26, 54, 103, 128	0
1	B	390/399 (97%)	0.59	33 (8%) 16 18	31, 53, 91, 125	1 (0%)
1	D	371/399 (92%)	0.81	49 (13%) 7 8	25, 56, 119, 160	0
1	E	391/399 (97%)	-0.03	10 (2%) 57 59	23, 40, 68, 82	0
All	All	1543/1596 (96%)	0.51	146 (9%) 14 15	23, 50, 101, 160	1 (0%)

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	7	PRO	6.8
1	D	24	PHE	5.9
1	B	233	SER	5.1
1	A	268	ASP	4.8
1	D	120	ALA	4.8
1	A	363	HIS	4.5
1	A	263	LEU	4.5
1	D	106	TRP	4.5
1	B	69	LYS	4.5
1	A	2	ALA	4.3
1	D	103	THR	4.3
1	D	27	GLU	4.2
1	A	233	SER	4.1
1	B	97	ARG	4.1
1	D	234	SER	4.0
1	B	3	ALA	4.0
1	B	70	ASP	4.0
1	D	121	PRO	4.0
1	D	99	LEU	3.9
1	A	337	GLY	3.9
1	A	260	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	99	LEU	3.7
1	B	231	LEU	3.6
1	D	231	LEU	3.6
1	A	270	VAL	3.6
1	A	360	ALA	3.6
1	D	184	ILE	3.6
1	D	95	ALA	3.5
1	A	305	ARG	3.5
1	B	232	ALA	3.5
1	A	303	PHE	3.5
1	D	373	GLY	3.4
1	D	21	ARG	3.4
1	D	233	SER	3.4
1	A	286	ARG	3.3
1	D	104	PRO	3.3
1	B	120	ALA	3.2
1	A	365	MET	3.1
1	D	93	PRO	3.1
1	B	214	SER	3.1
1	A	334	ALA	3.1
1	B	100	GLU	3.1
1	A	261	GLU	3.0
1	D	175	HIS	3.0
1	E	268	ASP	3.0
1	D	268	ASP	3.0
1	A	265	ALA	3.0
1	A	370	GLU	3.0
1	B	96	GLN	3.0
1	B	249	ALA	2.9
1	A	306	LEU	2.9
1	D	98	SER	2.9
1	D	119	ALA	2.9
1	B	80	GLU	2.9
1	D	163	ILE	2.9
1	A	230	SER	2.8
1	B	71	GLY	2.8
1	A	4	LEU	2.8
1	A	269	LEU	2.8
1	A	335	VAL	2.8
1	D	192	MET	2.8
1	A	364	ALA	2.8
1	E	3	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	213	LEU	2.8
1	A	331	ALA	2.8
1	A	368	ILE	2.8
1	A	214	SER	2.8
1	E	2	ALA	2.8
1	D	113	VAL	2.8
1	D	235	GLU	2.7
1	D	72	LEU	2.7
1	D	101	PRO	2.7
1	D	88	LEU	2.7
1	B	244	GLU	2.6
1	A	367	HIS	2.6
1	A	279	ARG	2.6
1	B	94	THR	2.6
1	B	92	LEU	2.6
1	D	23	GLU	2.6
1	D	96	GLN	2.6
1	A	302	ALA	2.6
1	D	167	ALA	2.6
1	D	162	THR	2.6
1	D	169	VAL	2.6
1	A	96	GLN	2.5
1	D	161	GLY	2.5
1	E	4	LEU	2.5
1	A	330	GLU	2.5
1	D	135	LEU	2.5
1	A	317	ASP	2.5
1	D	170	CYS	2.5
1	A	369	GLN	2.5
1	B	89	GLN	2.5
1	E	80	GLU	2.5
1	A	272	LYS	2.4
1	A	288	THR	2.4
1	A	275	PHE	2.4
1	A	366	ARG	2.4
1	D	165	ALA	2.4
1	B	88	LEU	2.4
1	A	80	GLU	2.4
1	D	122	LEU	2.4
1	B	163	ILE	2.3
1	D	89	GLN	2.3
1	A	362	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	87	ARG	2.3
1	D	105	ARG	2.3
1	D	107	ALA	2.3
1	A	245	GLU	2.3
1	A	355	LEU	2.3
1	E	217	LYS	2.3
1	A	336	PRO	2.3
1	A	251	GLY	2.3
1	A	300	TYR	2.3
1	B	126	SER	2.3
1	E	363	HIS	2.3
1	A	327	GLN	2.3
1	B	90	PHE	2.2
1	D	78	THR	2.2
1	A	277	ARG	2.2
1	A	340	GLY	2.2
1	A	249	ALA	2.2
1	A	361	ALA	2.2
1	B	83	ASP	2.2
1	D	269	LEU	2.2
1	B	169	VAL	2.2
1	A	359	SER	2.2
1	D	375	THR	2.2
1	A	338	VAL	2.1
1	A	259	GLN	2.1
1	A	332	ALA	2.1
1	B	253	ALA	2.1
1	B	72	LEU	2.1
1	B	228	ARG	2.1
1	D	172	GLN	2.1
1	B	91	PRO	2.1
1	D	90	PHE	2.1
1	B	114	ILE	2.1
1	D	129	VAL	2.1
1	B	248	ARG	2.1
1	B	95	ALA	2.0
1	D	185	MET	2.0
1	E	6	GLN	2.0
1	D	271	SER	2.0
1	A	252	ALA	2.0
1	E	10	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 [i](#)

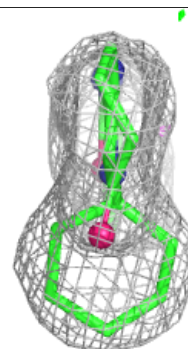
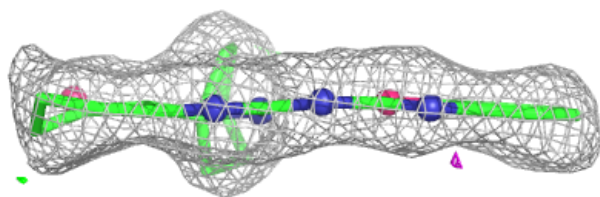
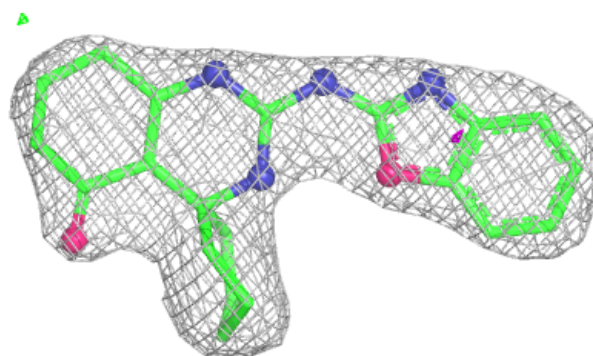
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.89	0.13	60,69,74,78	0
4	QKW	D	401	17/17	0.90	0.11	42,45,49,54	0
3	HFK	A	402	26/26	0.91	0.12	51,55,62,70	0
2	GAL	B	401	12/12	0.92	0.09	38,46,50,55	0
3	HFK	E	402	26/26	0.93	0.09	38,41,47,48	0
2	GAL	A	401	12/12	0.94	0.07	38,42,45,46	0
2	GAL	E	401	12/12	0.96	0.06	24,26,29,33	0

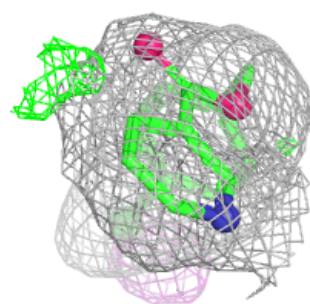
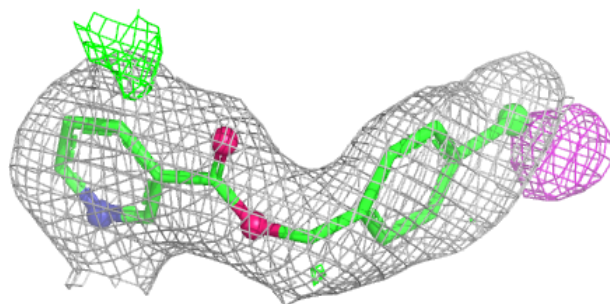
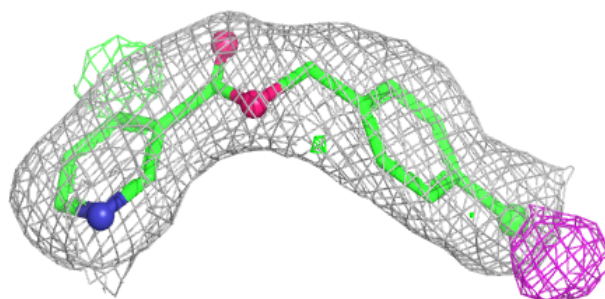
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

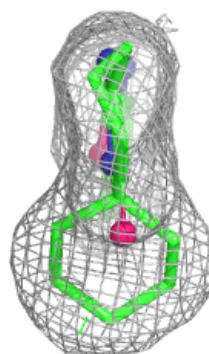
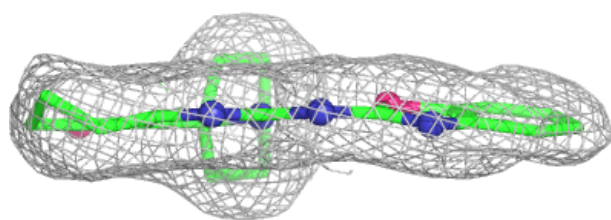
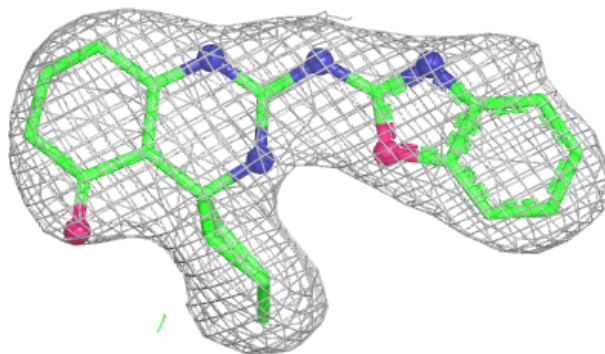
**Electron density around QKW D 401:**

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

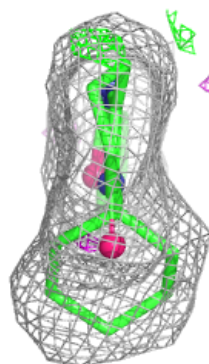
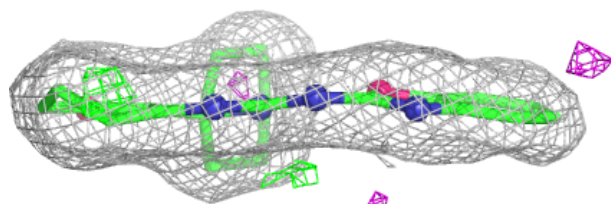
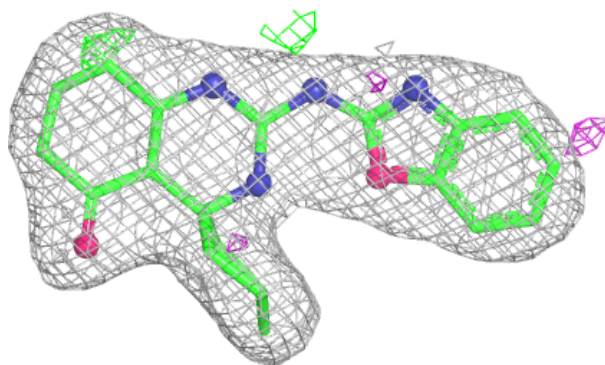


Electron density around HFK A 402:

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

**Electron density around HFK E 402:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.