



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:13 PM UTC

PDB ID : 6ZGX / pdb_00006zgx
Title : Structure of human galactokinase 1 bound with 2-(4-chlorophenyl)-N-(pyrimidin-2-yl)acetamide
Authors : Mackinnon, S.R.; Bezerra, G.A.; Zhang, M.; Foster, W.; Krojer, T.; Brandao-Neto, J.; Douangamath, A.; Arrowsmith, C.; Edwards, A.; Bountra, C.; Brennan, P.; Lai, K.; Yue, W.W.
Deposited on : 2020-06-20
Resolution : 1.86 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:

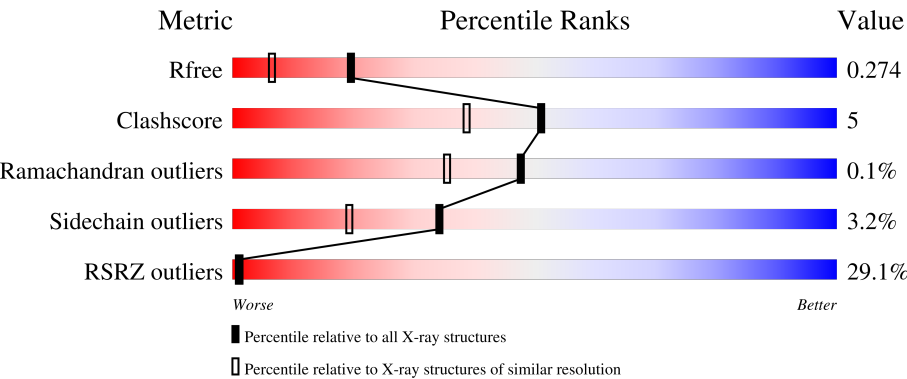
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.86 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	40% 85% 12% ..
1	B	399	27% 89% 8% ..
1	D	399	38% 79% 9% 10%
1	E	399	6% 89% 9% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11542 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
			2785	1750	491	528	16			
1	B	391	Total	C	N	O	S	0	0	0
			2793	1754	495	529	15			
1	D	359	Total	C	N	O	S	0	0	0
			2517	1580	443	481	13			
1	E	391	Total	C	N	O	S	0	0	0
			2859	1794	509	540	16			

There are 40 discrepancies between the modelled and reference sequences:

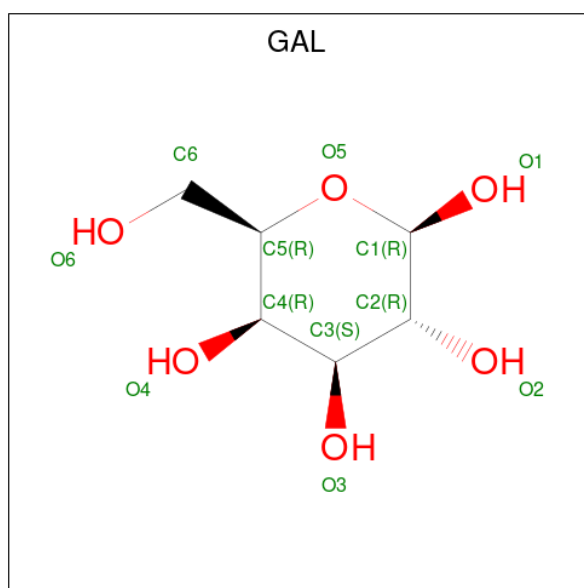
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP P51570
A	-5	ALA	-	expression tag	UNP P51570
A	-4	HIS	-	expression tag	UNP P51570
A	-3	HIS	-	expression tag	UNP P51570
A	-2	HIS	-	expression tag	UNP P51570
A	-1	HIS	-	expression tag	UNP P51570
A	0	HIS	-	expression tag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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
E	-6	MET	-	initiating methionine	UNP P51570
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

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



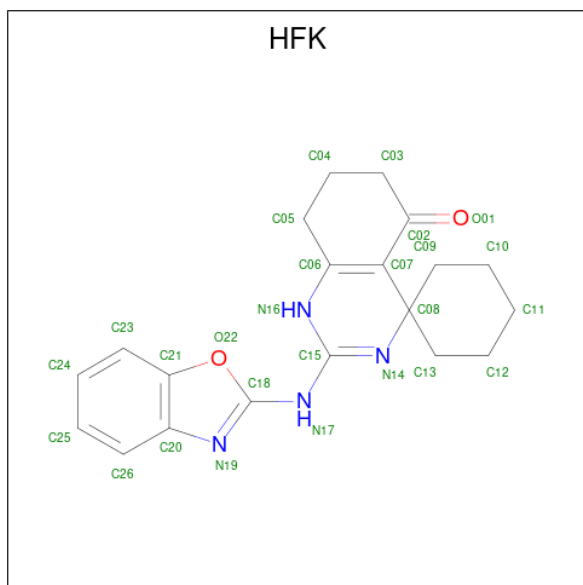
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

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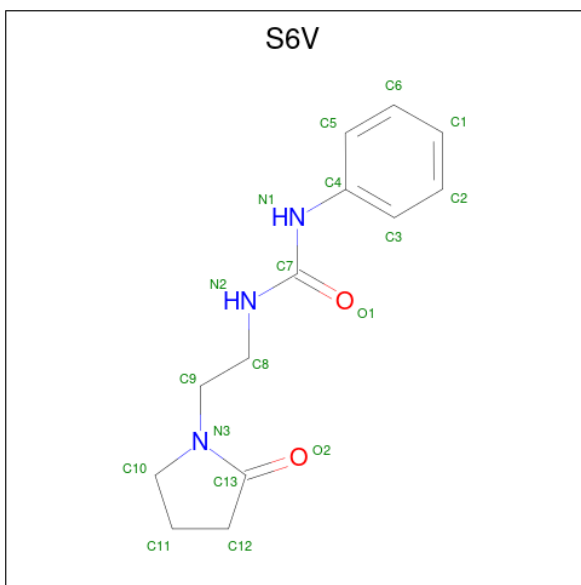
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			12	6	6		

- 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		

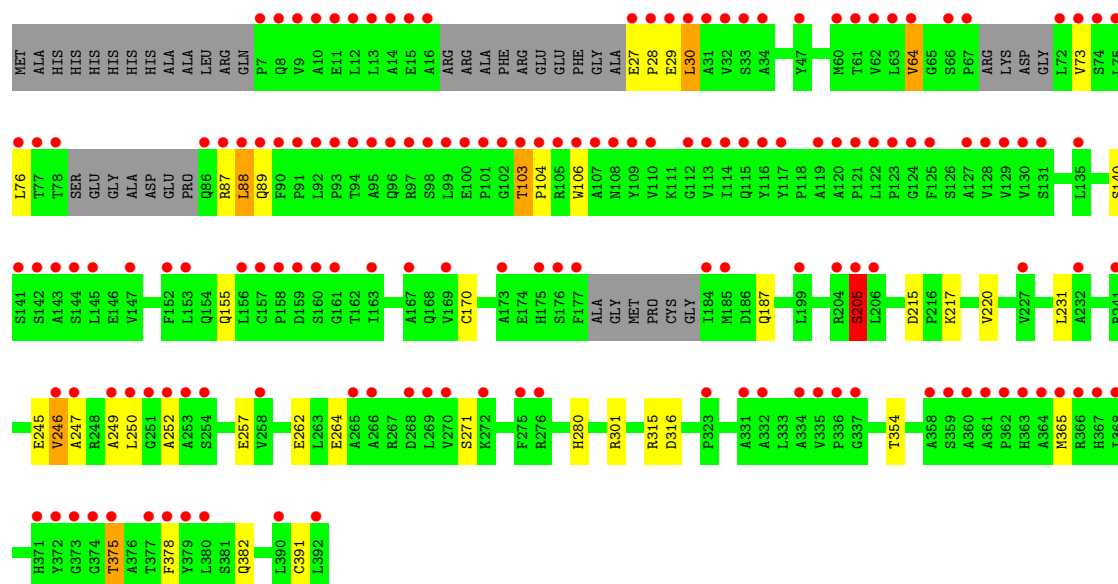
- Molecule 4 is 1-[2-(2-oxidanilidenpyrrolidin-1-yl)ethyl]-3-phenyl-urea (CCD ID: S6V) (formula: $C_{13}H_{17}N_3O_2$) (labeled as "Ligand of Interest" by depositor).



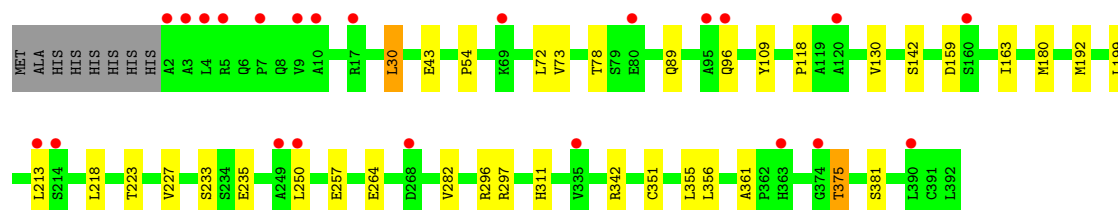
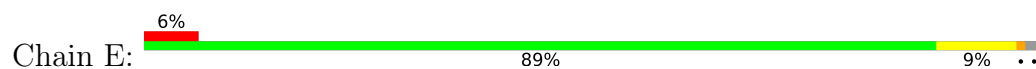
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			18	13	3	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	107	Total	O	0	0
			107	107		
5	B	102	Total	O	0	0
			102	102		
5	D	87	Total	O	0	0
			87	87		
5	E	160	Total	O	0	0
			160	160		



• 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	73.77Å 114.45Å 120.92Å 90.00° 100.55° 90.00°	Depositor
Resolution (Å)	82.59 – 1.86 82.59 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.4 (82.59-1.86) 99.5 (82.59-1.86)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.249 , 0.274 0.249 , 0.274	Depositor DCC
R_{free} test set	8248 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.0	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	11542	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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, S6V, GAL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.58	0/2839	1.06	3/3875 (0.1%)
1	B	0.57	0/2847	1.00	5/3884 (0.1%)
1	D	0.65	0/2556	1.08	7/3486 (0.2%)
1	E	0.59	0/2913	1.00	6/3965 (0.2%)
All	All	0.60	0/11155	1.03	21/15210 (0.1%)

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

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	205	SER	CA-C-O	-7.89	111.92	120.36
1	D	246	VAL	CB-CA-C	6.32	121.66	111.29
1	A	159	ASP	CA-C-N	-6.08	112.98	123.25
1	A	159	ASP	C-N-CA	-6.08	112.98	123.25
1	B	45	THR	OG1-CB-CG2	5.98	121.26	109.30
1	D	375	THR	CB-CA-C	5.97	119.98	110.19
1	B	45	THR	CB-CA-C	5.76	118.36	109.03
1	D	280	HIS	CA-CB-CG	-5.69	108.11	113.80
1	E	235	GLU	CB-CG-CD	5.61	122.14	112.60
1	D	246	VAL	CA-C-N	5.61	131.04	122.29
1	D	246	VAL	C-N-CA	5.61	131.04	122.29
1	D	205	SER	N-CA-C	-5.60	99.60	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	THR	N-CA-CB	-5.56	103.19	110.59
1	E	375	THR	CB-CA-C	5.36	119.06	110.16
1	B	82	ALA	CA-C-N	5.22	128.63	120.75
1	B	82	ALA	C-N-CA	5.22	128.63	120.75
1	E	72	LEU	N-CA-CB	-5.19	102.20	111.08
1	A	287	ARG	CG-CD-NE	-5.12	100.74	112.00
1	E	311	HIS	CA-CB-CG	-5.07	108.73	113.80
1	E	159	ASP	CA-C-N	-5.05	114.71	123.25
1	E	159	ASP	C-N-CA	-5.05	114.71	123.25

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	205	SER	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	2785	0	2662	42	0
1	B	2793	0	2671	25	0
1	D	2517	0	2389	30	0
1	E	2859	0	2801	19	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
2	E	12	0	12	0	0
3	A	26	0	0	0	0
3	B	26	0	0	0	0
3	E	26	0	0	0	0
4	D	18	0	0	1	0
5	A	107	0	0	2	0
5	B	102	0	0	1	0
5	D	87	0	0	3	0
5	E	160	0	0	4	0
All	All	11542	0	10559	112	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (112) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:ARG:HD2	1:D:316:ASP:OD1	1.67	0.95
1:B:45:THR:HG21	1:B:51:LEU:O	1.67	0.94
1:D:87:ARG:O	1:D:88:LEU:HD13	1.69	0.93
1:A:4:LEU:HB2	1:A:365:MET:HE1	1.61	0.82
1:E:163:ILE:HG21	1:E:192:MET:SD	2.20	0.81
1:D:301:ARG:CB	5:D:576:HOH:O	2.28	0.81
1:D:365:MET:HE2	1:D:378:PHE:HB3	1.64	0.78
1:B:12:LEU:HD22	1:B:130:VAL:HG23	1.66	0.78
1:B:45:THR:CG2	1:B:51:LEU:O	2.34	0.76
1:D:103:THR:CB	1:D:104:PRO:CD	2.64	0.76
1:E:257:GLU:HG3	5:E:561:HOH:O	1.84	0.76
1:A:163:ILE:HD11	1:B:194:GLN:CD	2.12	0.75
1:A:356:LEU:O	1:A:356:LEU:HD13	1.87	0.75
1:A:311:HIS:HD2	1:A:343:MET:H	1.33	0.74
1:A:287:ARG:NH2	1:A:310:SER:HA	2.04	0.72
1:B:12:LEU:HD22	1:B:130:VAL:CG2	2.19	0.72
1:A:263:LEU:CB	5:A:596:HOH:O	2.36	0.72
1:D:27:GLU:N	1:D:28:PRO:HD2	2.06	0.70
1:D:103:THR:CB	1:D:104:PRO:HD3	2.21	0.70
1:A:4:LEU:HB2	1:A:365:MET:CE	2.21	0.70
1:A:284:GLU:HA	1:A:287:ARG:HD3	1.78	0.66
1:A:327:GLN:NE2	1:A:373:GLY:H	1.95	0.64
1:A:184:ILE:HD12	1:A:184:ILE:C	2.24	0.63
1:A:163:ILE:HG21	1:A:192:MET:SD	2.40	0.62
1:A:290:GLN:NE2	5:A:501:HOH:O	2.35	0.60
1:D:205:SER:O	1:D:205:SER:OG	2.05	0.60
1:D:30:LEU:HD21	1:D:155:GLN:HG3	1.85	0.59
1:A:72:LEU:C	1:A:72:LEU:HD12	2.27	0.58
1:B:43:GLU:HB2	1:B:342:ARG:NH2	2.19	0.58
1:B:30:LEU:HD21	1:B:155:GLN:HB3	1.86	0.57
1:D:27:GLU:N	1:D:28:PRO:CD	2.67	0.57
1:A:43:GLU:HB2	1:A:342:ARG:NH2	2.18	0.57
1:E:96:GLN:N	1:E:96:GLN:OE1	2.36	0.57
1:A:356:LEU:HD13	1:A:356:LEU:C	2.29	0.57
1:D:262:GLU:OE1	5:D:502:HOH:O	2.18	0.55
1:D:315:ARG:CD	1:D:316:ASP:OD1	2.49	0.55
1:B:218:LEU:HD11	1:B:355:LEU:HG	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:LEU:HD21	1:D:155:GLN:CB	2.37	0.55
1:D:382:GLN:OE1	5:D:501:HOH:O	2.17	0.54
1:A:174:GLU:HG2	1:A:182:CYS:SG	2.48	0.54
1:A:305:ARG:O	1:A:309:GLU:HB2	2.06	0.53
1:A:49:GLN:O	1:A:256:ARG:HG3	2.09	0.53
1:D:245:GLU:C	1:D:247:ALA:H	2.17	0.53
1:A:163:ILE:HD11	1:B:194:GLN:OE1	2.08	0.53
1:D:365:MET:HE2	1:D:378:PHE:CB	2.37	0.53
1:B:45:THR:HG22	1:B:52:VAL:HG12	1.90	0.52
1:A:308:VAL:HG21	1:A:333:LEU:HD21	1.91	0.52
1:E:43:GLU:HB2	1:E:342:ARG:NH2	2.24	0.52
1:B:6:GLN:N	1:B:7:PRO:HD3	2.24	0.52
1:B:83:ASP:HB3	1:B:104:PRO:HB2	1.92	0.52
1:A:78:THR:OG1	1:A:130:VAL:HG12	2.10	0.52
1:A:287:ARG:HH21	1:A:309:GLU:C	2.17	0.51
1:A:28:PRO:CB	1:A:64:VAL:HG13	2.40	0.51
1:D:391:CYS:HB2	1:E:30:LEU:CD2	2.41	0.51
1:A:43:GLU:HB2	1:A:342:ARG:HH22	1.77	0.49
1:D:28:PRO:CB	1:D:64:VAL:HG13	2.41	0.49
1:E:296:ARG:NH1	5:E:504:HOH:O	2.44	0.49
1:A:311:HIS:CD2	1:A:343:MET:H	2.21	0.49
1:A:283:GLY:O	1:A:287:ARG:CD	2.60	0.49
1:A:68:ARG:CZ	1:A:72:LEU:HD11	2.42	0.48
1:A:287:ARG:NH2	1:A:309:GLU:O	2.47	0.48
1:A:303:PHE:CD1	1:A:355:LEU:HD22	2.48	0.48
1:E:218:LEU:HD11	1:E:355:LEU:HG	1.94	0.48
1:B:78:THR:OG1	1:B:130:VAL:HG12	2.14	0.48
1:B:43:GLU:HB2	1:B:342:ARG:HH22	1.79	0.48
1:A:283:GLY:O	1:A:287:ARG:HD3	2.14	0.47
1:D:87:ARG:C	1:D:88:LEU:HD22	2.39	0.47
1:E:78:THR:OG1	1:E:130:VAL:HG12	2.14	0.47
1:D:30:LEU:HD21	1:D:155:GLN:CG	2.45	0.47
1:E:180:MET:HE1	1:E:233:SER:HA	1.97	0.47
1:A:327:GLN:HE22	1:A:373:GLY:H	1.63	0.46
1:B:111:LYS:HE2	5:B:534:HOH:O	2.13	0.46
1:B:272:LYS:NZ	1:E:257:GLU:O	2.47	0.46
1:B:259:GLN:OE1	1:B:261:GLU:HB2	2.16	0.46
1:E:297:ARG:HD3	5:E:569:HOH:O	2.16	0.46
1:A:163:ILE:HG21	1:A:192:MET:CG	2.47	0.45
1:B:6:GLN:NE2	1:B:6:GLN:H	2.15	0.45
1:D:76:LEU:HD23	1:D:76:LEU:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:ARG:C	1:D:88:LEU:HD13	2.38	0.45
1:D:249:ALA:O	1:D:250:LEU:CB	2.64	0.45
1:A:311:HIS:CD2	1:A:329:VAL:HG21	2.52	0.45
1:A:356:LEU:O	1:A:356:LEU:CD1	2.62	0.45
1:A:356:LEU:C	1:A:356:LEU:CD1	2.90	0.45
1:E:356:LEU:HD11	1:E:361:ALA:HA	1.99	0.44
1:B:5:ARG:C	1:B:7:PRO:HD3	2.42	0.44
1:D:170:CYS:HB2	1:D:187:GLN:HG2	1.98	0.44
1:A:195:LYS:HE3	1:B:160:SER:O	2.18	0.43
1:A:73:VAL:O	1:A:89:GLN:HA	2.19	0.43
1:E:54:PRO:HD2	1:E:199:LEU:O	2.18	0.43
1:A:28:PRO:HG3	1:A:64:VAL:HG13	2.01	0.43
1:D:215:ASP:OD1	1:D:217:LYS:HG2	2.18	0.43
1:B:242:GLN:NE2	1:B:273:GLU:OE1	2.52	0.43
1:D:88:LEU:HD22	1:D:88:LEU:N	2.34	0.43
1:A:54:PRO:HD2	1:A:199:LEU:O	2.19	0.43
1:A:367:HIS:O	1:A:371:HIS:HD2	2.01	0.43
1:E:109:TYR:CE1	1:E:142:SER:HB2	2.53	0.42
1:E:73:VAL:O	1:E:89:GLN:HA	2.19	0.42
1:B:218:LEU:HD11	1:B:355:LEU:CG	2.49	0.42
1:E:43:GLU:HB2	1:E:342:ARG:HH22	1.84	0.42
4:D:401:S6V:O1	4:D:401:S6V:C5	2.67	0.42
1:B:109:TYR:CE1	1:B:142:SER:HB2	2.55	0.42
1:D:104:PRO:O	1:D:106:TRP:N	2.49	0.42
1:D:73:VAL:O	1:D:89:GLN:HA	2.20	0.41
1:B:252:ALA:HB1	1:B:257:GLU:HB2	2.01	0.41
1:B:54:PRO:HD2	1:B:199:LEU:O	2.21	0.41
1:A:308:VAL:HG23	1:A:340:GLY:HA2	2.03	0.41
1:E:118:PRO:HG3	5:E:576:HOH:O	2.20	0.41
1:D:220:VAL:HA	1:D:354:THR:O	2.20	0.41
1:E:223:THR:O	1:E:351:CYS:HA	2.21	0.40
1:D:252:ALA:HB1	1:D:257:GLU:HB2	2.03	0.40
1:A:171:GLN:NE2	1:A:184:ILE:HG22	2.37	0.40
1:E:218:LEU:HD11	1:E:355:LEU:CG	2.52	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	389/399 (98%)	384 (99%)	5 (1%)	0	100	100
1	B	389/399 (98%)	382 (98%)	7 (2%)	0	100	100
1	D	349/399 (88%)	337 (97%)	10 (3%)	2 (1%)	21	10
1	E	389/399 (98%)	384 (99%)	5 (1%)	0	100	100
All	All	1516/1596 (95%)	1487 (98%)	27 (2%)	2 (0%)	48	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	103	THR
1	D	246	VAL

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	270/315 (86%)	258 (96%)	12 (4%)	25	10
1	B	270/315 (86%)	265 (98%)	5 (2%)	50	38
1	D	240/315 (76%)	231 (96%)	9 (4%)	29	14
1	E	288/315 (91%)	280 (97%)	8 (3%)	38	23
All	All	1068/1260 (85%)	1034 (97%)	34 (3%)	34	19

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	41	ILE
1	A	64	VAL
1	A	72	LEU
1	A	168	GLN
1	A	188	PHE
1	A	230	SER
1	A	256	ARG
1	A	267	ARG
1	A	271	SER
1	A	333	LEU
1	A	356	LEU
1	B	5	ARG
1	B	45	THR
1	B	213	LEU
1	B	227	VAL
1	B	259	GLN
1	D	29	GLU
1	D	30	LEU
1	D	64	VAL
1	D	88	LEU
1	D	140	SER
1	D	231	LEU
1	D	264	GLU
1	D	271	SER
1	D	375	THR
1	E	30	LEU
1	E	213	LEU
1	E	227	VAL
1	E	250	LEU
1	E	264	GLU
1	E	282	VAL
1	E	375	THR
1	E	381	SER

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	6	GLN
1	A	171	GLN
1	A	290	GLN
1	A	311	HIS
1	A	327	GLN

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Mol	Chain	Res	Type
1	A	371	HIS
1	B	6	GLN
1	E	226	ASN

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 ⓘ

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	A	401	-	12,12,12	0.69	0	17,17,17	2.59	4 (23%)
2	GAL	E	401	-	12,12,12	0.91	0	17,17,17	3.10	5 (29%)
3	HFK	A	402	-	29,30,30	2.73	9 (31%)	32,44,44	1.78	11 (34%)
3	HFK	B	402	-	29,30,30	2.44	7 (24%)	32,44,44	2.21	12 (37%)
3	HFK	E	402	-	29,30,30	2.37	7 (24%)	32,44,44	2.22	13 (40%)
2	GAL	B	401	-	12,12,12	0.65	0	17,17,17	1.33	2 (11%)
4	S6V	D	401	-	19,19,19	1.76	4 (21%)	24,24,24	1.20	3 (12%)

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	A	401	-	-	2/2/22/22	0/1/1/1
2	GAL	E	401	-	-	1/2/22/22	0/1/1/1
3	HFK	A	402	-	-	2/4/43/43	0/5/5/5
3	HFK	B	402	-	-	2/4/43/43	0/5/5/5
3	HFK	E	402	-	-	2/4/43/43	0/5/5/5
2	GAL	B	401	-	-	1/2/22/22	0/1/1/1
4	S6V	D	401	-	-	1/10/20/20	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	HFK	C06-C07	10.73	1.50	1.37
3	B	402	HFK	C06-C07	9.61	1.49	1.37
3	E	402	HFK	C06-C07	8.96	1.48	1.37
3	A	402	HFK	C15-N14	6.08	1.46	1.30
3	B	402	HFK	C15-N14	5.73	1.45	1.30
3	E	402	HFK	C15-N14	5.59	1.44	1.30
4	D	401	S6V	C13-N3	3.78	1.43	1.34
4	D	401	S6V	C5-C4	3.39	1.45	1.39
3	A	402	HFK	C05-C06	3.03	1.54	1.49
3	A	402	HFK	C18-N19	3.03	1.35	1.30
4	D	401	S6V	C8-N2	3.03	1.53	1.46
3	B	402	HFK	C05-C06	2.94	1.54	1.49
3	E	402	HFK	C05-C06	2.89	1.54	1.49
3	A	402	HFK	C08-N14	2.77	1.49	1.46
3	E	402	HFK	C20-N19	-2.64	1.34	1.39
3	B	402	HFK	C03-C02	2.53	1.54	1.50
4	D	401	S6V	C6-C5	2.49	1.43	1.38
3	A	402	HFK	C15-N17	2.36	1.42	1.37
3	A	402	HFK	C26-C20	2.31	1.43	1.40
3	E	402	HFK	C13-C08	2.18	1.57	1.54
3	E	402	HFK	C15-N16	2.16	1.40	1.36
3	E	402	HFK	C15-N17	2.14	1.42	1.37
3	B	402	HFK	C15-N16	2.13	1.40	1.36
3	A	402	HFK	C18-N17	2.12	1.40	1.36
3	A	402	HFK	C15-N16	2.11	1.40	1.36
3	B	402	HFK	C15-N17	2.04	1.42	1.37
3	B	402	HFK	C18-N17	2.02	1.40	1.36

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	GAL	C1-O5-C5	-9.11	96.03	113.65
2	A	401	GAL	C1-O5-C5	-6.78	100.53	113.65
3	B	402	HFK	C07-C06-N16	-6.39	116.95	122.11
2	E	401	GAL	C1-C2-C3	-6.22	97.68	110.36
3	E	402	HFK	C07-C06-N16	-6.18	117.13	122.11
2	A	401	GAL	C1-C2-C3	-5.73	98.68	110.36
2	E	401	GAL	O1-C1-C2	4.85	123.06	108.98
2	A	401	GAL	O1-C1-C2	4.15	121.03	108.98
3	B	402	HFK	C23-C21-C20	-3.80	119.01	123.62
3	B	402	HFK	O22-C21-C23	3.72	134.31	126.49
3	E	402	HFK	C23-C21-C20	-3.69	119.14	123.62
3	A	402	HFK	C07-C06-N16	-3.63	119.18	122.11
3	E	402	HFK	N17-C15-N14	3.59	124.67	117.96
3	B	402	HFK	C02-C07-C06	-3.57	116.01	119.18
3	E	402	HFK	N17-C15-N16	-3.49	112.09	117.96
3	B	402	HFK	C09-C10-C11	3.09	116.17	111.35
3	E	402	HFK	C02-C07-C06	-3.07	116.45	119.18
3	E	402	HFK	O22-C18-N19	-3.05	110.09	115.57
3	A	402	HFK	N17-C15-N16	-2.99	112.93	117.96
3	E	402	HFK	O22-C21-C23	2.98	132.75	126.49
3	B	402	HFK	N17-C15-N16	-2.94	113.02	117.96
3	A	402	HFK	C13-C12-C11	2.94	115.93	111.35
3	A	402	HFK	N17-C15-N14	2.91	123.39	117.96
2	A	401	GAL	C3-C4-C5	2.89	115.47	110.23
3	B	402	HFK	N17-C15-N14	2.87	123.32	117.96
3	B	402	HFK	N17-C18-N19	-2.82	120.57	128.58
2	B	401	GAL	C1-C2-C3	-2.80	104.64	110.36
3	A	402	HFK	O22-C21-C20	-2.79	105.90	107.80
3	A	402	HFK	O22-C18-N19	-2.78	110.57	115.57
4	D	401	S6V	C8-N2-C7	-2.69	116.42	121.71
3	E	402	HFK	N17-C18-N19	-2.64	121.08	128.58
3	B	402	HFK	O01-C02-C07	-2.63	118.00	121.53
3	B	402	HFK	O22-C18-N19	-2.59	110.91	115.57
2	E	401	GAL	C6-C5-C4	2.56	119.31	113.02
3	E	402	HFK	C20-N19-C18	2.50	109.08	104.13
4	D	401	S6V	C4-N1-C7	-2.41	121.70	126.61
3	A	402	HFK	C02-C07-C06	-2.40	117.05	119.18
2	B	401	GAL	O5-C1-C2	-2.39	106.09	110.30
3	E	402	HFK	C04-C03-C02	2.31	118.02	113.57
3	E	402	HFK	O01-C02-C07	-2.29	118.45	121.53
3	A	402	HFK	C18-N17-C15	-2.28	119.70	125.27
3	B	402	HFK	C08-C07-C06	-2.27	119.19	121.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	HFK	C24-C25-C26	2.26	123.03	120.24
3	B	402	HFK	C05-C06-N16	2.23	118.63	115.46
3	A	402	HFK	C26-C20-C21	-2.12	117.61	120.31
4	D	401	S6V	C3-C4-C5	2.09	121.82	119.04
2	E	401	GAL	C3-C4-C5	2.07	113.99	110.23
3	A	402	HFK	O01-C02-C07	-2.05	118.78	121.53
3	E	402	HFK	C03-C02-C07	2.01	121.26	117.35
3	E	402	HFK	C05-C06-N16	2.01	118.32	115.46

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	O5-C5-C6-O6
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	B	402	HFK	N16-C15-N17-C18
3	E	402	HFK	N16-C15-N17-C18
4	D	401	S6V	C8-C9-N3-C10
3	E	402	HFK	N14-C15-N17-C18

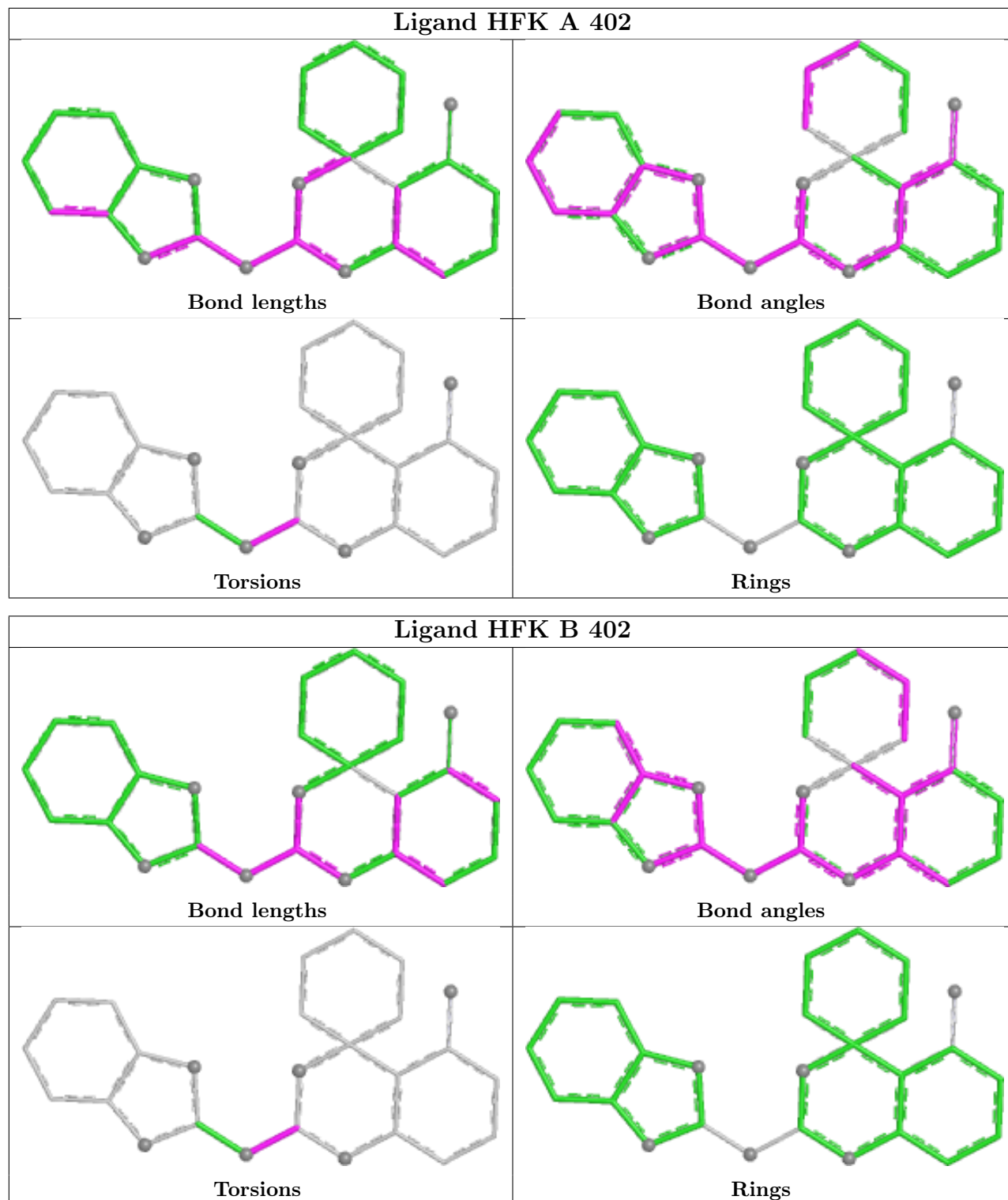
There are no ring outliers.

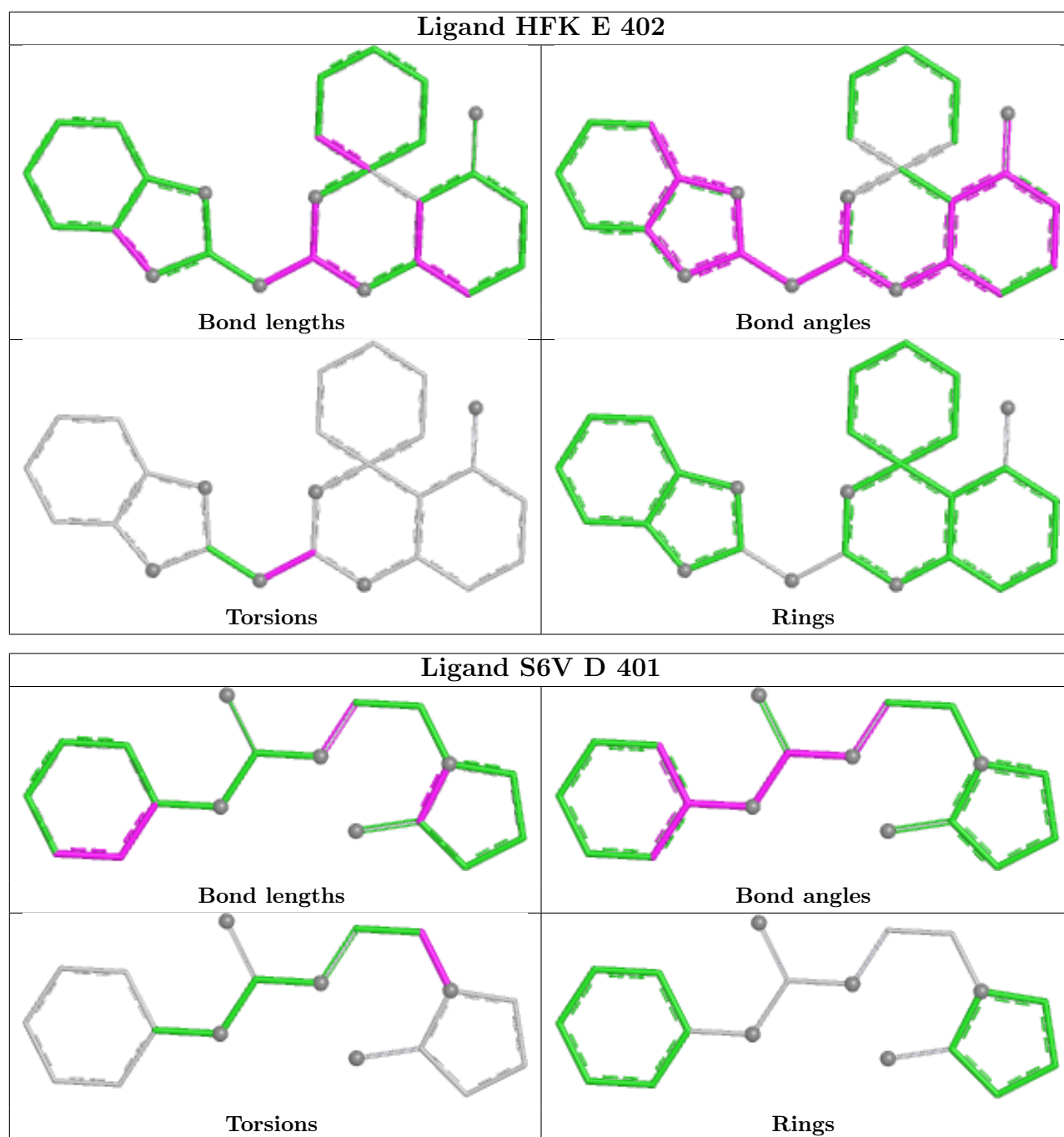
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	401	S6V	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	391/399 (97%)	2.04	161 (41%) 0 0	21, 41, 78, 101	0
1	B	391/399 (97%)	1.29	109 (27%) 1 1	21, 39, 70, 100	0
1	D	359/399 (89%)	1.88	153 (42%) 0 0	19, 42, 77, 113	0
1	E	391/399 (97%)	0.48	23 (5%) 28 31	17, 31, 52, 69	0
All	All	1532/1596 (95%)	1.41	446 (29%) 1 1	17, 38, 73, 113	0

All (446) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	250	LEU	8.3
1	A	269	LEU	7.8
1	A	263	LEU	7.6
1	D	249	ALA	7.4
1	A	265	ALA	7.2
1	D	106	TRP	7.0
1	A	268	ASP	6.9
1	A	337	GLY	6.8
1	A	360	ALA	6.7
1	A	275	PHE	6.7
1	A	332	ALA	6.6
1	A	255	LEU	6.4
1	D	99	LEU	6.4
1	A	361	ALA	6.4
1	A	340	GLY	6.4
1	A	266	ALA	6.3
1	A	261	GLU	6.3
1	A	249	ALA	6.2
1	A	274	GLY	6.1
1	D	95	ALA	6.1
1	B	92	LEU	6.1

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Mol	Chain	Res	Type	RSRZ
1	D	76	LEU	6.1
1	B	69	LYS	6.0
1	A	260	LEU	5.9
1	A	303	PHE	5.9
1	D	247	ALA	5.9
1	A	339	TYR	5.9
1	A	2	ALA	5.9
1	D	72	LEU	5.8
1	A	219	ALA	5.7
1	A	258	VAL	5.7
1	A	270	VAL	5.7
1	A	362	PRO	5.7
1	A	246	VAL	5.6
1	B	26	ALA	5.6
1	A	306	LEU	5.5
1	A	363	HIS	5.5
1	A	300	TYR	5.5
1	A	308	VAL	5.5
1	D	246	VAL	5.5
1	D	184	ILE	5.4
1	D	128	VAL	5.3
1	A	278	ALA	5.3
1	A	3	ALA	5.3
1	D	127	ALA	5.3
1	A	252	ALA	5.2
1	D	130	VAL	5.2
1	A	364	ALA	5.2
1	A	218	LEU	5.1
1	A	329	VAL	5.1
1	A	356	LEU	5.1
1	A	355	LEU	5.0
1	A	336	PRO	5.0
1	D	93	PRO	5.0
1	D	88	LEU	4.9
1	A	304	GLY	4.9
1	A	251	GLY	4.9
1	A	281	VAL	4.9
1	A	335	VAL	4.9
1	A	338	VAL	4.9
1	A	250	LEU	4.8
1	B	233	SER	4.8
1	A	358	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	62	VAL	4.8
1	B	2	ALA	4.8
1	D	92	LEU	4.8
1	A	354	THR	4.8
1	A	330	GLU	4.7
1	B	232	ALA	4.7
1	B	99	LEU	4.7
1	A	328	LEU	4.7
1	B	231	LEU	4.7
1	A	214	SER	4.7
1	A	310	SER	4.7
1	A	264	GLU	4.6
1	A	277	ARG	4.6
1	A	314	LEU	4.6
1	A	245	GLU	4.6
1	B	106	TRP	4.6
1	D	7	PRO	4.6
1	D	362	PRO	4.6
1	D	94	THR	4.6
1	D	64	VAL	4.6
1	B	70	ASP	4.6
1	B	25	GLY	4.6
1	A	331	ALA	4.5
1	A	334	ALA	4.5
1	A	231	LEU	4.5
1	A	368	ILE	4.5
1	A	247	ALA	4.5
1	D	129	VAL	4.4
1	A	295	LEU	4.4
1	D	63	LEU	4.4
1	A	311	HIS	4.4
1	D	275	PHE	4.4
1	D	27	GLU	4.4
1	D	98	SER	4.4
1	A	288	THR	4.4
1	A	357	GLU	4.4
1	D	373	GLY	4.4
1	D	12	LEU	4.4
1	D	30	LEU	4.4
1	D	251	GLY	4.3
1	D	96	GLN	4.3
1	B	90	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	13	LEU	4.3
1	D	175	HIS	4.3
1	A	271	SER	4.3
1	A	294	ALA	4.3
1	A	302	ALA	4.3
1	D	90	PHE	4.3
1	A	267	ARG	4.3
1	D	78	THR	4.2
1	A	373	GLY	4.2
1	B	91	PRO	4.2
1	D	77	THR	4.2
1	B	392	LEU	4.1
1	B	128	VAL	4.1
1	A	291	ALA	4.1
1	D	67	PRO	4.1
1	A	298	GLY	4.1
1	A	316	ASP	4.1
1	A	301	ARG	4.0
1	A	341	SER	4.0
1	A	221	LEU	4.0
1	A	220	VAL	4.0
1	A	282	VAL	4.0
1	A	262	GLU	4.0
1	D	152	PHE	4.0
1	D	377	THR	4.0
1	D	108	ASN	4.0
1	B	24	PHE	4.0
1	B	87	ARG	3.9
1	A	279	ARG	3.9
1	D	10	ALA	3.9
1	A	259	GLN	3.9
1	D	206	LEU	3.9
1	D	97	ARG	3.8
1	D	86	GLN	3.8
1	A	359	SER	3.8
1	A	333	LEU	3.8
1	D	269	LEU	3.8
1	A	323	PRO	3.8
1	A	280	HIS	3.8
1	D	253	ALA	3.8
1	A	243	CYS	3.8
1	A	285	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	335	VAL	3.8
1	B	249	ALA	3.7
1	E	95	ALA	3.7
1	B	98	SER	3.7
1	A	287	ARG	3.7
1	D	15	GLU	3.7
1	B	89	GLN	3.7
1	B	96	GLN	3.7
1	B	95	ALA	3.7
1	B	83	ASP	3.7
1	B	122	LEU	3.6
1	A	305	ARG	3.6
1	B	97	ARG	3.6
1	D	374	GLY	3.6
1	A	223	THR	3.6
1	A	370	GLU	3.6
1	B	88	LEU	3.6
1	A	217	LYS	3.6
1	A	273	GLU	3.6
1	D	91	PRO	3.6
1	A	4	LEU	3.6
1	A	289	ALA	3.5
1	A	325	LEU	3.6
1	A	372	TYR	3.5
1	D	177	PHE	3.5
1	A	232	ALA	3.5
1	D	145	LEU	3.5
1	D	205	SER	3.5
1	D	28	PRO	3.5
1	A	293	ALA	3.5
1	D	153	LEU	3.5
1	D	104	PRO	3.5
1	A	253	ALA	3.5
1	A	292	ALA	3.5
1	B	30	LEU	3.5
1	D	87	ARG	3.5
1	E	4	LEU	3.5
1	D	31	ALA	3.4
1	D	135	LEU	3.4
1	A	318	TYR	3.4
1	D	110	VAL	3.4
1	A	283	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	107	ALA	3.4
1	B	72	LEU	3.4
1	A	276	ARG	3.4
1	A	371	HIS	3.4
1	D	9	VAL	3.4
1	E	2	ALA	3.4
1	D	101	PRO	3.4
1	D	119	ALA	3.3
1	A	365	MET	3.3
1	D	185	MET	3.3
1	B	123	PRO	3.3
1	A	327	GLN	3.3
1	B	300	TYR	3.3
1	A	222	ILE	3.3
1	D	120	ALA	3.3
1	D	100	GLU	3.3
1	A	272	LYS	3.3
1	B	248	ARG	3.3
1	B	74	SER	3.3
1	A	257	GLU	3.2
1	D	29	GLU	3.2
1	D	109	TYR	3.2
1	E	213	LEU	3.2
1	D	8	GLN	3.2
1	A	312	ARG	3.2
1	B	114	ILE	3.2
1	D	379	TYR	3.2
1	B	120	ALA	3.2
1	B	246	VAL	3.2
1	D	73	VAL	3.2
1	D	336	PRO	3.2
1	D	337	GLY	3.2
1	D	47	TYR	3.2
1	B	156	LEU	3.2
1	D	176	SER	3.2
1	B	21	ARG	3.2
1	D	368	ILE	3.1
1	B	7	PRO	3.1
1	A	367	HIS	3.1
1	B	247	ALA	3.1
1	D	252	ALA	3.1
1	B	71	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	380	LEU	3.1
1	D	157	CYS	3.1
1	A	216	PRO	3.1
1	D	334	ALA	3.1
1	D	102	GLY	3.1
1	A	307	MET	3.1
1	A	315	ARG	3.1
1	A	313	SER	3.1
1	D	375	THR	3.1
1	D	123	PRO	3.1
1	B	126	SER	3.0
1	D	75	LEU	3.0
1	A	48	ASN	3.0
1	E	80	GLU	3.0
1	B	118	PRO	3.0
1	E	268	ASP	3.0
1	A	376	ALA	3.0
1	D	16	ALA	3.0
1	A	41	ILE	3.0
1	A	353	VAL	3.0
1	D	117	TYR	3.0
1	B	79	SER	3.0
1	D	158	PRO	3.0
1	B	127	ALA	3.0
1	A	254	SER	2.9
1	B	73	VAL	2.9
1	A	375	THR	2.9
1	B	3	ALA	2.9
1	D	131	SER	2.9
1	A	299	ASP	2.9
1	B	116	TYR	2.9
1	B	100	GLU	2.9
1	E	10	ALA	2.9
1	D	105	ARG	2.9
1	D	163	ILE	2.9
1	B	93	PRO	2.9
1	A	242	GLN	2.9
1	B	253	ALA	2.9
1	D	14	ALA	2.9
1	D	89	GLN	2.9
1	E	249	ALA	2.9
1	D	142	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	40	LEU	2.9
1	B	295	LEU	2.9
1	B	104	PRO	2.8
1	B	20	PHE	2.8
1	B	252	ALA	2.8
1	D	125	PHE	2.8
1	D	66	SER	2.8
1	D	122	LEU	2.8
1	B	102	GLY	2.8
1	D	103	THR	2.8
1	B	68	ARG	2.8
1	D	323	PRO	2.8
1	D	34	ALA	2.8
1	A	286	ARG	2.8
1	A	215	ASP	2.8
1	D	371	HIS	2.8
1	A	80	GLU	2.8
1	B	119	ALA	2.7
1	A	378	PHE	2.7
1	B	22	GLU	2.7
1	A	317	ASP	2.7
1	D	121	PRO	2.7
1	B	8	GLN	2.7
1	D	143	ALA	2.7
1	D	361	ALA	2.7
1	B	103	THR	2.7
1	B	250	LEU	2.7
1	A	163	ILE	2.7
1	B	9	VAL	2.7
1	B	64	VAL	2.7
1	B	238	VAL	2.7
1	D	360	ALA	2.7
1	B	125	PHE	2.7
1	D	365	MET	2.7
1	A	256	ARG	2.7
1	D	204	ARG	2.7
1	B	76	LEU	2.7
1	D	114	ILE	2.7
1	A	320	VAL	2.7
1	B	14	ALA	2.6
1	D	358	ALA	2.6
1	D	156	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	258	VAL	2.6
1	A	95	ALA	2.6
1	B	173	ALA	2.6
1	D	167	ALA	2.6
1	A	326	ASP	2.6
1	D	159	ASP	2.6
1	D	363	HIS	2.6
1	E	363	HIS	2.6
1	D	60	MET	2.6
1	E	374	GLY	2.6
1	B	19	ALA	2.6
1	D	147	VAL	2.6
1	E	9	VAL	2.6
1	B	77	THR	2.6
1	D	372	TYR	2.5
1	A	168	GLN	2.5
1	A	290	GLN	2.5
1	B	177	PHE	2.5
1	A	309	GLU	2.5
1	A	72	LEU	2.5
1	D	268	ASP	2.5
1	D	380	LEU	2.5
1	D	392	LEU	2.5
1	B	163	ILE	2.5
1	D	144	SER	2.5
1	D	160	SER	2.5
1	B	110	VAL	2.5
1	D	270	VAL	2.5
1	A	96	GLN	2.5
1	A	79	SER	2.5
1	A	248	ARG	2.5
1	D	367	HIS	2.5
1	D	266	ALA	2.5
1	D	169	VAL	2.5
1	B	214	SER	2.5
1	B	245	GLU	2.5
1	B	107	ALA	2.5
1	D	112	GLY	2.4
1	A	379	TYR	2.4
1	D	276	ARG	2.4
1	B	218	LEU	2.4
1	D	378	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	390	LEU	2.4
1	B	85	PRO	2.4
1	A	347	GLY	2.4
1	A	319	GLU	2.4
1	B	80	GLU	2.4
1	B	367	HIS	2.4
1	A	348	PHE	2.4
1	A	103	THR	2.4
1	E	3	ALA	2.4
1	A	241	ARG	2.4
1	A	5	ARG	2.4
1	B	228	ARG	2.4
1	B	82	ALA	2.4
1	D	173	ALA	2.4
1	A	382	GLN	2.4
1	D	161	GLY	2.4
1	D	116	TYR	2.3
1	B	78	THR	2.3
1	B	10	ALA	2.3
1	B	265	ALA	2.3
1	B	298	GLY	2.3
1	D	124	GLY	2.3
1	D	33	SER	2.3
1	E	160	SER	2.3
1	A	51	LEU	2.3
1	B	236	TYR	2.3
1	B	67	PRO	2.3
1	D	366	ARG	2.3
1	B	243	CYS	2.3
1	D	390	LEU	2.3
1	B	108	ASN	2.3
1	B	363	HIS	2.3
1	E	69	LYS	2.3
1	D	331	ALA	2.3
1	A	374	GLY	2.3
1	D	32	VAL	2.3
1	B	75	LEU	2.3
1	B	94	THR	2.3
1	D	241	ARG	2.2
1	B	27	GLU	2.2
1	B	81	GLY	2.2
1	B	160	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	230	SER	2.2
1	D	254	SER	2.2
1	A	369	GLN	2.2
1	B	86	GLN	2.2
1	D	113	VAL	2.2
1	E	250	LEU	2.2
1	E	214	SER	2.2
1	A	227	VAL	2.2
1	A	238	VAL	2.2
1	D	61	THR	2.2
1	D	115	GLN	2.2
1	D	141	SER	2.2
1	A	366	ARG	2.2
1	E	17	ARG	2.2
1	A	377	THR	2.2
1	D	199	LEU	2.2
1	B	266	ALA	2.2
1	D	265	ALA	2.2
1	B	244	GLU	2.1
1	B	184	ILE	2.1
1	B	113	VAL	2.1
1	A	392	LEU	2.1
1	B	63	LEU	2.1
1	B	121	PRO	2.1
1	D	272	LYS	2.1
1	A	15	GLU	2.1
1	D	364	ALA	2.1
1	A	45	THR	2.1
1	D	74	SER	2.1
1	B	62	VAL	2.1
1	E	5	ARG	2.1
1	A	322	CYS	2.1
1	B	180	MET	2.1
1	B	12	LEU	2.1
1	B	369	GLN	2.1
1	A	184	ILE	2.1
1	A	344	THR	2.1
1	E	335	VAL	2.1
1	D	332	ALA	2.1
1	E	120	ALA	2.1
1	D	11	GLU	2.0
1	D	359	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	96	GLN	2.0
1	D	227	VAL	2.0
1	E	7	PRO	2.0
1	D	232	ALA	2.0
1	B	129	VAL	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](#)

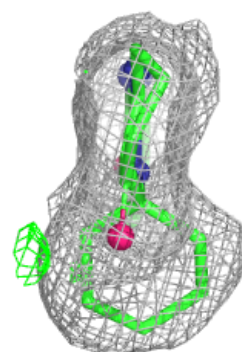
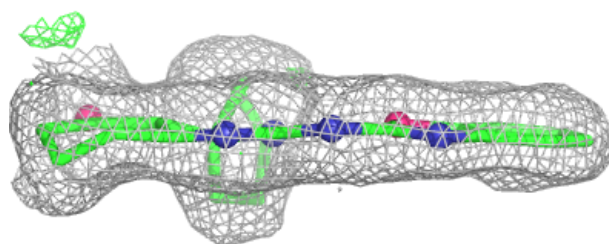
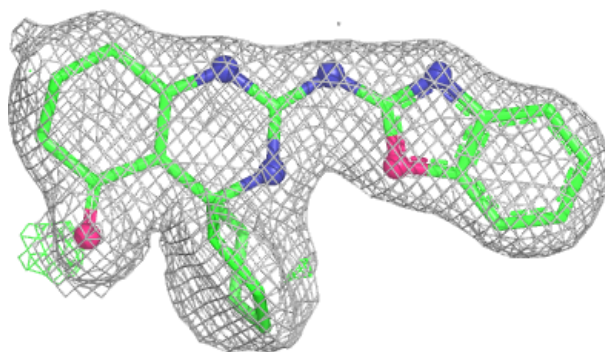
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	HFK	B	402	26/26	0.85	0.14	40,48,52,56	0
3	HFK	A	402	26/26	0.91	0.11	25,39,46,52	0
2	GAL	A	401	12/12	0.92	0.09	25,30,35,40	0
2	GAL	B	401	12/12	0.92	0.09	27,34,37,53	0
4	S6V	D	401	18/18	0.92	0.10	20,27,43,46	0
3	HFK	E	402	26/26	0.93	0.09	22,31,36,36	0
2	GAL	E	401	12/12	0.95	0.06	18,21,23,35	0

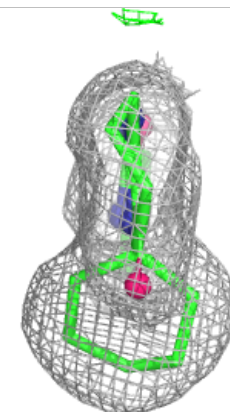
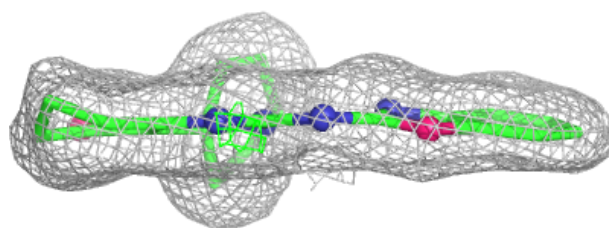
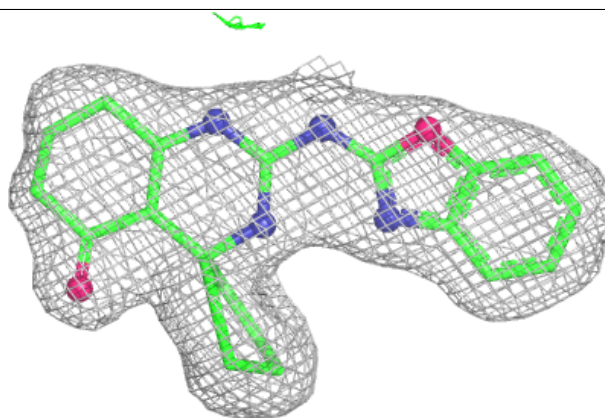
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

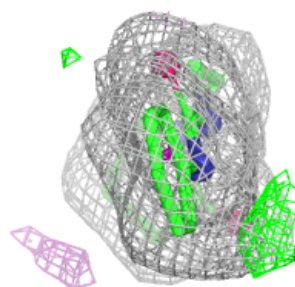
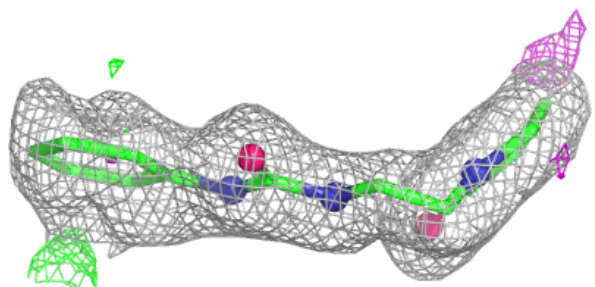
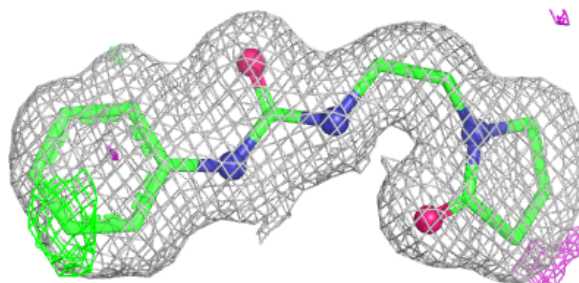
**Electron density around HFK A 402:**

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

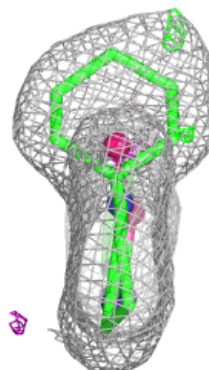
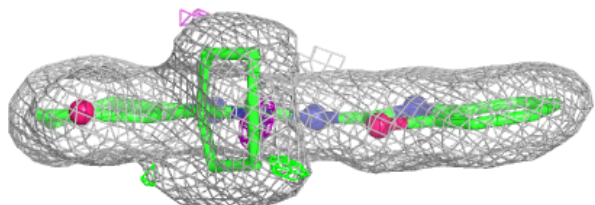
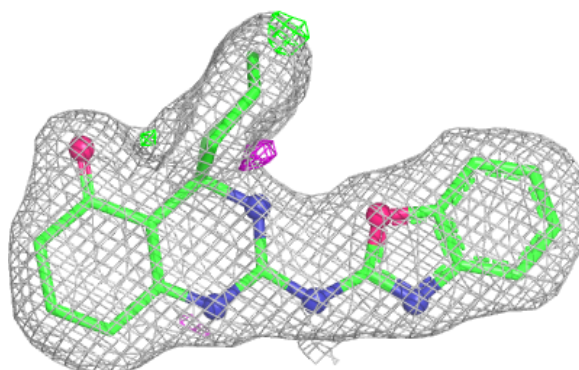


Electron density around S6V D 401:

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

**Electron density around HFK 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.