



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:15 AM UTC

PDB ID : 6ZGZ / pdb_00006zgz
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 : 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

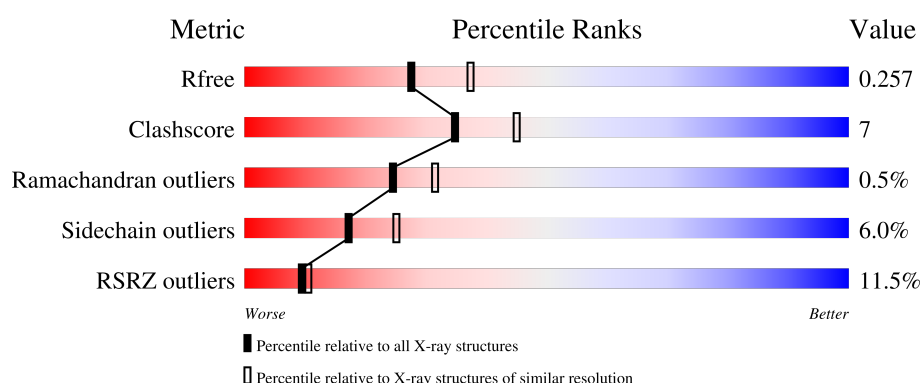
1 Overall quality at a glance

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	17% 66% 23% 7% • •
1	B	399	6% 80% 16% • •
1	D	399	20% 70% 18% 5% • 8%
1	E	399	2% 82% 16% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11599 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	388	Total	C	N	O	S	0	0	0
			2700	1692	476	516	16			
1	B	388	Total	C	N	O	S	0	1	0
			2765	1738	486	525	16			
1	E	390	Total	C	N	O	S	0	1	0
			2834	1780	497	541	16			
1	D	368	Total	C	N	O	S	0	2	0
			2594	1628	452	501	13			

There are 40 discrepancies between the modelled and reference sequences:

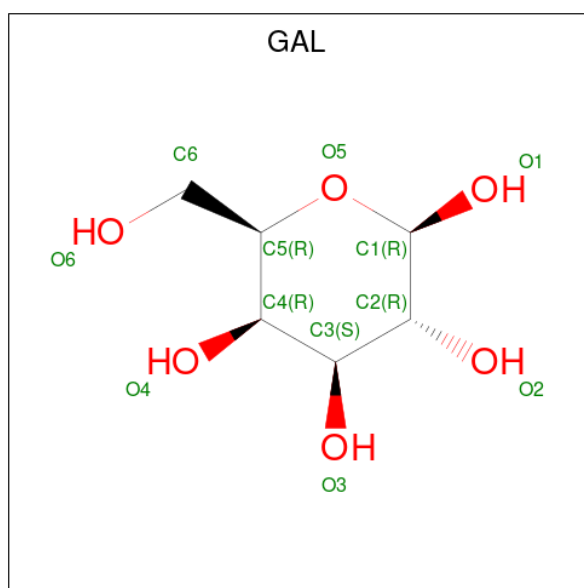
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP P51570
A	-5	ALA	-	expression tag	UNP P51570
A	-4	HIS	-	expression tag	UNP P51570
A	-3	HIS	-	expression tag	UNP P51570
A	-2	HIS	-	expression tag	UNP P51570
A	-1	HIS	-	expression tag	UNP P51570
A	0	HIS	-	expression tag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



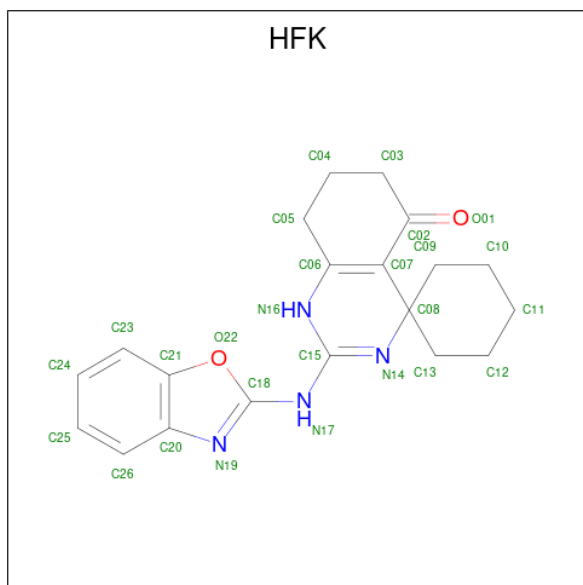
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

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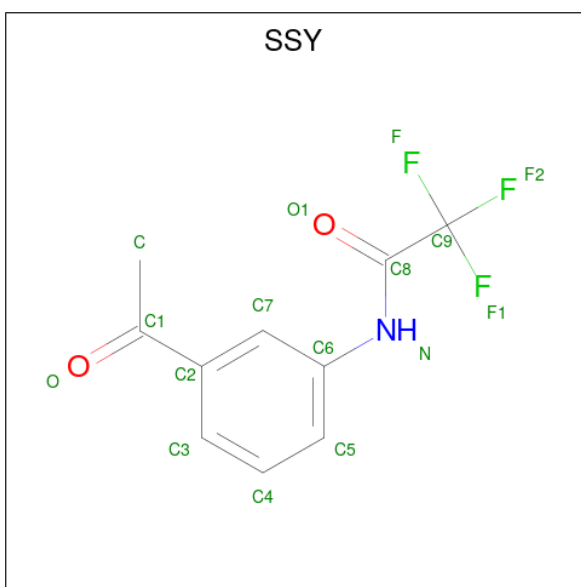
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			12	6	6		

- 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 {N}-(3-ethanoylphenyl)-2,2,2-tris(fluoranyl)ethanamide (CCD ID: SSY) (formula: $C_{10}H_8F_3NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	F	N	O	0	0
			16	10	3	1	2		

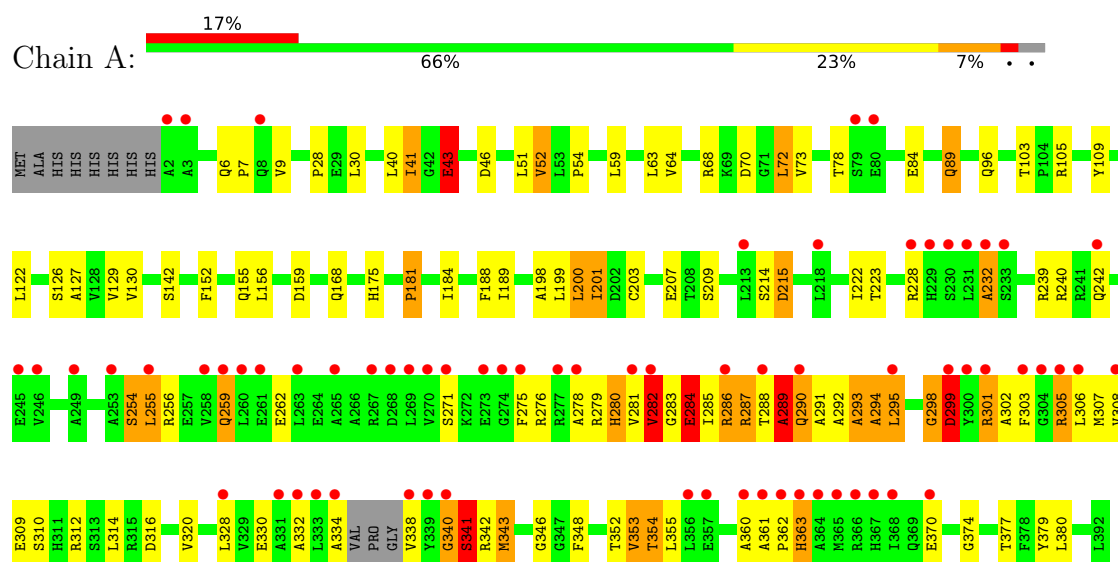
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	130	Total	O	0	0
			130	130		
5	B	131	Total	O	0	0
			131	131		
5	E	207	Total	O	0	0
			207	207		
5	D	108	Total	O	0	0
			108	108		

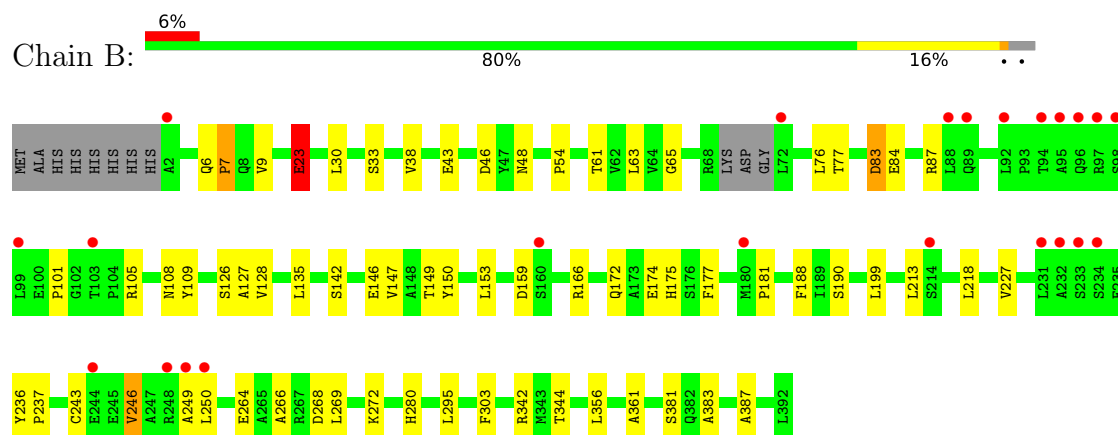
3 Residue-property plots [i](#)

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.

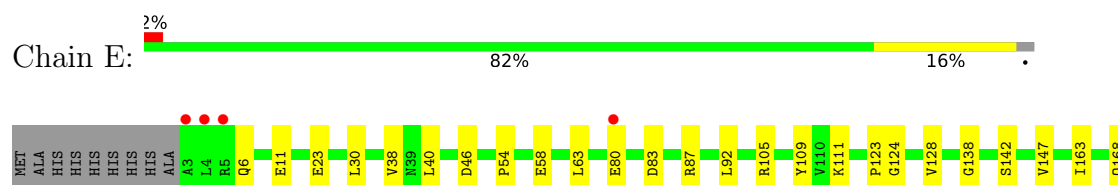
• Molecule 1: Galactokinase

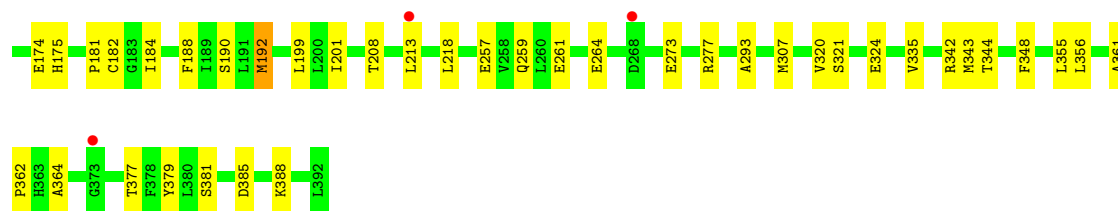


• Molecule 1: Galactokinase

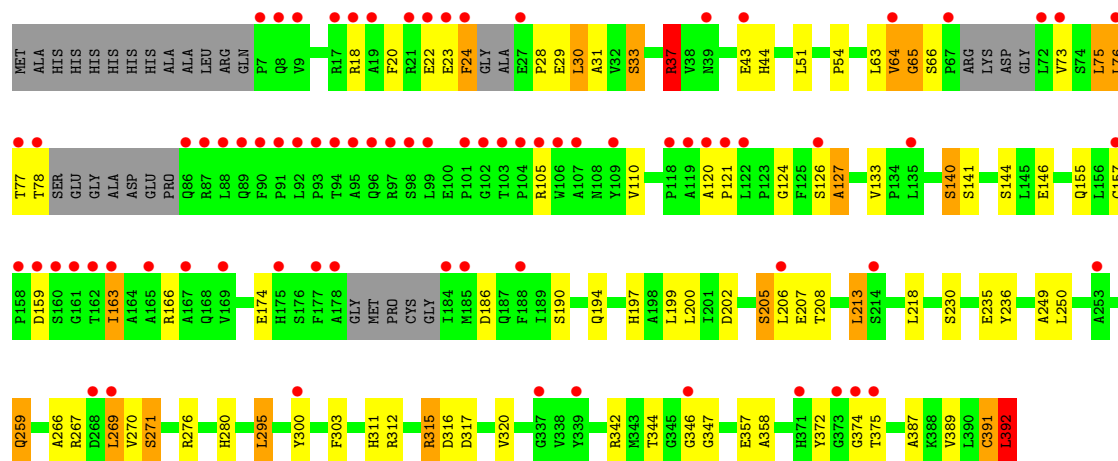


• Molecule 1: Galactokinase





● 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	73.21Å 114.30Å 120.81Å 90.00° 100.54° 90.00°	Depositor
Resolution (Å)	82.49 – 2.30 82.49 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (82.49-2.30) 99.8 (82.49-2.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.214 , 0.256 0.217 , 0.257	Depositor DCC
R_{free} test set	5872 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.673	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.5	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	11599	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, HFK, SSY

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	1.99	66/2749 (2.4%)	1.70	34/3756 (0.9%)
1	B	1.21	3/2819 (0.1%)	1.55	6/3846 (0.2%)
1	D	1.38	19/2641 (0.7%)	1.58	15/3602 (0.4%)
1	E	1.21	3/2891 (0.1%)	1.49	7/3939 (0.2%)
All	All	1.48	91/11100 (0.8%)	1.58	62/15143 (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	A	0	10
1	B	0	1
All	All	0	11

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	295	LEU	C-O	22.32	1.50	1.24
1	A	301	ARG	C-O	20.09	1.47	1.24
1	D	24	PHE	C-O	19.82	1.63	1.23
1	A	316	ASP	CG-OD1	18.98	1.61	1.25
1	A	299	ASP	CG-OD2	17.92	1.59	1.25
1	A	328	LEU	C-O	16.11	1.43	1.24
1	A	299	ASP	CG-OD1	14.96	1.53	1.25
1	A	41	ILE	C-O	14.67	1.41	1.24
1	A	370	GLU	C-O	13.66	1.42	1.24
1	A	308	VAL	C-O	13.43	1.39	1.24
1	A	295	LEU	CA-C	12.61	1.69	1.52
1	A	294	ALA	C-O	11.78	1.38	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	290	GLN	C-O	11.69	1.37	1.24
1	A	353	VAL	C-O	11.61	1.36	1.24
1	D	391	CYS	C-O	11.45	1.37	1.23
1	A	289	ALA	C-O	11.37	1.37	1.24
1	A	282	VAL	C-O	10.81	1.36	1.24
1	A	40	LEU	C-O	10.33	1.37	1.24
1	A	291	ALA	C-N	9.90	1.45	1.33
1	A	301	ARG	C-N	9.58	1.45	1.33
1	A	51	LEU	C-O	9.43	1.36	1.24
1	A	198	ALA	C-O	9.31	1.35	1.23
1	A	334	ALA	C-O	9.05	1.41	1.23
1	A	293	ALA	C-N	8.57	1.46	1.33
1	A	286	ARG	CA-C	8.53	1.63	1.52
1	D	127	ALA	C-O	8.44	1.34	1.23
1	A	298	GLY	C-O	8.38	1.35	1.23
1	D	389	VAL	C-O	8.36	1.32	1.24
1	D	28	PRO	CA-C	8.31	1.61	1.53
1	A	282	VAL	C-N	8.30	1.45	1.33
1	A	89	GLN	C-O	7.87	1.33	1.23
1	A	279	ARG	C-O	7.82	1.34	1.24
1	A	275	PHE	C-O	7.75	1.33	1.24
1	A	207	GLU	CD-OE2	7.72	1.40	1.25
1	A	299	ASP	CA-C	7.12	1.62	1.52
1	D	124	GLY	C-O	7.10	1.33	1.23
1	A	284	GLU	CA-C	7.09	1.62	1.52
1	A	288	THR	C-O	6.98	1.32	1.24
1	A	299	ASP	C-O	6.96	1.32	1.24
1	A	316	ASP	CG-OD2	6.95	1.38	1.25
1	E	343	MET	C-O	6.83	1.32	1.23
1	A	301	ARG	CA-C	6.74	1.61	1.52
1	D	266	ALA	C-O	6.70	1.33	1.23
1	A	286	ARG	C-O	6.65	1.31	1.24
1	A	43	GLU	CD-OE2	6.57	1.37	1.25
1	A	316	ASP	C-N	6.55	1.42	1.33
1	A	288	THR	C-N	6.50	1.42	1.33
1	A	291	ALA	C-O	6.41	1.31	1.24
1	A	201	ILE	C-O	6.32	1.31	1.24
1	A	280	HIS	C-N	6.29	1.41	1.33
1	D	250	LEU	C-O	6.29	1.32	1.24
1	D	29	GLU	CD-OE2	6.24	1.37	1.25
1	A	341	SER	C-O	6.24	1.31	1.23
1	D	65	GLY	C-N	6.19	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	GLY	C-N	6.18	1.41	1.33
1	A	310	SER	C-N	6.16	1.41	1.33
1	D	73	VAL	C-O	6.10	1.30	1.24
1	A	259	GLN	CA-C	6.06	1.59	1.52
1	A	285	ILE	N-CA	6.02	1.53	1.46
1	B	268	ASP	CB-CG	6.01	1.67	1.52
1	D	33	SER	CB-OG	5.98	1.54	1.42
1	D	110	VAL	C-O	5.94	1.30	1.24
1	A	52	VAL	C-O	5.94	1.29	1.24
1	A	346	GLY	C-O	-5.87	1.17	1.24
1	A	332	ALA	C-O	5.86	1.31	1.24
1	E	138	GLY	C-O	5.81	1.32	1.24
1	A	43	GLU	CD-OE1	5.78	1.36	1.25
1	D	392	LEU	C-O	5.69	1.34	1.23
1	A	330	GLU	C-O	5.65	1.30	1.24
1	A	288	THR	CA-C	5.64	1.60	1.52
1	A	293	ALA	C-O	5.62	1.31	1.24
1	A	289	ALA	C-N	5.52	1.41	1.33
1	B	266	ALA	C-O	-5.52	1.15	1.23
1	A	207	GLU	CG-CD	5.52	1.65	1.52
1	D	28	PRO	C-N	5.50	1.41	1.33
1	A	284	GLU	CD-OE1	5.50	1.35	1.25
1	A	374	GLY	C-O	5.49	1.29	1.23
1	A	276	ARG	C-O	5.48	1.30	1.24
1	A	200	LEU	C-O	5.46	1.30	1.24
1	A	299	ASP	C-N	5.44	1.41	1.33
1	D	124	GLY	C-N	5.43	1.40	1.33
1	A	377	THR	C-O	5.38	1.30	1.24
1	D	270	VAL	C-O	5.34	1.30	1.23
1	B	127	ALA	C-O	5.29	1.30	1.23
1	D	65	GLY	CA-C	5.26	1.59	1.51
1	D	271	SER	C-O	5.24	1.31	1.23
1	A	295	LEU	N-CA	5.17	1.52	1.46
1	A	41	ILE	C-N	5.14	1.41	1.33
1	E	80	GLU	C-O	5.06	1.30	1.23
1	A	222	ILE	C-O	5.06	1.30	1.24
1	A	307	MET	SD-CE	5.01	1.92	1.79

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	LEU	O-C-N	11.96	134.87	122.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	LEU	CA-C-O	-10.41	109.62	121.07
1	A	299	ASP	CA-C-O	9.89	130.83	120.54
1	A	282	VAL	CA-C-O	-9.49	111.40	121.27
1	D	346	GLY	N-CA-C	-8.51	101.16	112.14
1	A	295	LEU	N-CA-C	-8.00	101.25	111.02
1	A	299	ASP	CB-CG-OD2	-8.00	100.01	118.40
1	B	280	HIS	CA-CB-CG	-6.99	106.81	113.80
1	A	310	SER	CA-C-O	6.97	128.31	121.00
1	A	289	ALA	CA-C-O	-6.68	113.47	120.55
1	B	46	ASP	CA-CB-CG	6.62	119.22	112.60
1	A	286	ARG	N-CA-C	-6.57	104.04	111.07
1	D	346	GLY	CA-C-O	-6.46	114.92	121.90
1	A	295	LEU	CB-CA-C	6.27	120.90	110.92
1	A	305	ARG	O-C-N	6.24	128.58	122.09
1	A	281	VAL	CA-C-N	6.08	128.44	120.60
1	A	281	VAL	C-N-CA	6.08	128.44	120.60
1	A	46	ASP	CA-CB-CG	5.97	118.57	112.60
1	A	284	GLU	CB-CA-C	-5.97	99.59	110.63
1	A	289	ALA	O-C-N	5.95	128.43	122.12
1	A	308	VAL	O-C-N	5.66	127.36	121.87
1	D	259	GLN	CB-CA-C	5.65	118.85	109.53
1	E	46	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	305	ARG	CA-C-O	-5.63	114.87	120.90
1	D	280	HIS	CA-CB-CG	-5.51	108.29	113.80
1	A	298	GLY	O-C-N	-5.44	115.71	122.34
1	A	282	VAL	O-C-N	5.38	127.32	121.94
1	D	37	ARG	CG-CD-NE	-5.34	100.26	112.00
1	D	163	ILE	CA-C-N	5.32	127.36	120.44
1	D	163	ILE	C-N-CA	5.32	127.36	120.44
1	E	293	ALA	N-CA-C	-5.32	105.56	111.36
1	B	159	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	7	PRO	N-CA-C	-5.31	102.85	111.14
1	D	344	THR	CA-CB-OG1	-5.31	101.64	109.60
1	D	315	ARG	CG-CD-NE	5.29	123.64	112.00
1	D	358	ALA	CA-C-N	5.26	127.34	120.28
1	D	358	ALA	C-N-CA	5.26	127.34	120.28
1	A	70	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	240	ARG	CB-CA-C	5.21	119.07	110.88
1	A	288	THR	CB-CA-C	5.21	119.70	110.85
1	B	7	PRO	N-CA-CB	-5.20	97.79	103.25
1	A	159	ASP	CB-CA-C	5.19	118.92	109.83
1	E	324	GLU	CA-C-O	-5.18	115.56	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	205	SER	CA-C-O	-5.17	114.75	120.60
1	A	360	ALA	CA-C-N	5.17	128.51	120.60
1	A	360	ALA	C-N-CA	5.17	128.51	120.60
1	A	181	PRO	CA-C-N	5.13	128.50	120.75
1	A	181	PRO	C-N-CA	5.13	128.50	120.75
1	B	246	VAL	N-CA-CB	5.13	116.44	110.65
1	A	280	HIS	CA-CB-CG	-5.13	108.67	113.80
1	E	111	LYS	CA-C-N	5.11	125.61	119.94
1	E	111	LYS	C-N-CA	5.11	125.61	119.94
1	A	328	LEU	O-C-N	5.11	127.53	122.12
1	D	374	GLY	CA-C-O	-5.10	116.96	122.47
1	A	298	GLY	CA-C-O	5.08	126.19	119.58
1	E	168	GLN	CB-CG-CD	5.08	121.24	112.60
1	D	372	TYR	CA-C-N	5.07	125.58	120.00
1	D	372	TYR	C-N-CA	5.07	125.58	120.00
1	A	286	ARG	O-C-N	5.07	127.29	122.07
1	A	159	ASP	O-C-N	-5.05	117.28	122.94
1	E	307	MET	O-C-N	5.02	127.44	122.12
1	B	77	THR	CA-CB-OG1	-5.01	102.08	109.60

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	282	VAL	Mainchain
1	A	284	GLU	Mainchain
1	A	289	ALA	Mainchain
1	A	293	ALA	Mainchain
1	A	295	LEU	Mainchain
1	A	298	GLY	Mainchain
1	A	299	ASP	Sidechain
1	A	301	ARG	Mainchain
1	A	303	PHE	Peptide
1	A	312	ARG	Mainchain
1	B	23	GLU	Sidechain

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	2700	0	2527	57	0
1	B	2765	0	2632	27	0
1	D	2594	0	2411	46	0
1	E	2834	0	2754	32	0
2	A	12	0	12	0	0
2	B	12	0	12	0	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	0	0
4	D	16	0	0	3	0
5	A	130	0	0	4	1
5	B	131	0	0	0	0
5	D	108	0	0	1	0
5	E	207	0	0	1	1
All	All	11599	0	10359	160	1

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:LEU:HB3	1:A:343:MET:HE3	1.18	1.13
1:D:37:ARG:NH1	1:D:186:ASP:OD1	1.80	1.12
1:A:320:VAL:HG23	1:A:343:MET:HE1	1.41	1.00
1:A:314:LEU:CB	1:A:343:MET:HE3	2.03	0.89
1:A:223:THR:HG22	5:A:569:HOH:O	1.73	0.87
1:A:299:ASP:OD2	1:A:302:ALA:HB2	1.75	0.85
1:A:314:LEU:HB3	1:A:343:MET:CE	2.08	0.79
1:D:159:ASP:O	1:D:159:ASP:OD1	2.05	0.74
1:A:72:LEU:C	1:A:72:LEU:HD12	2.14	0.73
1:A:63:LEU:HD11	1:A:129:VAL:HG22	1.73	0.70
1:B:23:GLU:HG3	1:B:76:LEU:HD22	1.73	0.69
1:D:315:ARG:NH1	1:D:316:ASP:OD1	2.26	0.68
1:B:83[A]:ASP:OD1	1:B:84:GLU:N	2.27	0.68
1:B:236:TYR:HB3	1:B:237:PRO:HD3	1.77	0.67
1:A:280:HIS:O	1:A:284:GLU:N	2.27	0.65
1:B:147:VAL:HG21	1:B:190:SER:HB3	1.79	0.65
1:D:249:ALA:HB1	1:D:269:LEU:HD22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:SER:OG	1:D:235:GLU:OE1	2.15	0.63
1:A:354:THR:HG23	5:A:569:HOH:O	1.98	0.62
1:A:239:ARG:HD3	1:A:242:GLN:HE21	1.66	0.61
1:E:361:ALA:HB3	1:E:362:PRO:HD3	1.82	0.60
1:E:30:LEU:CD2	1:D:391:CYS:HB2	2.33	0.59
1:D:121:PRO:HD2	1:D:157:CYS:SG	2.43	0.59
1:D:312:ARG:HD3	5:D:514:HOH:O	2.03	0.59
1:D:295:LEU:HD13	1:D:303:PHE:CD2	2.38	0.58
1:A:105:ARG:NH1	3:A:402:HFK:O01	2.37	0.58
1:D:159:ASP:OD1	1:D:159:ASP:C	2.47	0.58
1:A:59:LEU:HD11	1:A:379:TYR:CD2	2.40	0.56
1:D:31:ALA:HB2	1:D:392:LEU:HD21	1.87	0.56
1:D:18:ARG:O	1:D:22:GLU:HG3	2.06	0.55
1:B:213:LEU:HD12	1:B:383:ALA:HB2	1.89	0.55
1:E:38:VAL:HG23	1:E:344:THR:HG21	1.89	0.55
1:A:63:LEU:CD1	1:A:129:VAL:HG22	2.36	0.54
1:E:192:MET:CE	1:E:208:THR:HG21	2.37	0.54
1:A:259:GLN:O	1:A:262:GLU:N	2.40	0.54
1:B:150:TYR:CZ	1:B:166:ARG:HG2	2.42	0.54
1:D:20:PHE:CE2	1:D:65:GLY:HA2	2.42	0.54
1:D:120:ALA:HB3	1:D:121:PRO:HD3	1.90	0.54
1:A:214:SER:O	1:A:215:ASP:C	2.51	0.54
1:E:192:MET:HE1	1:E:208:THR:CB	2.38	0.53
1:A:54:PRO:HD2	1:A:199:LEU:O	2.08	0.53
1:A:168:GLN:NE2	5:A:506:HOH:O	2.36	0.53
1:B:101:PRO:HG3	1:B:177:PHE:HA	1.91	0.53
1:E:192:MET:HE1	1:E:208:THR:OG1	2.09	0.53
1:B:54:PRO:HD2	1:B:199:LEU:O	2.09	0.52
1:A:30:LEU:HD21	1:A:155:GLN:HB3	1.92	0.52
1:A:109:TYR:CE1	1:A:142:SER:HB2	2.45	0.52
1:D:44:HIS:CD2	1:D:236:TYR:CE1	2.97	0.52
1:A:43:GLU:HB3	1:A:314:LEU:HD21	1.92	0.51
1:D:205:SER:O	1:D:205:SER:OG	2.23	0.51
1:A:68:ARG:CZ	1:A:72:LEU:HD11	2.40	0.51
1:A:299:ASP:CG	1:A:302:ALA:HB2	2.36	0.51
1:A:223:THR:CG2	1:A:352:THR:OG1	2.59	0.51
1:D:44:HIS:CD2	1:D:236:TYR:HE1	2.29	0.50
1:D:24:PHE:CE1	1:D:126:SER:HB3	2.47	0.50
1:A:28:PRO:HG3	1:A:64:VAL:CG1	2.41	0.50
1:E:6:GLN:NE2	1:E:379:TYR:HB3	2.27	0.50
1:D:194[B]:GLN:HG3	1:D:197:HIS:ND1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:GLU:CB	1:D:44:HIS:ND1	2.75	0.49
1:D:276:ARG:NH1	1:D:317:ASP:OD1	2.46	0.49
1:E:109:TYR:CE1	1:E:142:SER:HB2	2.47	0.49
1:A:306:LEU:N	1:A:306:LEU:HD12	2.27	0.49
1:B:105:ARG:HA	1:B:108:ASN:ND2	2.28	0.49
1:A:289:ALA:O	1:A:292:ALA:HB3	2.14	0.48
1:E:213:LEU:O	1:E:213:LEU:HG	2.11	0.48
1:D:54:PRO:HD2	1:D:199:LEU:O	2.14	0.48
1:E:92:LEU:HD11	1:E:123:PRO:C	2.39	0.48
1:D:205:SER:C	1:D:207:GLU:H	2.21	0.48
1:D:300:TYR:CD1	4:D:401:SSY:C	2.97	0.48
1:D:30:LEU:HD21	1:D:155:GLN:HG3	1.96	0.48
1:E:199:LEU:HD23	1:E:201:ILE:HD11	1.95	0.48
1:E:273:GLU:O	1:E:277:ARG:HG2	2.13	0.48
1:A:72:LEU:HD12	1:A:72:LEU:O	2.12	0.48
1:E:259:GLN:CB	5:E:642:HOH:O	2.62	0.48
1:D:30:LEU:O	1:D:64:VAL:HA	2.14	0.48
1:A:43:GLU:HB2	1:A:342:ARG:NH2	2.29	0.48
1:E:40:LEU:O	1:E:342:ARG:HD3	2.13	0.47
1:A:232:ALA:HA	1:A:348:PHE:CD2	2.50	0.47
1:B:272:LYS:NZ	1:E:257:GLU:O	2.47	0.47
1:A:184:ILE:HD12	1:A:184:ILE:C	2.40	0.47
1:E:320:VAL:HA	1:E:348:PHE:CZ	2.50	0.47
1:D:30:LEU:HD21	1:D:155:GLN:CB	2.45	0.47
1:A:354:THR:CG2	5:A:569:HOH:O	2.59	0.47
1:E:192:MET:HE2	1:E:208:THR:HG21	1.97	0.47
1:A:72:LEU:C	1:A:72:LEU:CD1	2.84	0.46
1:A:341:SER:HA	1:A:353:VAL:O	2.15	0.46
1:A:184:ILE:HD11	1:A:203:CYS:SG	2.55	0.46
1:B:23:GLU:OE1	1:B:87:ARG:NE	2.42	0.46
1:E:385:ASP:OD2	1:E:388:LYS:HE3	2.15	0.46
1:A:30:LEU:HD21	1:A:155:GLN:CB	2.45	0.46
1:A:52:VAL:O	1:A:200:LEU:HD12	2.16	0.46
1:A:290:GLN:O	1:A:294:ALA:N	2.48	0.46
1:E:335:VAL:HG11	1:E:364:ALA:HA	1.97	0.46
1:D:23:GLU:HB3	1:D:24:PHE:CE2	2.51	0.46
1:E:218:LEU:HD11	1:E:355:LEU:CD1	2.45	0.45
1:D:194[B]:GLN:CG	1:D:197:HIS:ND1	2.79	0.45
1:A:152:PHE:HE1	1:A:156:LEU:HD11	1.82	0.45
1:E:174:GLU:HG2	1:E:182:CYS:SG	2.55	0.45
1:A:73:VAL:O	1:A:89:GLN:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:GLY:C	1:A:287:ARG:HE	2.24	0.45
1:E:23:GLU:CD	1:E:87:ARG:HE	2.25	0.45
1:A:78:THR:OG1	1:A:130:VAL:HG12	2.17	0.45
1:B:43:GLU:HB2	1:B:342:ARG:NH2	2.32	0.45
1:D:200:LEU:O	1:D:208:THR:HA	2.17	0.45
1:D:300:TYR:CE1	4:D:401:SSY:C	3.00	0.44
1:A:361:ALA:HA	1:A:363:HIS:H	1.82	0.44
1:D:75:LEU:HA	1:D:127:ALA:O	2.17	0.44
1:D:320:VAL:O	1:D:347:GLY:HA3	2.18	0.44
1:B:356:LEU:HD11	1:B:361:ALA:HA	1.99	0.44
1:D:51:LEU:HD23	1:D:202:ASP:HA	1.99	0.44
1:A:283:GLY:O	1:A:286:ARG:N	2.49	0.44
1:B:76:LEU:O	1:B:128:VAL:HA	2.18	0.43
1:B:175:HIS:CD2	1:B:181:PRO:HA	2.52	0.43
1:B:246:VAL:HG12	1:B:250:LEU:HD12	2.00	0.43
1:E:92:LEU:HD11	1:E:124:GLY:N	2.34	0.43
1:E:192:MET:HE1	1:E:208:THR:HG21	1.99	0.43
1:B:109:TYR:CE1	1:B:142:SER:HB2	2.53	0.43
1:E:147:VAL:HG21	1:E:190:SER:HB3	1.99	0.43
1:A:340:GLY:O	1:A:354:THR:HA	2.18	0.43
1:E:54:PRO:HD2	1:E:199:LEU:O	2.18	0.43
1:A:152:PHE:CE1	1:A:156:LEU:HD11	2.53	0.43
1:B:38:VAL:HG23	1:B:344:THR:HG21	1.99	0.43
1:E:63:LEU:HA	1:E:128:VAL:O	2.19	0.43
1:A:64:VAL:O	1:A:127:ALA:HA	2.19	0.43
1:D:141:SER:O	1:D:144:SER:HB3	2.17	0.43
1:B:295:LEU:HD13	1:B:303:PHE:CD2	2.54	0.43
1:E:83:ASP:OD2	1:E:105:ARG:N	2.47	0.43
1:D:133:VAL:HG11	1:D:141:SER:HA	2.01	0.43
1:B:246:VAL:O	1:B:249:ALA:N	2.51	0.42
1:D:315:ARG:NH1	1:D:316:ASP:CG	2.78	0.42
1:B:146:GLU:OE2	1:B:174:GLU:OE1	2.37	0.42
1:A:199:LEU:HD23	1:A:201:ILE:HD11	2.01	0.42
1:A:380:LEU:HD23	1:A:380:LEU:HA	1.81	0.42
1:D:163:ILE:O	1:D:166:ARG:HB2	2.19	0.42
1:A:254:SER:OG	1:A:256:ARG:HB3	2.20	0.42
1:E:184:ILE:O	1:E:188:PHE:HB2	2.20	0.41
1:B:150:TYR:CE1	1:B:166:ARG:HG2	2.55	0.41
1:A:175:HIS:CD2	1:A:181:PRO:HA	2.55	0.41
1:A:306:LEU:HD12	1:A:306:LEU:H	1.86	0.41
1:D:311:HIS:HB2	1:D:342:ARG:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ALA:O	1:A:282:VAL:HB	2.21	0.41
1:B:33:SER:O	1:B:387:ALA:HA	2.20	0.41
1:B:65:GLY:HA3	1:B:126:SER:O	2.20	0.41
1:E:163:ILE:HG21	1:E:192:MET:CG	2.50	0.41
1:D:20:PHE:CD1	1:D:20:PHE:C	2.99	0.41
1:E:6:GLN:OE1	1:E:58:GLU:HB2	2.20	0.41
1:D:33:SER:O	1:D:387:ALA:HA	2.21	0.41
1:D:140:SER:O	1:D:144:SER:HB2	2.20	0.41
1:D:146:GLU:OE2	1:D:174:GLU:OE1	2.38	0.41
1:B:33:SER:HA	1:B:61:THR:O	2.21	0.41
1:B:48:ASN:HD21	1:B:243:CYS:CB	2.34	0.41
1:B:149:THR:O	1:B:153:LEU:HG	2.21	0.41
1:A:361:ALA:HA	1:A:363:HIS:N	2.35	0.41
1:D:76:LEU:HD12	1:D:77:THR:N	2.36	0.41
1:A:305:ARG:O	1:A:309:GLU:CB	2.69	0.40
1:E:175:HIS:CD2	1:E:181:PRO:HA	2.56	0.40
1:A:68:ARG:HD2	1:A:126:SER:OG	2.21	0.40
1:D:77:THR:O	1:D:78:THR:C	2.65	0.40
1:D:213:LEU:O	4:D:401:SSY:F	2.30	0.40
1:A:255:LEU:HD12	1:A:255:LEU:HA	1.93	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:564:HOH:O	5:E:609:HOH:O[1_656]	2.18	0.02

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	384/399 (96%)	360 (94%)	20 (5%)	4 (1%)	12 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	385/399 (96%)	367 (95%)	17 (4%)	1 (0%)	36	46
1	D	360/399 (90%)	334 (93%)	24 (7%)	2 (1%)	21	27
1	E	389/399 (98%)	377 (97%)	12 (3%)	0	100	100
All	All	1518/1596 (95%)	1438 (95%)	73 (5%)	7 (0%)	24	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	105	ARG
1	A	96	GLN
1	A	215	ASP
1	A	232	ALA
1	B	7	PRO
1	A	271	SER
1	D	206	LEU

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	252/315 (80%)	230 (91%)	22 (9%)	9	12
1	B	266/315 (84%)	251 (94%)	15 (6%)	19	28
1	D	244/315 (78%)	225 (92%)	19 (8%)	11	16
1	E	285/315 (90%)	277 (97%)	8 (3%)	38	56
All	All	1047/1260 (83%)	983 (94%)	64 (6%)	17	24

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

Mol	Chain	Res	Type
1	A	6	GLN
1	A	9	VAL
1	A	41	ILE
1	A	43	GLU

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Mol	Chain	Res	Type
1	A	72	LEU
1	A	84	GLU
1	A	103	THR
1	A	122	LEU
1	A	188	PHE
1	A	189	ILE
1	A	209	SER
1	A	228	ARG
1	A	254	SER
1	A	255	LEU
1	A	287	ARG
1	A	338	VAL
1	A	341	SER
1	A	343	MET
1	A	354	THR
1	A	355	LEU
1	A	362	PRO
1	A	363	HIS
1	B	6	GLN
1	B	9	VAL
1	B	23	GLU
1	B	30	LEU
1	B	63	LEU
1	B	83[A]	ASP
1	B	83[B]	ASP
1	B	135	LEU
1	B	172	GLN
1	B	188	PHE
1	B	218	LEU
1	B	227	VAL
1	B	264	GLU
1	B	269	LEU
1	B	381	SER
1	E	11	GLU
1	E	192	MET
1	E	261	GLU
1	E	264	GLU
1	E	321	SER
1	E	356	LEU
1	E	377	THR
1	E	381	SER
1	D	30	LEU

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Mol	Chain	Res	Type
1	D	37	ARG
1	D	63	LEU
1	D	64	VAL
1	D	66	SER
1	D	75	LEU
1	D	76	LEU
1	D	140	SER
1	D	190	SER
1	D	213	LEU
1	D	218	LEU
1	D	259	GLN
1	D	267	ARG
1	D	269	LEU
1	D	271	SER
1	D	295	LEU
1	D	357	GLU
1	D	375	THR
1	D	392	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	172	GLN
1	A	226	ASN
1	A	242	GLN
1	A	327	GLN
1	A	363	HIS
1	B	48	ASN
1	B	49	GLN
1	B	172	GLN
1	B	367	HIS
1	B	371	HIS
1	E	226	ASN
1	E	327	GLN

5.3.3 RNA ⓘ

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	$\# Z > 2$
3	HFK	B	402	-	29,30,30	2.68	9 (31%)	32,44,44	2.22	14 (43%)
2	GAL	E	401	-	12,12,12	1.03	1 (8%)	17,17,17	2.89	8 (47%)
2	GAL	A	401	-	12,12,12	0.71	0	17,17,17	2.17	5 (29%)
4	SSY	D	401	-	16,16,16	1.54	4 (25%)	23,23,23	1.38	2 (8%)
3	HFK	A	402	-	29,30,30	2.94	11 (37%)	32,44,44	1.63	8 (25%)
2	GAL	B	401	-	12,12,12	0.96	0	17,17,17	2.40	6 (35%)
3	HFK	E	402	-	29,30,30	2.59	11 (37%)	32,44,44	2.18	10 (31%)

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
3	HFK	B	402	-	-	2/4/43/43	0/5/5/5
2	GAL	E	401	-	-	2/2/22/22	0/1/1/1
2	GAL	A	401	-	-	2/2/22/22	0/1/1/1
4	SSY	D	401	-	-	0/14/14/14	0/1/1/1
3	HFK	A	402	-	-	2/4/43/43	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	B	401	-	-	1/2/22/22	0/1/1/1
3	HFK	E	402	-	-	2/4/43/43	0/5/5/5

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	HFK	C06-C07	9.96	1.49	1.37
3	B	402	HFK	C06-C07	9.57	1.49	1.37
3	E	402	HFK	C06-C07	8.84	1.48	1.37
3	A	402	HFK	C15-N14	6.56	1.47	1.30
3	B	402	HFK	C15-N14	5.40	1.44	1.30
3	E	402	HFK	C15-N14	5.06	1.43	1.30
3	A	402	HFK	C18-N19	4.56	1.38	1.30
3	A	402	HFK	C08-N14	4.09	1.50	1.46
3	E	402	HFK	C18-N17	4.00	1.44	1.36
3	E	402	HFK	C03-C02	3.97	1.56	1.50
3	B	402	HFK	C05-C06	3.75	1.55	1.49
4	D	401	SSY	C9-C8	3.60	1.62	1.53
3	A	402	HFK	C15-N17	3.55	1.45	1.37
3	A	402	HFK	C18-N17	3.48	1.43	1.36
3	B	402	HFK	C18-N19	3.40	1.36	1.30
3	B	402	HFK	C18-N17	3.40	1.43	1.36
3	B	402	HFK	C15-N16	3.36	1.42	1.36
3	B	402	HFK	C15-N17	3.21	1.44	1.37
3	E	402	HFK	C15-N17	3.20	1.44	1.37
3	E	402	HFK	C05-C06	3.08	1.54	1.49
3	A	402	HFK	C15-N16	3.04	1.41	1.36
3	E	402	HFK	C20-N19	-2.82	1.34	1.39
4	D	401	SSY	C8-N	2.52	1.41	1.35
2	E	401	GAL	O1-C1	-2.40	1.32	1.39
3	B	402	HFK	O22-C21	2.35	1.42	1.38
3	E	402	HFK	C18-N19	2.35	1.34	1.30
3	E	402	HFK	C15-N16	2.35	1.40	1.36
3	E	402	HFK	O22-C21	2.35	1.42	1.38
3	A	402	HFK	C06-N16	2.22	1.41	1.37
3	A	402	HFK	C26-C20	2.19	1.43	1.40
3	E	402	HFK	C06-N16	2.17	1.41	1.37
3	B	402	HFK	C03-C02	2.15	1.53	1.50
3	A	402	HFK	C23-C21	2.14	1.44	1.39
4	D	401	SSY	F1-C9	2.08	1.40	1.32
4	D	401	SSY	C4-C3	-2.04	1.35	1.38
3	A	402	HFK	C05-C06	2.03	1.53	1.49

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	GAL	C1-O5-C5	-7.87	98.43	113.65
2	B	401	GAL	C1-O5-C5	-6.96	100.19	113.65
2	E	401	GAL	C1-C2-C3	-6.22	97.66	110.36
3	B	402	HFK	C07-C06-N16	-6.19	117.11	122.11
3	E	402	HFK	C07-C06-N16	-5.62	117.58	122.11
2	A	401	GAL	C1-C2-C3	-5.03	100.09	110.36
2	A	401	GAL	C1-O5-C5	-4.67	104.61	113.65
3	B	402	HFK	C23-C21-C20	-4.54	118.09	123.62
3	E	402	HFK	C09-C10-C11	4.06	117.67	111.35
3	B	402	HFK	C09-C10-C11	3.97	117.53	111.35
3	E	402	HFK	O22-C18-N19	-3.88	108.60	115.57
3	E	402	HFK	C23-C21-C20	-3.66	119.17	123.62
3	B	402	HFK	O22-C21-C23	3.60	134.05	126.49
3	A	402	HFK	C23-C21-C20	-3.48	119.39	123.62
2	A	401	GAL	O1-C1-C2	3.38	118.78	108.98
3	E	402	HFK	C20-N19-C18	3.37	110.81	104.13
3	A	402	HFK	N17-C15-N14	3.34	124.19	117.96
3	E	402	HFK	O22-C21-C23	3.23	133.28	126.49
2	B	401	GAL	C1-C2-C3	-3.21	103.81	110.36
3	B	402	HFK	C05-C06-N16	3.09	119.86	115.46
2	B	401	GAL	O5-C5-C6	3.02	113.91	106.44
2	E	401	GAL	C3-C4-C5	2.96	115.60	110.23
3	A	402	HFK	O22-C21-C23	2.95	132.69	126.49
3	E	402	HFK	C13-C12-C11	2.94	115.92	111.35
2	B	401	GAL	O2-C2-C3	2.90	117.22	110.38
3	A	402	HFK	C05-C06-N16	2.84	119.50	115.46
3	B	402	HFK	N17-C18-N19	-2.81	120.60	128.58
3	E	402	HFK	C05-C06-N16	2.78	119.42	115.46
2	A	401	GAL	O2-C2-C1	2.73	115.54	109.25
2	E	401	GAL	O6-C6-C5	-2.72	102.06	111.33
3	B	402	HFK	O22-C18-N19	-2.66	110.79	115.57
4	D	401	SSY	F1-C9-C8	2.62	119.69	111.85
3	B	402	HFK	C02-C07-C06	-2.61	116.87	119.18
4	D	401	SSY	C3-C2-C1	-2.57	114.99	120.83
3	E	402	HFK	N17-C15-N14	2.57	122.76	117.96
3	B	402	HFK	C08-C07-C06	-2.49	118.94	121.75
2	E	401	GAL	C6-C5-C4	2.47	119.09	113.02
3	A	402	HFK	C07-C06-N16	-2.47	120.12	122.11
2	A	401	GAL	O5-C1-C2	-2.46	105.97	110.30
3	E	402	HFK	O01-C02-C07	-2.37	118.36	121.53
3	A	402	HFK	C04-C03-C02	-2.35	109.05	113.57
3	B	402	HFK	C13-C12-C11	-2.34	107.71	111.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	HFK	O22-C18-N19	-2.33	111.38	115.57
2	B	401	GAL	C4-C3-C2	-2.32	106.76	110.83
3	B	402	HFK	C05-C04-C03	2.28	119.43	112.03
3	B	402	HFK	C04-C03-C02	2.21	117.82	113.57
2	B	401	GAL	O5-C5-C4	2.17	113.60	109.70
3	A	402	HFK	C05-C06-C07	-2.16	119.78	122.72
2	E	401	GAL	O1-C1-O5	-2.15	104.02	110.41
2	E	401	GAL	O3-C3-C4	2.09	115.31	110.38
2	E	401	GAL	O4-C4-C5	-2.06	104.24	109.32
3	B	402	HFK	C04-C05-C06	2.02	115.22	110.97
3	B	402	HFK	C20-N19-C18	2.00	108.10	104.13

There are no chirality outliers.

All (11) torsion outliers are listed below:

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

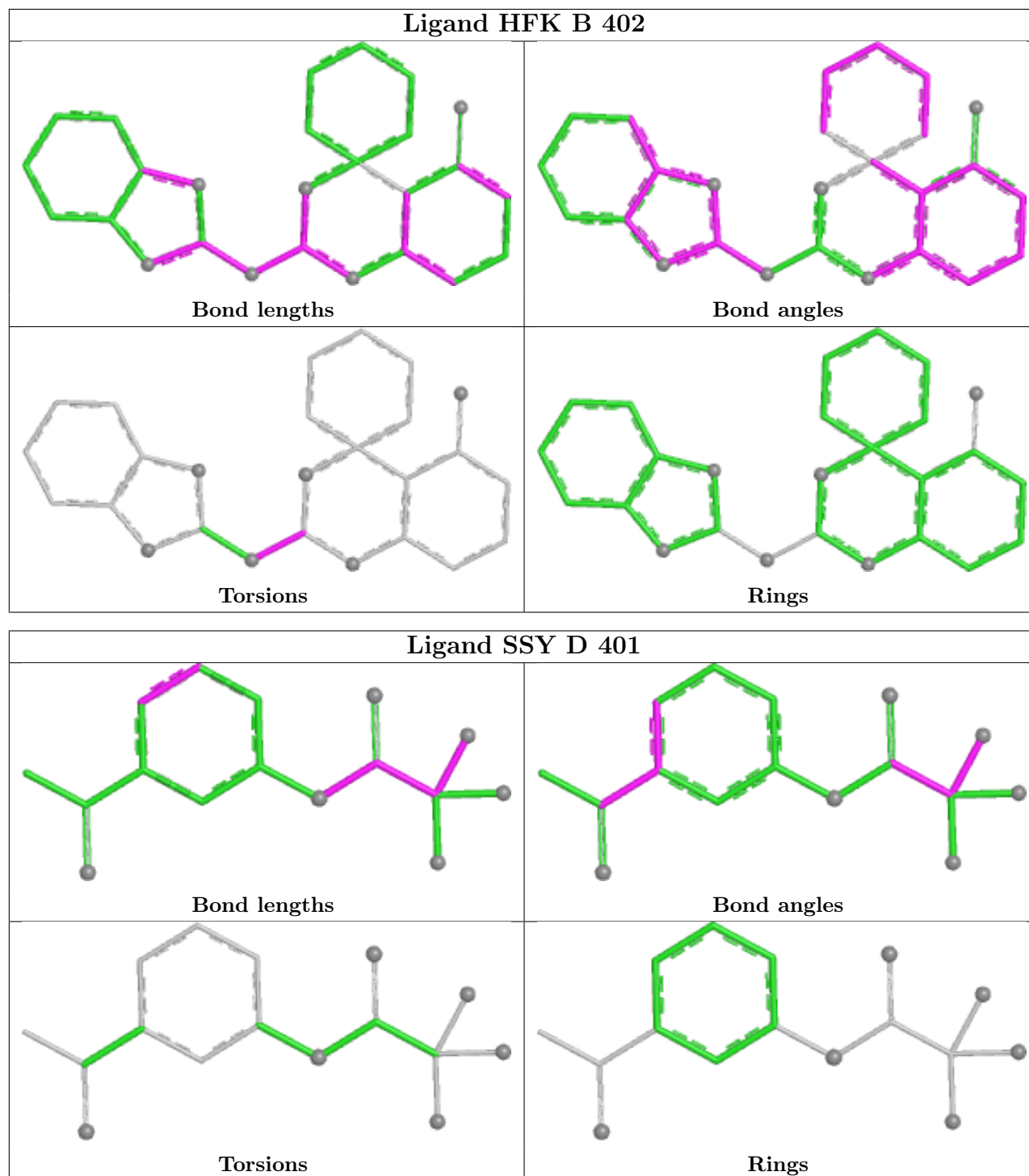
There are no ring outliers.

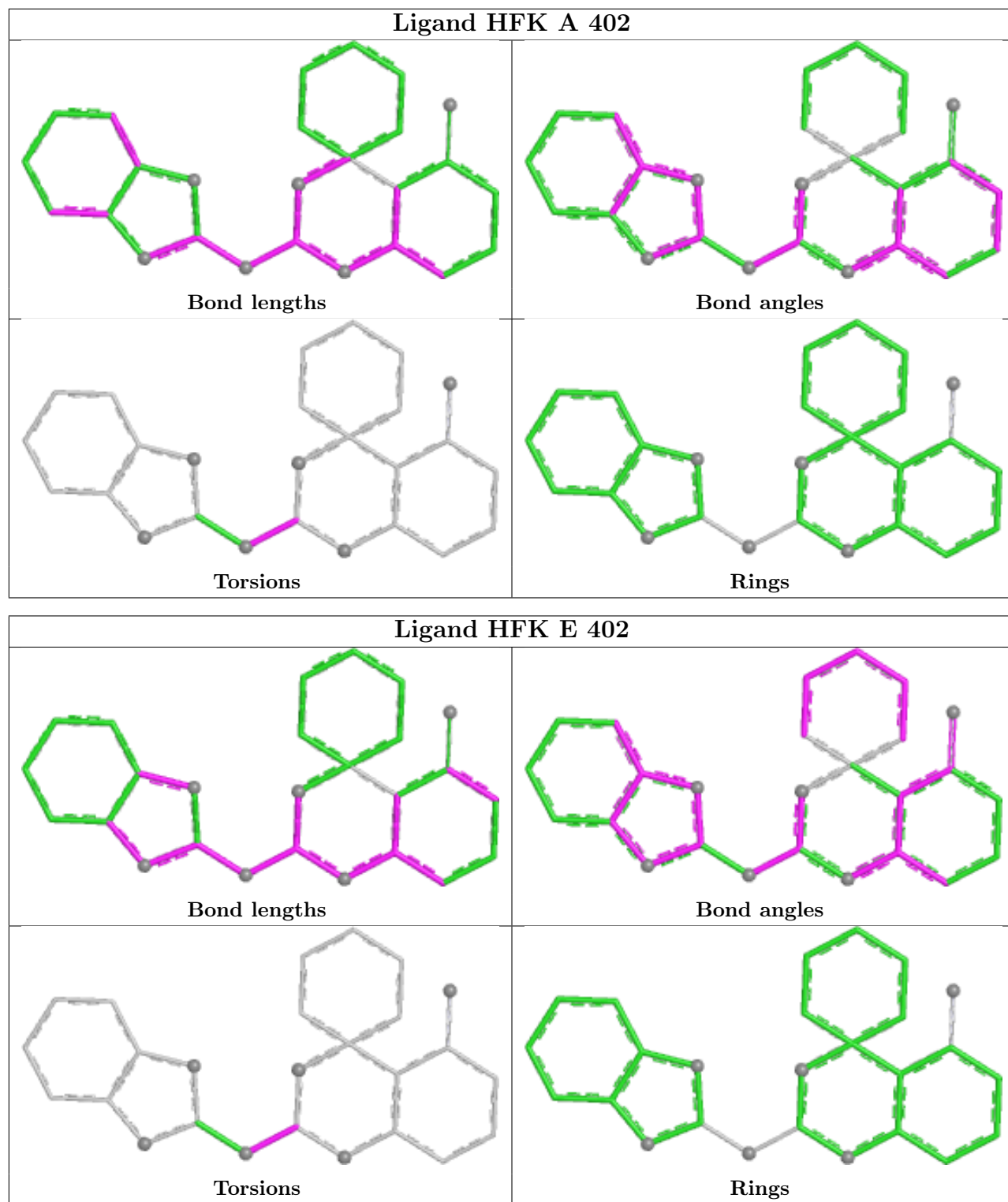
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	401	SSY	3	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.





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	388/399 (97%)	0.84	69 (17%) 4 4	26, 50, 100, 128	0
1	B	388/399 (97%)	0.41	23 (5%) 28 30	26, 44, 77, 113	1 (0%)
1	D	368/399 (92%)	1.09	78 (21%) 2 3	15, 53, 111, 147	2 (0%)
1	E	390/399 (97%)	-0.04	7 (1%) 67 69	15, 36, 59, 73	1 (0%)
All	All	1534/1596 (96%)	0.57	177 (11%) 9 10	15, 44, 96, 147	4 (0%)

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	ALA	8.2
1	A	268	ASP	6.6
1	D	72	LEU	5.4
1	D	43	GLU	5.4
1	D	88	LEU	5.2
1	A	233	SER	5.2
1	A	361	ALA	5.2
1	D	7	PRO	5.1
1	D	99	LEU	5.0
1	D	184	ILE	5.0
1	D	106	TRP	4.8
1	B	99	LEU	4.8
1	B	72	LEU	4.8
1	A	303	PHE	4.7
1	B	96	GLN	4.6
1	D	24	PHE	4.6
1	D	120	ALA	4.6
1	A	2	ALA	4.5
1	A	270	VAL	4.3
1	D	95	ALA	4.3
1	A	288	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	273	GLU	4.2
1	A	275	PHE	4.2
1	D	105	ARG	4.1
1	D	104	PRO	4.1
1	D	163	ILE	4.1
1	B	234	SER	4.1
1	A	269	LEU	4.1
1	D	122	LEU	4.1
1	A	259	GLN	4.1
1	B	214	SER	4.1
1	D	27	GLU	4.1
1	B	233	SER	4.0
1	D	78	THR	3.9
1	A	260	LEU	3.8
1	D	103	THR	3.8
1	D	121	PRO	3.7
1	D	373	GLY	3.7
1	D	39[A]	ASN	3.7
1	B	232	ALA	3.7
1	B	2	ALA	3.6
1	B	103	THR	3.5
1	D	89	GLN	3.5
1	D	300	TYR	3.5
1	D	76	LEU	3.5
1	A	363	HIS	3.4
1	A	230	SER	3.4
1	B	231	LEU	3.4
1	D	161	GLY	3.4
1	A	261	GLU	3.3
1	D	96	GLN	3.3
1	A	263	LEU	3.3
1	E	3	ALA	3.2
1	B	92	LEU	3.2
1	D	94	THR	3.2
1	A	3	ALA	3.2
1	D	178	ALA	3.2
1	A	249	ALA	3.2
1	A	300	TYR	3.2
1	D	19	ALA	3.2
1	D	374	GLY	3.2
1	A	370	GLU	3.1
1	D	93	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	102	GLY	3.1
1	A	331	ALA	3.1
1	D	91	PRO	3.0
1	E	4	LEU	3.0
1	D	119	ALA	3.0
1	D	9	VAL	3.0
1	A	258	VAL	3.0
1	A	333	LEU	3.0
1	A	271	SER	3.0
1	D	175	HIS	2.9
1	A	364	ALA	2.9
1	A	282	VAL	2.9
1	E	268	ASP	2.9
1	D	98	SER	2.9
1	D	101	PRO	2.9
1	A	305	ARG	2.9
1	A	265	ALA	2.9
1	A	267	ARG	2.8
1	A	231	LEU	2.8
1	A	299	ASP	2.8
1	B	97	ARG	2.8
1	D	21	ARG	2.8
1	A	332	ALA	2.8
1	E	373	GLY	2.8
1	D	214	SER	2.8
1	D	86	GLN	2.8
1	A	295	LEU	2.8
1	A	301	ARG	2.8
1	D	97	ARG	2.8
1	D	268	ASP	2.8
1	B	98	SER	2.8
1	D	177	PHE	2.8
1	A	229	HIS	2.7
1	D	135	LEU	2.7
1	B	95	ALA	2.7
1	D	87	ARG	2.7
1	A	246	VAL	2.7
1	A	253	ALA	2.7
1	D	92	LEU	2.7
1	A	360	ALA	2.6
1	D	160	SER	2.6
1	A	242	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	73	VAL	2.6
1	A	218	LEU	2.6
1	A	80	GLU	2.6
1	D	107	ALA	2.6
1	D	77	THR	2.6
1	A	339	TYR	2.6
1	B	88	LEU	2.5
1	D	18	ARG	2.5
1	B	249	ALA	2.5
1	A	328	LEU	2.5
1	D	118	PRO	2.5
1	D	346	GLY	2.5
1	D	90	PHE	2.5
1	D	188	PHE	2.5
1	A	338	VAL	2.5
1	A	274	GLY	2.5
1	D	339	TYR	2.4
1	A	245	GLU	2.4
1	D	67	PRO	2.4
1	D	185	MET	2.4
1	A	306	LEU	2.4
1	B	248	ARG	2.4
1	D	23	GLU	2.4
1	A	304	GLY	2.4
1	D	167	ALA	2.4
1	A	286	ARG	2.4
1	D	159	ASP	2.4
1	A	255	LEU	2.4
1	B	250	LEU	2.4
1	D	269	LEU	2.4
1	D	8	GLN	2.4
1	D	169	VAL	2.3
1	A	356	LEU	2.3
1	D	109	TYR	2.3
1	D	253	ALA	2.3
1	E	213	LEU	2.3
1	D	157	CYS	2.3
1	D	158	PRO	2.3
1	A	232	ALA	2.3
1	A	277	ARG	2.3
1	B	94	THR	2.3
1	D	375	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	366	ARG	2.2
1	B	180	MET	2.2
1	A	278	ALA	2.2
1	B	89	GLN	2.2
1	D	162	THR	2.2
1	A	308	VAL	2.2
1	E	80	GLU	2.2
1	A	290	GLN	2.2
1	A	367	HIS	2.2
1	D	165	ALA	2.2
1	A	365	MET	2.1
1	D	64	VAL	2.1
1	A	357	GLU	2.1
1	A	362	PRO	2.1
1	D	371	HIS	2.1
1	E	5	ARG	2.1
1	A	368	ILE	2.1
1	A	340	GLY	2.1
1	D	337	GLY	2.1
1	D	17	ARG	2.1
1	D	22	GLU	2.1
1	A	8	GLN	2.1
1	A	281	VAL	2.1
1	B	160	SER	2.0
1	D	126	SER	2.0
1	A	213	LEU	2.0
1	A	228	ARG	2.0
1	A	79	SER	2.0
1	B	244	GLU	2.0
1	D	206	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

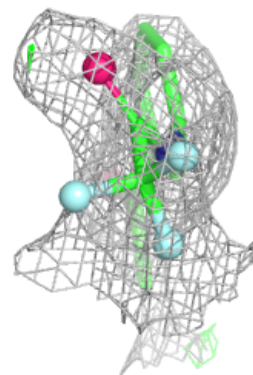
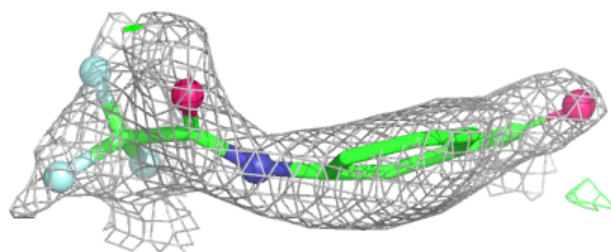
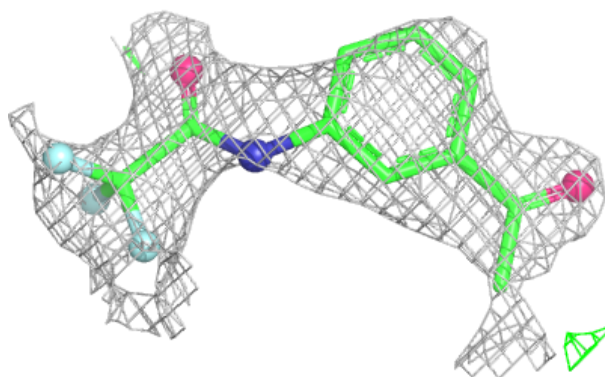
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SSY	D	401	16/16	0.83	0.18	37,44,50,52	16
3	HFK	B	402	26/26	0.87	0.14	51,56,65,66	0
3	HFK	A	402	26/26	0.89	0.13	48,55,59,60	0
3	HFK	E	402	26/26	0.93	0.09	33,38,44,45	0
2	GAL	B	401	12/12	0.93	0.09	29,35,38,41	0
2	GAL	A	401	12/12	0.94	0.07	36,40,44,44	0
2	GAL	E	401	12/12	0.95	0.06	24,25,27,30	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.

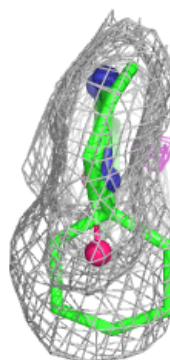
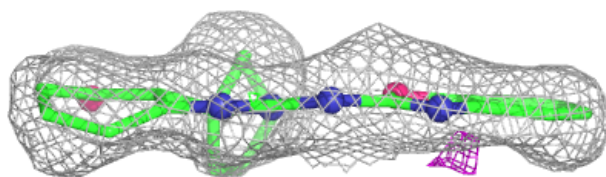
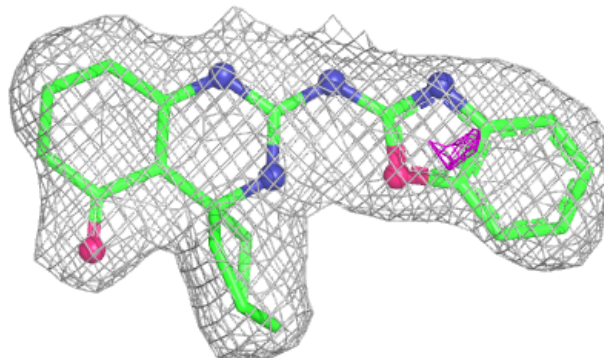
Electron density around SSY D 401:

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

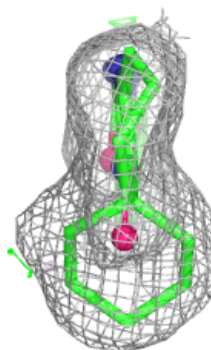
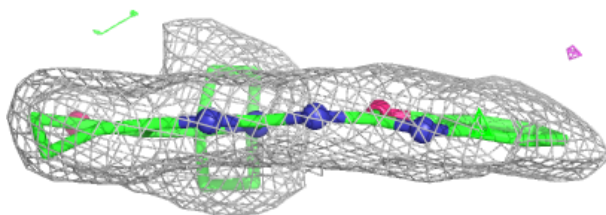
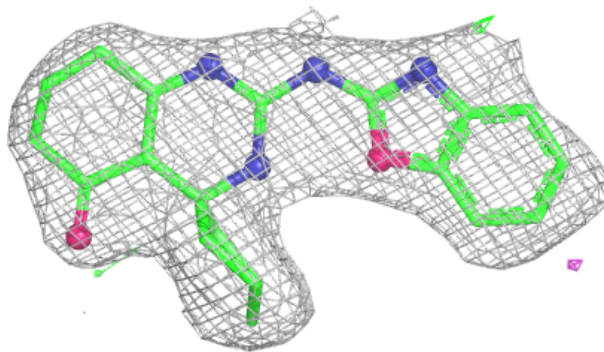


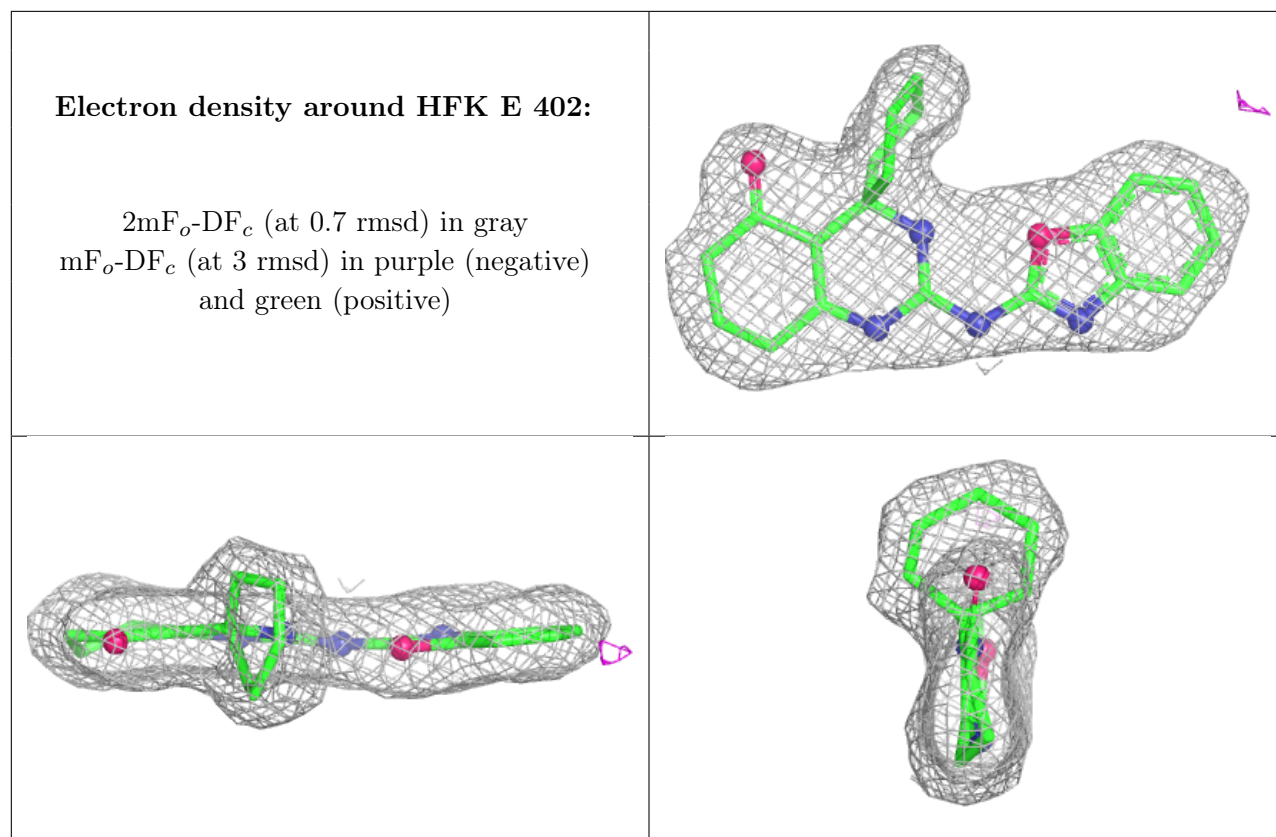
Electron density around HFK B 402:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.