



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 04:58 AM UTC

PDB ID : 6TBH / pdb_00006tbh
Title : Structure of a beta galactosidase with inhibitor
Authors : Offen, W.; Davies, G.
Deposited on : 2019-11-01
Resolution : 1.50 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 ⓘ](#)) were used in the production of this report:

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

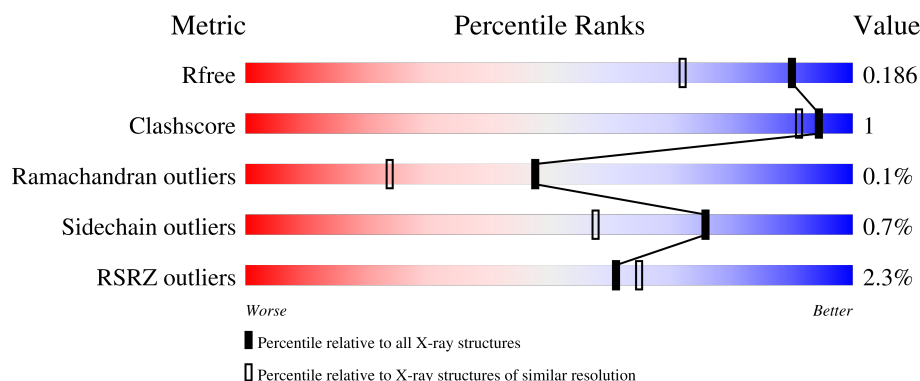
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	550	4% 91% 7%
1	B	550	2% 89% 7%
1	C	550	2% 91% 6%
1	D	550	% 92% 6%
1	E	550	% 93% 5%

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Mol	Chain	Length	Quality of chain
1	F	550	2% 90% 7% . .
1	G	550	3% 91% 7% .
1	H	550	3% 86% 10% . .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 38555 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 Beta-galactosidase, putative, bgl35A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	0	6	0
			4274	2736	721	801	16			
1	B	530	Total	C	N	O	S	0	6	0
			4219	2700	719	785	15			
1	C	533	Total	C	N	O	S	0	8	0
			4252	2722	725	789	16			
1	D	539	Total	C	N	O	S	0	10	0
			4298	2750	725	807	16			
1	E	538	Total	C	N	O	S	0	9	0
			4321	2769	732	804	16			
1	F	536	Total	C	N	O	S	0	15	0
			4353	2783	740	814	16			
1	G	540	Total	C	N	O	S	0	13	0
			4348	2780	740	812	16			
1	H	534	Total	C	N	O	S	0	13	0
			4296	2750	728	802	16			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	initiating methionine	UNP B3PBE0
A	27	GLY	-	expression tag	UNP B3PBE0
A	28	SER	-	expression tag	UNP B3PBE0
A	29	SER	-	expression tag	UNP B3PBE0
A	30	HIS	-	expression tag	UNP B3PBE0
A	31	HIS	-	expression tag	UNP B3PBE0
A	32	HIS	-	expression tag	UNP B3PBE0
A	33	HIS	-	expression tag	UNP B3PBE0
A	34	HIS	-	expression tag	UNP B3PBE0
A	35	HIS	-	expression tag	UNP B3PBE0
B	26	MET	-	initiating methionine	UNP B3PBE0
B	27	GLY	-	expression tag	UNP B3PBE0
B	28	SER	-	expression tag	UNP B3PBE0

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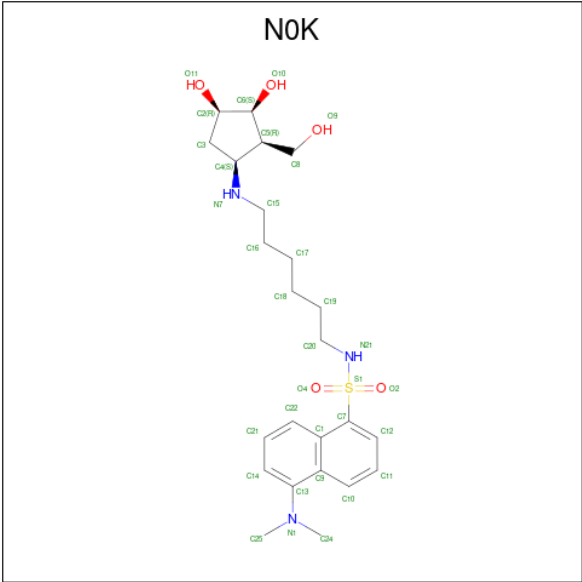
Chain	Residue	Modelled	Actual	Comment	Reference
B	29	SER	-	expression tag	UNP B3PBE0
B	30	HIS	-	expression tag	UNP B3PBE0
B	31	HIS	-	expression tag	UNP B3PBE0
B	32	HIS	-	expression tag	UNP B3PBE0
B	33	HIS	-	expression tag	UNP B3PBE0
B	34	HIS	-	expression tag	UNP B3PBE0
B	35	HIS	-	expression tag	UNP B3PBE0
C	26	MET	-	initiating methionine	UNP B3PBE0
C	27	GLY	-	expression tag	UNP B3PBE0
C	28	SER	-	expression tag	UNP B3PBE0
C	29	SER	-	expression tag	UNP B3PBE0
C	30	HIS	-	expression tag	UNP B3PBE0
C	31	HIS	-	expression tag	UNP B3PBE0
C	32	HIS	-	expression tag	UNP B3PBE0
C	33	HIS	-	expression tag	UNP B3PBE0
C	34	HIS	-	expression tag	UNP B3PBE0
C	35	HIS	-	expression tag	UNP B3PBE0
D	26	MET	-	initiating methionine	UNP B3PBE0
D	27	GLY	-	expression tag	UNP B3PBE0
D	28	SER	-	expression tag	UNP B3PBE0
D	29	SER	-	expression tag	UNP B3PBE0
D	30	HIS	-	expression tag	UNP B3PBE0
D	31	HIS	-	expression tag	UNP B3PBE0
D	32	HIS	-	expression tag	UNP B3PBE0
D	33	HIS	-	expression tag	UNP B3PBE0
D	34	HIS	-	expression tag	UNP B3PBE0
D	35	HIS	-	expression tag	UNP B3PBE0
E	26	MET	-	initiating methionine	UNP B3PBE0
E	27	GLY	-	expression tag	UNP B3PBE0
E	28	SER	-	expression tag	UNP B3PBE0
E	29	SER	-	expression tag	UNP B3PBE0
E	30	HIS	-	expression tag	UNP B3PBE0
E	31	HIS	-	expression tag	UNP B3PBE0
E	32	HIS	-	expression tag	UNP B3PBE0
E	33	HIS	-	expression tag	UNP B3PBE0
E	34	HIS	-	expression tag	UNP B3PBE0
E	35	HIS	-	expression tag	UNP B3PBE0
F	26	MET	-	initiating methionine	UNP B3PBE0
F	27	GLY	-	expression tag	UNP B3PBE0
F	28	SER	-	expression tag	UNP B3PBE0
F	29	SER	-	expression tag	UNP B3PBE0
F	30	HIS	-	expression tag	UNP B3PBE0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	31	HIS	-	expression tag	UNP B3PBE0
F	32	HIS	-	expression tag	UNP B3PBE0
F	33	HIS	-	expression tag	UNP B3PBE0
F	34	HIS	-	expression tag	UNP B3PBE0
F	35	HIS	-	expression tag	UNP B3PBE0
G	26	MET	-	initiating methionine	UNP B3PBE0
G	27	GLY	-	expression tag	UNP B3PBE0
G	28	SER	-	expression tag	UNP B3PBE0
G	29	SER	-	expression tag	UNP B3PBE0
G	30	HIS	-	expression tag	UNP B3PBE0
G	31	HIS	-	expression tag	UNP B3PBE0
G	32	HIS	-	expression tag	UNP B3PBE0
G	33	HIS	-	expression tag	UNP B3PBE0
G	34	HIS	-	expression tag	UNP B3PBE0
G	35	HIS	-	expression tag	UNP B3PBE0
H	26	MET	-	initiating methionine	UNP B3PBE0
H	27	GLY	-	expression tag	UNP B3PBE0
H	28	SER	-	expression tag	UNP B3PBE0
H	29	SER	-	expression tag	UNP B3PBE0
H	30	HIS	-	expression tag	UNP B3PBE0
H	31	HIS	-	expression tag	UNP B3PBE0
H	32	HIS	-	expression tag	UNP B3PBE0
H	33	HIS	-	expression tag	UNP B3PBE0
H	34	HIS	-	expression tag	UNP B3PBE0
H	35	HIS	-	expression tag	UNP B3PBE0

- Molecule 2 is 5-[ethyl(methyl)amino]- {N}-[6-[(1 {S},2 {R},3 {S},4 {R})-2-(hydroxymethyl)-3,4-bis(oxidanyl)cyclopentyl]amino]hexyl]naphthalene-1-sulfonamide (CCD ID: N0K) (formula: C₂₄H₃₇N₃O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			21	13	2	5	1		
2	B	1	Total	C	N	O	S	0	0
			21	13	2	5	1		
2	C	1	Total	C	N	O	S	0	0
			21	13	2	5	1		
2	D	1	Total	C	N	O	S	0	0
			21	13	2	5	1		
2	E	1	Total	C	N	O	S	0	0
			21	13	2	5	1		
2	F	1	Total	C	N	O	S	0	0
			21	13	2	5	1		
2	G	1	Total	C	N	O	S	0	0
			21	13	2	5	1		
2	H	1	Total	C	N	O	S	0	0
			21	13	2	5	1		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total Na 4 4	0	0
4	B	2	Total Na 2 2	0	0
4	C	4	Total Na 4 4	0	0
4	D	5	Total Na 5 5	0	0
4	E	4	Total Na 4 4	0	0
4	F	5	Total Na 5 5	0	0
4	G	4	Total Na 4 4	0	0
4	H	4	Total Na 4 4	0	0

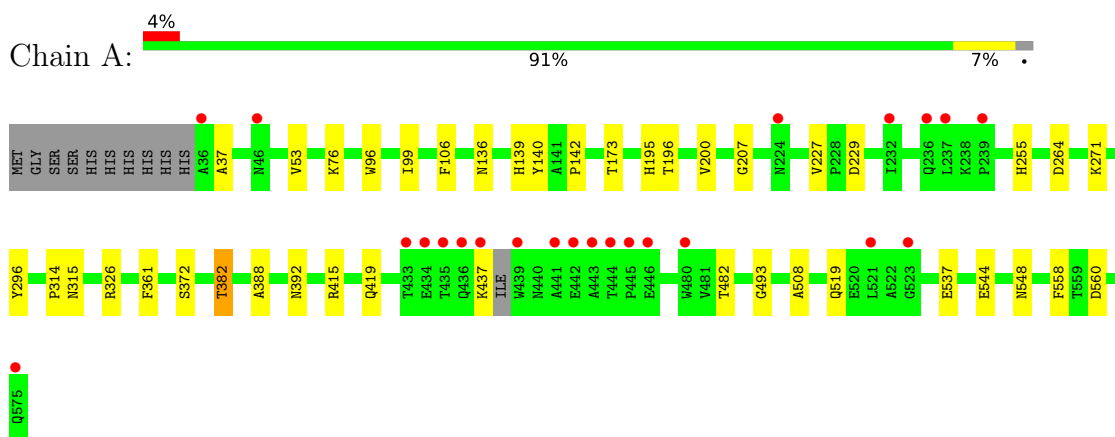
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	424	Total 424	O 424	0	0
5	B	482	Total 482	O 482	0	0
5	C	458	Total 458	O 458	0	0
5	D	562	Total 562	O 562	0	0
5	E	542	Total 542	O 542	0	0
5	F	534	Total 534	O 534	0	0
5	G	572	Total 572	O 572	0	0
5	H	404	Total 404	O 404	0	0

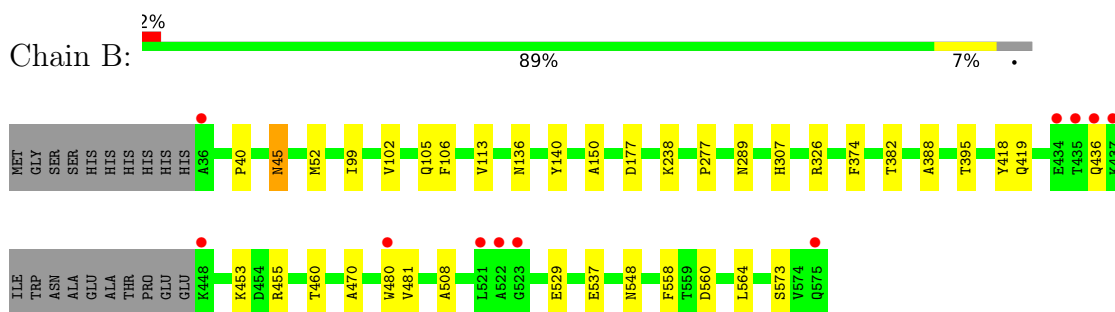
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

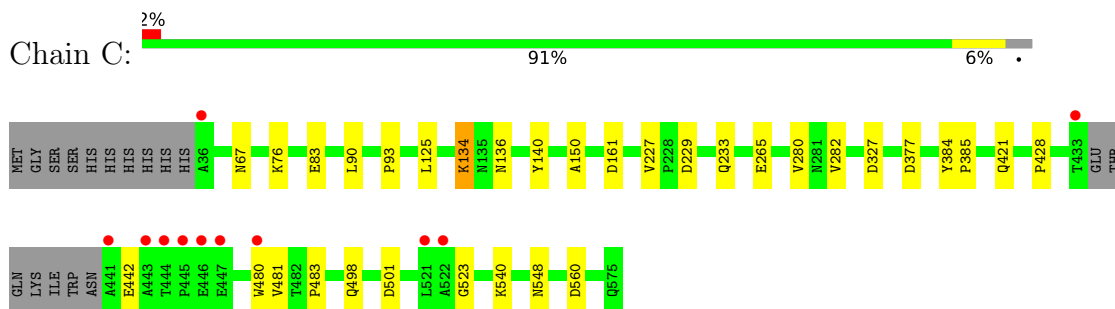
- Molecule 1: Beta-galactosidase, putative, bgl35A



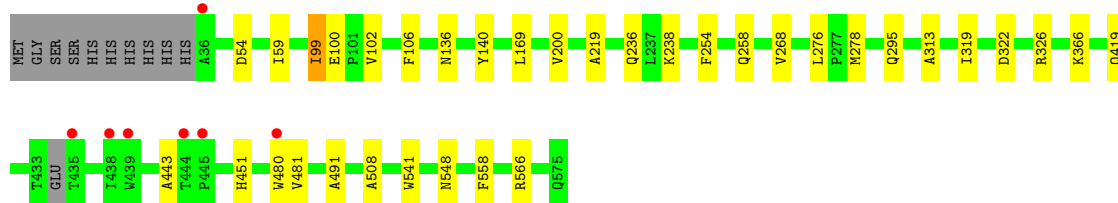
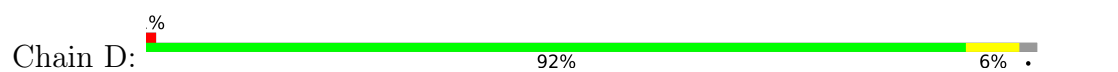
- Molecule 1: Beta-galactosidase, putative, bgl35A



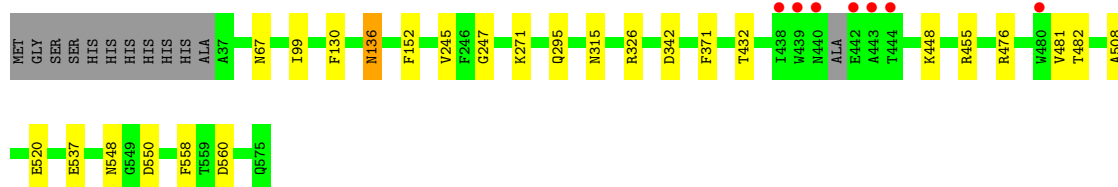
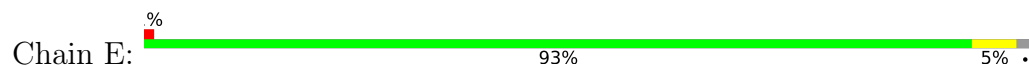
- Molecule 1: Beta-galactosidase, putative, bgl35A



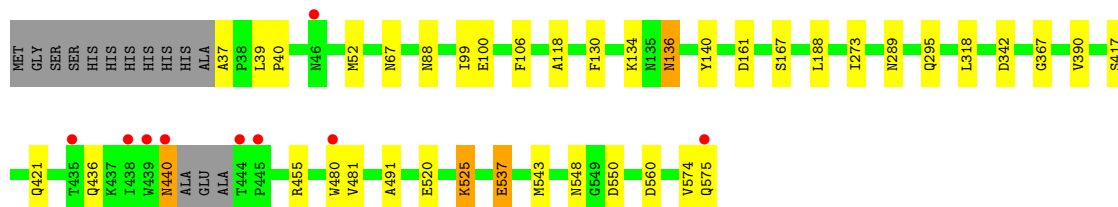
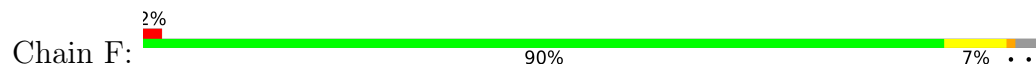
- Molecule 1: Beta-galactosidase, putative, bgl35A



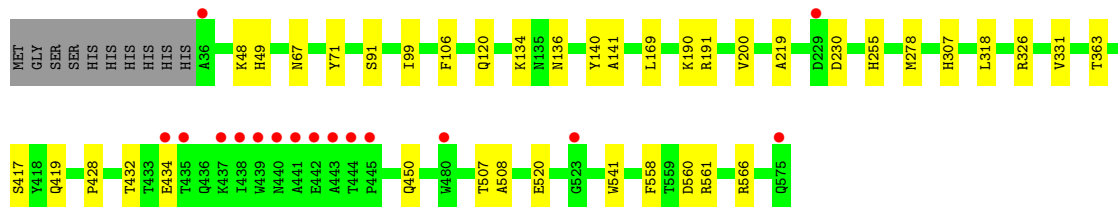
- Molecule 1: Beta-galactosidase, putative, bgl35A



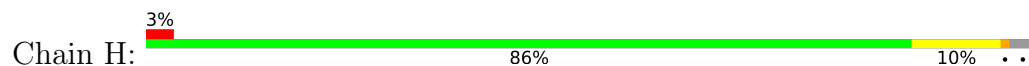
- Molecule 1: Beta-galactosidase, putative, bgl35A

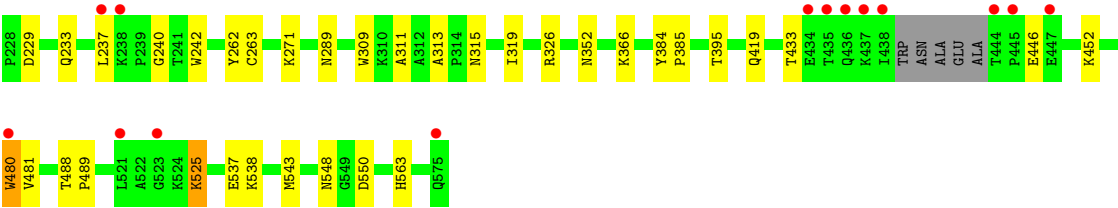


- Molecule 1: Beta-galactosidase, putative, bgl35A



- Molecule 1: Beta-galactosidase, putative, bgl35A





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	99.10Å 115.39Å 115.72Å 90.21° 89.99° 89.85°	Depositor
Resolution (Å)	81.86 – 1.50 81.86 – 1.50	Depositor EDS
% Data completeness (in resolution range)	96.1 (81.86-1.50) 96.1 (81.86-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.131 , 0.182 0.141 , 0.186	Depositor DCC
R_{free} test set	39674 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for h,l,-k 0.013 for h,-l,k 0.013 for h,-k,-l 0.008 for -h,k,-l 0.009 for -h,-k,l 0.006 for -h,l,k 0.007 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	38555	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.17% 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: NA, ACT, N0K

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	1.26	14/4387 (0.3%)	1.32	10/5979 (0.2%)
1	B	1.23	12/4334 (0.3%)	1.28	8/5906 (0.1%)
1	C	1.22	13/4365 (0.3%)	1.29	8/5946 (0.1%)
1	D	1.24	6/4414 (0.1%)	1.32	13/6014 (0.2%)
1	E	1.20	3/4439 (0.1%)	1.33	16/6043 (0.3%)
1	F	1.26	5/4466 (0.1%)	1.37	24/6075 (0.4%)
1	G	1.28	13/4462 (0.3%)	1.30	7/6076 (0.1%)
1	H	1.27	18/4412 (0.4%)	1.31	14/6008 (0.2%)
All	All	1.25	84/35279 (0.2%)	1.32	100/48047 (0.2%)

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

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

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	HIS	CE1-NE2	8.14	1.40	1.32
1	G	520	GLU	C-O	8.00	1.33	1.23
1	A	195	HIS	CE1-NE2	7.76	1.40	1.32
1	F	390	VAL	C-O	7.59	1.32	1.24
1	B	307	HIS	CE1-NE2	7.49	1.40	1.32
1	G	363	THR	C-O	7.31	1.32	1.24
1	H	153	PRO	C-O	7.13	1.31	1.23
1	F	520	GLU	C-O	7.01	1.32	1.23
1	B	45	ASN	C-O	6.82	1.32	1.23
1	D	326	ARG	C-O	6.75	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	560	ASP	CG-OD2	-6.66	1.12	1.25
1	H	446	GLU	C-O	6.61	1.31	1.24
1	B	326	ARG	C-O	6.57	1.32	1.24
1	G	255	HIS	CE1-NE2	6.56	1.39	1.32
1	B	560	ASP	CG-OD1	-6.46	1.13	1.25
1	G	428	PRO	C-O	-6.41	1.16	1.24
1	G	434	GLU	C-N	6.41	1.41	1.33
1	B	564	LEU	C-O	6.37	1.31	1.24
1	C	523	GLY	C-O	6.35	1.32	1.23
1	H	480	TRP	C-O	6.33	1.31	1.24
1	C	327	ASP	C-O	6.28	1.31	1.24
1	C	125	LEU	C-O	6.28	1.31	1.23
1	H	156	VAL	C-O	6.26	1.31	1.24
1	H	262	TYR	C-O	6.17	1.31	1.24
1	H	326	ARG	C-O	6.16	1.32	1.24
1	A	326	ARG	C-O	6.09	1.32	1.24
1	A	372	SER	CA-CB	-6.09	1.46	1.53
1	H	203	GLN	C-O	6.07	1.31	1.24
1	H	161	ASP	C-O	6.03	1.32	1.23
1	C	282	VAL	C-O	6.02	1.31	1.24
1	A	392	ASN	C-O	-6.00	1.16	1.23
1	G	49	HIS	CE1-NE2	5.96	1.38	1.32
1	G	560	ASP	CG-OD2	-5.96	1.14	1.25
1	E	560	ASP	CG-OD1	-5.90	1.14	1.25
1	F	560	ASP	CG-OD2	-5.79	1.14	1.25
1	B	455	ARG	NE-CZ	-5.78	1.26	1.33
1	D	319	ILE	C-O	-5.75	1.18	1.24
1	H	237	LEU	C-O	5.74	1.31	1.23
1	A	264	ASP	C-O	5.66	1.30	1.24
1	C	560	ASP	CG-OD1	-5.66	1.14	1.25
1	A	229	ASP	C-O	5.65	1.30	1.24
1	B	395	THR	C-O	5.64	1.30	1.24
1	A	296	TYR	C-O	5.63	1.31	1.23
1	B	529	GLU	C-O	5.62	1.30	1.24
1	A	200	VAL	C-O	-5.56	1.18	1.24
1	C	93	PRO	C-O	-5.56	1.17	1.23
1	C	280	VAL	C-O	5.47	1.29	1.24
1	D	102	VAL	C-O	-5.43	1.18	1.24
1	A	560	ASP	CG-OD2	-5.41	1.15	1.25
1	G	307	HIS	CE1-NE2	5.41	1.38	1.32
1	H	452	LYS	C-O	5.39	1.30	1.24
1	A	53	VAL	C-O	5.38	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	314	PRO	C-O	-5.38	1.17	1.24
1	C	428	PRO	C-O	-5.34	1.17	1.24
1	H	49	HIS	CE1-NE2	5.33	1.37	1.32
1	H	240	GLY	C-O	5.32	1.31	1.23
1	E	520	GLU	C-O	5.31	1.30	1.23
1	C	265	GLU	C-O	5.30	1.30	1.24
1	F	525	LYS	CG-CD	-5.29	1.36	1.52
1	G	450	GLN	C-O	5.28	1.30	1.24
1	C	150	ALA	C-O	5.28	1.30	1.24
1	B	102	VAL	C-O	5.27	1.29	1.24
1	B	573	SER	C-O	5.26	1.30	1.23
1	G	507	THR	C-O	-5.26	1.17	1.23
1	C	540	LYS	C-O	5.24	1.30	1.23
1	G	561	ARG	NE-CZ	5.23	1.38	1.33
1	H	433	THR	C-O	5.20	1.30	1.23
1	H	395	THR	C-O	5.20	1.30	1.24
1	D	268	VAL	C-O	-5.20	1.18	1.24
1	H	263	CYS	N-CA	5.18	1.52	1.46
1	E	448	LYS	C-O	5.16	1.30	1.24
1	A	195	HIS	CG-ND1	5.15	1.44	1.38
1	H	69	SER	CA-CB	-5.14	1.45	1.53
1	C	501	ASP	C-O	5.11	1.30	1.24
1	G	91	SER	CA-CB	-5.08	1.46	1.53
1	G	331	VAL	C-O	5.07	1.29	1.24
1	F	37	ALA	N-CA	5.07	1.55	1.46
1	B	113	VAL	N-CA	5.06	1.52	1.46
1	H	311	ALA	C-O	-5.05	1.18	1.24
1	A	139	HIS	CE1-NE2	5.04	1.37	1.32
1	D	59	ILE	C-O	5.04	1.29	1.24
1	D	54	ASP	CG-OD2	-5.03	1.15	1.25
1	H	563	HIS	CE1-NE2	5.03	1.37	1.32
1	B	470	ALA	C-O	5.01	1.30	1.24

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	440	ASN	CA-CB-CG	8.01	120.61	112.60
1	D	276	LEU	CA-C-N	7.83	127.88	119.90
1	D	276	LEU	C-N-CA	7.83	127.88	119.90
1	E	130	PHE	CA-CB-CG	7.82	121.62	113.80
1	E	476	ARG	O-C-N	-7.47	116.20	121.65
1	B	177	ASP	CA-CB-CG	7.25	119.85	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	432	THR	CA-CB-OG1	-7.06	99.01	109.60
1	A	482	THR	CA-CB-OG1	-6.95	99.17	109.60
1	C	483	PRO	O-C-N	-6.77	118.20	121.31
1	E	455	ARG	NE-CZ-NH1	-6.61	114.89	121.50
1	F	537	GLU	CB-CA-C	6.46	120.88	110.16
1	G	434	GLU	CA-C-O	-6.45	113.48	121.02
1	F	67	ASN	CA-CB-CG	6.43	119.03	112.60
1	H	313	ALA	CA-C-N	6.38	126.06	119.56
1	H	313	ALA	C-N-CA	6.38	126.06	119.56
1	D	100	GLU	O-C-N	-6.26	115.94	121.20
1	B	277	PRO	N-CA-CB	6.22	108.72	103.25
1	G	434	GLU	O-C-N	6.21	129.71	122.20
1	A	227	VAL	CA-C-N	6.20	126.22	119.90
1	A	227	VAL	C-N-CA	6.20	126.22	119.90
1	B	238	LYS	CB-CA-C	6.19	117.60	108.87
1	H	167	SER	CA-C-N	6.15	125.85	119.82
1	H	167	SER	C-N-CA	6.15	125.85	119.82
1	F	289	ASN	CA-CB-CG	6.11	118.71	112.60
1	E	537	GLU	CB-CG-CD	6.10	122.97	112.60
1	F	136	ASN	CA-CB-CG	6.08	118.68	112.60
1	E	295	GLN	N-CA-C	-6.08	104.58	111.14
1	F	421	GLN	CB-CG-CD	-6.04	102.33	112.60
1	F	550	ASP	CA-CB-CG	5.95	118.55	112.60
1	E	550	ASP	CA-CB-CG	5.93	118.53	112.60
1	D	443	ALA	CA-C-N	5.93	129.67	120.60
1	D	443	ALA	C-N-CA	5.93	129.67	120.60
1	H	242	TRP	CA-C-N	5.85	128.40	120.38
1	H	242	TRP	C-N-CA	5.85	128.40	120.38
1	A	382	THR	CA-CB-OG1	-5.85	100.82	109.60
1	C	227	VAL	CA-C-N	5.84	125.85	119.90
1	C	227	VAL	C-N-CA	5.84	125.85	119.90
1	F	100	GLU	O-C-N	-5.83	115.75	121.17
1	F	295	GLN	N-CA-C	-5.83	104.85	111.14
1	A	37	ALA	O-C-N	-5.80	116.62	121.38
1	F	167	SER	CA-C-N	5.80	125.91	119.87
1	F	167	SER	C-N-CA	5.80	125.91	119.87
1	G	141	ALA	O-C-N	-5.79	115.16	121.53
1	H	227	VAL	CA-C-N	5.78	126.11	119.93
1	H	227	VAL	C-N-CA	5.78	126.11	119.93
1	E	152	PHE	O-C-N	-5.76	116.19	121.37
1	A	196	THR	N-CA-C	-5.72	104.95	111.07
1	H	134	LYS	CB-CA-C	5.70	119.22	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	313	ALA	CA-C-N	5.68	125.39	119.82
1	D	313	ALA	C-N-CA	5.68	125.39	119.82
1	E	136	ASN	CA-CB-CG	5.67	118.27	112.60
1	H	289	ASN	CA-CB-CG	5.66	118.26	112.60
1	D	295	GLN	N-CA-C	-5.65	105.04	111.14
1	E	67	ASN	CA-CB-CG	5.65	118.25	112.60
1	A	519	GLN	CA-C-O	-5.64	114.73	121.11
1	E	520	GLU	CB-CG-CD	-5.62	103.04	112.60
1	F	318	LEU	O-C-N	5.60	129.41	123.42
1	A	537	GLU	CB-CG-CD	5.59	122.10	112.60
1	G	67	ASN	CA-CB-CG	5.59	118.19	112.60
1	A	544	GLU	N-CA-C	-5.58	106.36	113.34
1	F	188	LEU	CA-C-O	-5.58	114.50	120.42
1	C	134	LYS	CB-CA-C	5.53	118.70	110.62
1	B	453	LYS	CB-CA-C	5.51	119.53	110.88
1	F	134	LYS	CB-CA-C	5.47	118.88	110.62
1	F	574	VAL	CA-C-O	-5.45	115.02	119.97
1	C	161	ASP	CA-CB-CG	5.42	118.02	112.60
1	D	322	ASP	CA-CB-CG	5.39	117.99	112.60
1	F	161	ASP	CA-CB-CG	5.37	117.97	112.60
1	F	39	LEU	CA-C-N	5.33	125.26	119.78
1	F	39	LEU	C-N-CA	5.33	125.26	119.78
1	H	352	ASN	OD1-CG-ND2	5.32	127.92	122.60
1	F	520	GLU	CB-CA-C	5.31	118.54	109.72
1	E	247	GLY	CA-C-N	5.31	128.13	120.38
1	E	247	GLY	C-N-CA	5.31	128.13	120.38
1	E	371	PHE	CA-CB-CG	5.30	119.11	113.80
1	F	130	PHE	CA-CB-CG	5.30	119.10	113.80
1	F	273	ILE	N-CA-C	-5.30	106.52	111.45
1	E	99	ILE	CA-C-O	-5.30	113.49	119.42
1	D	451	HIS	N-CA-C	-5.28	105.52	111.28
1	B	289	ASN	CA-CB-CG	5.28	117.88	112.60
1	C	377	ASP	CA-CB-CG	5.26	117.86	112.60
1	F	118	ALA	N-CA-C	-5.24	105.48	111.14
1	A	207	GLY	CA-C-O	-5.21	117.23	121.76
1	H	550	ASP	CA-CB-CG	5.20	117.80	112.60
1	G	230	ASP	CA-CB-CG	5.19	117.79	112.60
1	F	136	ASN	OD1-CG-ND2	5.17	127.77	122.60
1	H	67	ASN	CA-CB-CG	5.14	117.74	112.60
1	F	88	ASN	CA-CB-CG	5.13	117.73	112.60
1	H	550	ASP	CA-C-O	-5.13	115.08	120.63
1	C	67	ASN	CA-CB-CG	5.12	117.72	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	90	LEU	CA-C-O	-5.12	114.85	120.43
1	G	120	GLN	N-CA-C	-5.11	105.72	111.28
1	D	238	LYS	CB-CA-C	5.10	116.06	108.87
1	E	245	VAL	CA-C-O	-5.07	115.28	120.71
1	B	150	ALA	N-CA-C	-5.06	105.84	111.36
1	D	99	ILE	CA-C-N	-5.06	116.97	122.59
1	D	99	ILE	C-N-CA	-5.06	116.97	122.59
1	B	436	GLN	N-CA-C	-5.05	105.87	112.23
1	B	374	PHE	CA-CB-CG	-5.04	108.75	113.80
1	G	434	GLU	CB-CA-C	5.01	119.15	110.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	71	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4274	0	4085	10	0
1	B	4219	0	4054	11	0
1	C	4252	0	4085	7	0
1	D	4298	0	4111	11	0
1	E	4321	0	4170	11	0
1	F	4353	0	4183	10	0
1	G	4348	0	4173	16	0
1	H	4296	0	4117	20	0
2	A	21	0	0	0	0
2	B	21	0	0	0	0
2	C	21	0	0	0	0
2	D	21	0	0	0	0
2	E	21	0	0	0	0
2	F	21	0	0	0	0
2	G	21	0	0	0	0
2	H	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	4	0	3	0	0
3	D	4	0	3	0	0
3	F	4	0	3	0	0
3	G	4	0	3	1	0
4	A	4	0	0	0	0
4	B	2	0	0	0	0
4	C	4	0	0	0	0
4	D	5	0	0	0	0
4	E	4	0	0	0	0
4	F	5	0	0	0	0
4	G	4	0	0	0	0
4	H	4	0	0	0	0
5	A	424	0	0	1	0
5	B	482	0	0	2	0
5	C	458	0	0	0	0
5	D	562	0	0	2	0
5	E	542	0	0	2	0
5	F	534	0	0	1	0
5	G	572	0	0	3	0
5	H	404	0	0	4	0
All	All	38555	0	32990	89	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 1.

All (89) 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:H:76:LYS:CE	5:H:879:HOH:O	2.23	0.85
1:G:326[B]:ARG:NH1	5:G:701:HOH:O	2.21	0.73
1:E:326[B]:ARG:HH11	1:E:326[B]:ARG:HG3	1.52	0.72
1:A:76:LYS:CE	5:A:957:HOH:O	2.40	0.69
1:H:543[B]:MET:O	1:H:543[B]:MET:HG3	1.91	0.69
1:B:45:ASN:ND2	1:B:418:TYR:OH	2.26	0.66
1:D:419:GLN:NE2	5:D:802:HOH:O	2.29	0.66
1:E:326[B]:ARG:NH1	5:E:701:HOH:O	2.26	0.66
1:G:432:THR:CB	3:G:601:ACT:H1	2.26	0.65
1:E:326[B]:ARG:HD3	5:E:1102:HOH:O	1.99	0.62
1:A:415:ARG:O	1:A:419:GLN:HG3	2.00	0.62
1:B:105:GLN:HG3	5:B:1148:HOH:O	2.00	0.61
1:H:179:LYS:CD	5:H:774:HOH:O	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:525:LYS:HD2	5:H:1023:HOH:O	2.03	0.58
1:H:169:LEU:CD1	1:H:219:ALA:HA	2.35	0.56
1:G:190:LYS:HG3	1:G:191:ARG:HG2	1.88	0.55
1:F:455[B]:ARG:HD3	5:F:783:HOH:O	2.07	0.54
1:D:99:ILE:O	1:D:106:PHE:HA	2.09	0.52
1:H:99:ILE:O	1:H:106:PHE:HA	2.10	0.52
1:A:548:ASN:HB3	1:B:140:TYR:CZ	2.45	0.51
1:B:460:THR:O	5:B:701:HOH:O	2.19	0.51
1:E:326[B]:ARG:HG3	1:E:326[B]:ARG:NH1	2.24	0.51
1:A:271:LYS:HE3	1:A:315:ASN:O	2.11	0.50
1:F:480:TRP:CG	1:F:481:VAL:H	2.30	0.50
1:A:99:ILE:O	1:A:106:PHE:HA	2.12	0.49
1:B:99:ILE:O	1:B:106:PHE:HA	2.12	0.49
1:H:384:TYR:CD1	1:H:385:PRO:HA	2.47	0.49
1:F:40:PRO:HA	1:F:52:MET:O	2.12	0.49
1:C:140:TYR:CZ	1:H:548:ASN:HB3	2.47	0.49
1:E:326[B]:ARG:NH1	1:E:326[B]:ARG:CG	2.76	0.48
1:G:326[B]:ARG:HD3	5:G:1146:HOH:O	2.13	0.48
1:D:548:ASN:HB3	1:F:140:TYR:CZ	2.49	0.48
1:E:326[B]:ARG:HH11	1:E:326[B]:ARG:CG	2.18	0.48
1:H:525:LYS:CD	5:H:1023:HOH:O	2.61	0.48
1:A:140:TYR:CZ	1:C:548:ASN:HB3	2.49	0.48
1:A:508:ALA:HB3	1:A:558:PHE:CD1	2.49	0.47
1:G:169:LEU:HD13	1:G:219:ALA:HA	1.96	0.47
1:D:508:ALA:HB3	1:D:558:PHE:CD1	2.49	0.47
1:G:99:ILE:O	1:G:106:PHE:HA	2.15	0.46
1:H:271[A]:LYS:HE3	1:H:315:ASN:O	2.15	0.46
1:E:508:ALA:HB3	1:E:558:PHE:CD1	2.51	0.46
1:A:96:TRP:CG	1:A:142:PRO:HD3	2.52	0.46
1:F:99:ILE:O	1:F:106:PHE:HA	2.17	0.45
1:F:367:GLY:HA2	1:F:417[A]:SER:OG	2.16	0.45
1:F:548:ASN:HB3	1:G:140:TYR:CZ	2.52	0.45
1:H:40:PRO:HA	1:H:52:MET:O	2.17	0.45
1:C:421:GLN:NE2	1:C:498:GLN:OE1	2.50	0.44
1:B:508:ALA:HB3	1:B:558:PHE:CD1	2.52	0.44
1:C:134:LYS:HD3	1:C:134:LYS:C	2.43	0.44
1:H:229:ASP:O	1:H:233:GLN:HG3	2.18	0.44
1:G:318:LEU:C	1:G:318:LEU:HD12	2.43	0.44
1:H:157:LYS:HE3	1:H:161:ASP:HB2	2.00	0.44
1:C:384:TYR:CD1	1:C:385:PRO:HA	2.53	0.43
1:C:480:TRP:CG	1:C:481:VAL:H	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:VAL:O	1:D:278:MET:HA	2.17	0.43
1:H:309:TRP:HB3	1:H:319:ILE:HD11	2.00	0.43
1:H:488[A]:THR:O	1:H:488[A]:THR:HG23	2.19	0.43
1:F:543[B]:MET:HE2	1:F:543[B]:MET:HB3	1.86	0.43
1:H:537:GLU:O	1:H:538:LYS:C	2.61	0.43
1:E:342:ASP:OD1	1:E:342:ASP:C	2.61	0.43
1:E:481:VAL:O	1:E:482:THR:C	2.62	0.43
1:G:541:TRP:CE2	1:G:566:ARG:HD3	2.54	0.42
1:B:480:TRP:CG	1:B:481:VAL:H	2.37	0.42
1:D:169:LEU:CD1	1:D:219:ALA:HA	2.50	0.42
1:G:508:ALA:HB3	1:G:558:PHE:CD1	2.54	0.42
1:F:436:GLN:O	1:F:440:ASN:CG	2.63	0.42
1:G:48[B]:LYS:CE	5:G:726:HOH:O	2.67	0.42
1:H:480:TRP:CG	1:H:481:VAL:H	2.37	0.42
1:C:229:ASP:HB3	1:C:233:GLN:NE2	2.35	0.42
1:B:418:TYR:CD2	1:B:419[A]:GLN:HG3	2.55	0.41
1:G:134:LYS:HD3	1:G:134:LYS:C	2.46	0.41
1:B:548:ASN:HB3	1:H:140:TYR:CZ	2.56	0.41
1:F:342:ASP:OD1	1:F:342:ASP:C	2.64	0.41
1:D:480:TRP:CG	1:D:481:VAL:H	2.39	0.41
1:G:169:LEU:HD23	1:G:169:LEU:HA	1.98	0.41
1:D:254:PHE:O	1:D:258:GLN:HG2	2.21	0.41
1:D:366:LYS:NZ	5:D:824:HOH:O	2.54	0.41
1:D:541:TRP:CE2	1:D:566:ARG:HD3	2.56	0.41
1:A:382:THR:OG1	1:A:388:ALA:O	2.30	0.41
1:B:382[B]:THR:OG1	1:B:388:ALA:O	2.35	0.41
1:B:40:PRO:HA	1:B:52:MET:O	2.21	0.40
1:A:361:PHE:CD2	1:A:493:GLY:HA3	2.56	0.40
1:D:140:TYR:CZ	1:E:548:ASN:HB3	2.56	0.40
1:H:488[B]:THR:HA	1:H:489:PRO:HA	1.90	0.40
1:E:271:LYS:HE3	1:E:315:ASN:O	2.21	0.40
1:G:48[A]:LYS:CE	1:G:417[A]:SER:O	2.69	0.40
1:G:169:LEU:CD1	1:G:219:ALA:HA	2.51	0.40
1:G:200:VAL:O	1:G:278:MET:HA	2.20	0.40
1:H:480:TRP:CD1	1:H:481:VAL:H	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	541/550 (98%)	522 (96%)	19 (4%)	0	100	100
1	B	532/550 (97%)	515 (97%)	17 (3%)	0	100	100
1	C	537/550 (98%)	518 (96%)	18 (3%)	1 (0%)	43	22
1	D	545/550 (99%)	526 (96%)	18 (3%)	1 (0%)	43	22
1	E	543/550 (99%)	528 (97%)	15 (3%)	0	100	100
1	F	548/550 (100%)	531 (97%)	16 (3%)	1 (0%)	43	22
1	G	551/550 (100%)	529 (96%)	22 (4%)	0	100	100
1	H	543/550 (99%)	521 (96%)	22 (4%)	0	100	100
All	All	4340/4400 (99%)	4190 (96%)	147 (3%)	3 (0%)	48	24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	442	GLU
1	D	491	ALA
1	F	491	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	437/461 (95%)	434 (99%)	3 (1%)	76	57
1	B	435/461 (94%)	433 (100%)	2 (0%)	81	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	436/461 (95%)	432 (99%)	4 (1%)	70	49
1	D	441/461 (96%)	439 (100%)	2 (0%)	81	66
1	E	448/461 (97%)	447 (100%)	1 (0%)	87	77
1	F	450/461 (98%)	446 (99%)	4 (1%)	70	49
1	G	446/461 (97%)	444 (100%)	2 (0%)	84	71
1	H	441/461 (96%)	434 (98%)	7 (2%)	55	28
All	All	3534/3688 (96%)	3509 (99%)	25 (1%)	76	57

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	173	THR
1	A	437	LYS
1	B	136	ASN
1	B	537	GLU
1	C	76	LYS
1	C	83[A]	GLU
1	C	83[B]	GLU
1	C	136	ASN
1	D	136	ASN
1	D	236	GLN
1	E	136	ASN
1	F	136	ASN
1	F	525	LYS
1	F	537	GLU
1	F	575	GLN
1	G	136	ASN
1	G	419	GLN
1	H	136	ASN
1	H	158	GLU
1	H	173	THR
1	H	190	LYS
1	H	366	LYS
1	H	419	GLN
1	H	525	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	66	ASN
1	A	233	GLN
1	A	275	ASN
1	A	419	GLN
1	B	45	ASN
1	B	46	ASN
1	B	64	GLN
1	B	171	GLN
1	B	201	GLN
1	B	275	ASN
1	B	498	GLN
1	C	64	GLN
1	C	66	ASN
1	C	233	GLN
1	C	275	ASN
1	C	315	ASN
1	C	421	GLN
1	C	451	HIS
1	D	64	GLN
1	D	275	ASN
1	D	354	GLN
1	D	451	HIS
1	E	45	ASN
1	E	64	GLN
1	E	66	ASN
1	E	451	HIS
1	F	64	GLN
1	F	105	GLN
1	F	201	GLN
1	F	275	ASN
1	F	354	GLN
1	F	419	GLN
1	G	64	GLN
1	G	275	ASN
1	G	354	GLN
1	G	421	GLN
1	G	451	HIS
1	H	64	GLN
1	H	275	ASN
1	H	419	GLN
1	H	451	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 44 ligands modelled in this entry, 32 are monoatomic - leaving 12 for Mogul analysis.

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	N0K	B	601	-	21,21,35	1.53	3 (14%)	20,28,49	2.59	4 (20%)
3	ACT	G	601	-	3,3,3	0.50	0	3,3,3	1.20	0
3	ACT	F	602	-	3,3,3	0.98	0	3,3,3	0.99	0
2	N0K	D	701	-	21,21,35	2.22	6 (28%)	20,28,49	3.01	7 (35%)
3	ACT	A	602	-	3,3,3	0.86	0	3,3,3	0.60	0
2	N0K	G	602	-	21,21,35	1.45	3 (14%)	20,28,49	4.00	5 (25%)
3	ACT	D	702	-	3,3,3	1.00	0	3,3,3	1.35	0
2	N0K	C	601	-	21,21,35	1.43	3 (14%)	20,28,49	1.98	4 (20%)
2	N0K	F	601	-	21,21,35	1.41	4 (19%)	20,28,49	2.55	5 (25%)
2	N0K	A	601	-	21,21,35	1.95	3 (14%)	20,28,49	3.73	6 (30%)
2	N0K	E	601	-	21,21,35	1.95	4 (19%)	20,28,49	4.20	2 (10%)
2	N0K	H	601	-	21,21,35	1.84	4 (19%)	20,28,49	4.40	5 (25%)

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	NOK	B	601	-	-	3/14/30/40	0/1/1/3
2	NOK	D	701	-	-	4/14/30/40	0/1/1/3
2	NOK	G	602	-	-	2/14/30/40	0/1/1/3
2	NOK	C	601	-	-	7/14/30/40	0/1/1/3
2	NOK	F	601	-	-	5/14/30/40	0/1/1/3
2	NOK	A	601	-	-	4/14/30/40	0/1/1/3
2	NOK	E	601	-	-	3/14/30/40	0/1/1/3
2	NOK	H	601	-	-	3/14/30/40	0/1/1/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	601	NOK	C7-S1	-6.32	1.61	1.75
2	D	701	NOK	C7-S1	-6.32	1.61	1.75
2	A	601	NOK	C7-S1	-5.98	1.62	1.75
2	E	601	NOK	C7-S1	-5.34	1.63	1.75
2	D	701	NOK	O2-S1	4.87	1.51	1.43
2	C	601	NOK	C7-S1	-4.72	1.64	1.75
2	A	601	NOK	O2-S1	4.67	1.51	1.43
2	B	601	NOK	C7-S1	-4.50	1.65	1.75
2	G	602	NOK	C7-S1	-3.82	1.66	1.75
2	E	601	NOK	C8-C5	-3.61	1.46	1.52
2	D	701	NOK	C4-N7	3.09	1.53	1.47
2	G	602	NOK	C8-C5	2.97	1.57	1.52
2	D	701	NOK	O4-S1	-2.94	1.38	1.43
2	H	601	NOK	C3-C4	-2.93	1.49	1.54
2	F	601	NOK	C7-S1	-2.89	1.69	1.75
2	F	601	NOK	C5-C6	-2.74	1.49	1.53
2	F	601	NOK	C5-C4	2.64	1.58	1.54
2	E	601	NOK	S1-N21	2.55	1.65	1.60
2	H	601	NOK	C2-C6	-2.51	1.49	1.53
2	E	601	NOK	O2-S1	-2.36	1.39	1.43
2	C	601	NOK	C16-C17	2.33	1.63	1.51
2	B	601	NOK	C3-C4	-2.28	1.50	1.54
2	C	601	NOK	C3-C4	2.26	1.58	1.54
2	D	701	NOK	C5-C4	2.25	1.57	1.54
2	B	601	NOK	C4-N7	2.17	1.52	1.47
2	F	601	NOK	C2-C6	-2.17	1.50	1.53
2	A	601	NOK	C2-C6	-2.16	1.50	1.53
2	H	601	NOK	C5-C6	-2.16	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	602	N0K	C4-N7	2.12	1.51	1.47
2	D	701	N0K	C5-C6	-2.09	1.50	1.53

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	601	N0K	C7-S1-N21	17.92	119.53	107.82
2	E	601	N0K	C7-S1-N21	17.47	119.24	107.82
2	G	602	N0K	C7-S1-N21	16.06	118.32	107.82
2	A	601	N0K	O2-S1-O4	-11.30	103.73	118.87
2	D	701	N0K	C7-S1-N21	10.70	114.81	107.82
2	B	601	N0K	C7-S1-N21	8.45	113.34	107.82
2	F	601	N0K	C7-S1-N21	8.44	113.34	107.82
2	A	601	N0K	C7-S1-N21	-6.71	103.43	107.82
2	B	601	N0K	O2-S1-O4	-6.69	109.91	118.87
2	C	601	N0K	C7-S1-N21	6.57	112.12	107.82
2	A	601	N0K	O2-S1-N21	6.57	116.48	107.33
2	E	601	N0K	O4-S1-N21	-5.62	99.50	107.33
2	A	601	N0K	O4-S1-C7	5.52	116.99	108.26
2	H	601	N0K	O2-S1-O4	-5.15	111.97	118.87
2	G	602	N0K	O2-S1-O4	-5.11	112.02	118.87
2	F	601	N0K	O2-S1-N21	-4.42	101.18	107.33
2	D	701	N0K	O2-S1-O4	-4.16	113.29	118.87
2	G	602	N0K	C15-N7-C4	-3.68	108.68	114.05
2	C	601	N0K	O4-S1-N21	3.03	111.56	107.33
2	H	601	N0K	O4-S1-N21	-2.94	103.24	107.33
2	C	601	N0K	O2-S1-O4	-2.81	115.11	118.87
2	D	701	N0K	O4-S1-C7	2.81	112.70	108.26
2	D	701	N0K	C15-N7-C4	-2.78	109.99	114.05
2	F	601	N0K	O2-S1-C7	2.65	112.45	108.26
2	H	601	N0K	O2-S1-N21	-2.44	103.93	107.33
2	F	601	N0K	C15-N7-C4	-2.44	110.49	114.05
2	G	602	N0K	C5-C4-N7	2.43	117.40	113.53
2	D	701	N0K	C19-C20-N21	2.28	115.80	111.03
2	F	601	N0K	C5-C4-N7	2.26	117.13	113.53
2	A	601	N0K	C15-N7-C4	-2.26	110.76	114.05
2	C	601	N0K	O2-S1-C7	-2.24	104.71	108.26
2	H	601	N0K	O4-S1-C7	2.22	111.77	108.26
2	B	601	N0K	C15-N7-C4	-2.22	110.82	114.05
2	D	701	N0K	O9-C8-C5	-2.15	106.16	111.22
2	G	602	N0K	O4-S1-N21	-2.13	104.36	107.33
2	A	601	N0K	C19-C20-N21	-2.10	106.63	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	N0K	O2-S1-C7	-2.09	104.95	108.26
2	B	601	N0K	O11-C2-C3	2.07	118.06	110.88

There are no chirality outliers.

All (31) torsion outliers are listed below:

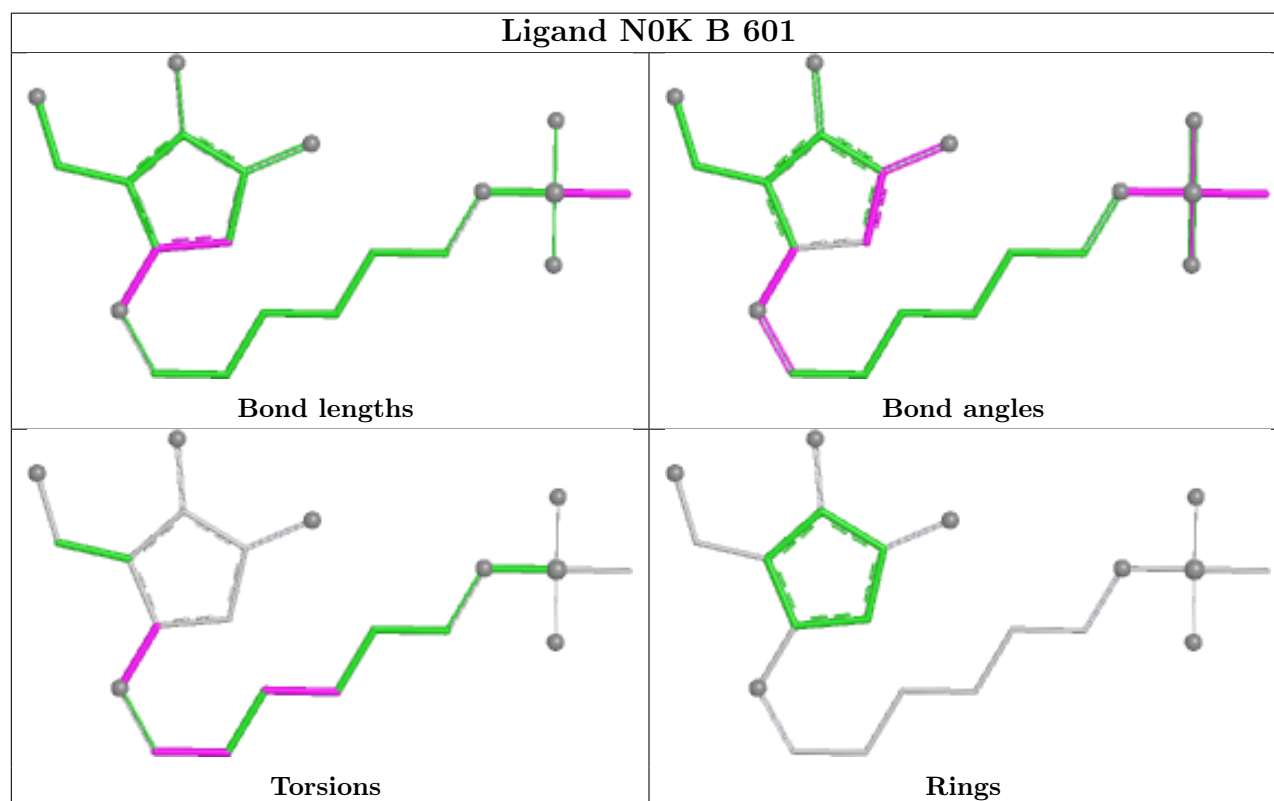
Mol	Chain	Res	Type	Atoms
2	A	601	N0K	C20-N21-S1-C7
2	A	601	N0K	C18-C19-C20-N21
2	C	601	N0K	C20-N21-S1-C7
2	C	601	N0K	C20-N21-S1-O2
2	C	601	N0K	C18-C19-C20-N21
2	D	701	N0K	C3-C4-N7-C15
2	E	601	N0K	C18-C19-C20-N21
2	D	701	N0K	N7-C15-C16-C17
2	H	601	N0K	C15-C16-C17-C18
2	F	601	N0K	N7-C15-C16-C17
2	F	601	N0K	C17-C18-C19-C20
2	A	601	N0K	C16-C17-C18-C19
2	H	601	N0K	C17-C18-C19-C20
2	B	601	N0K	N7-C15-C16-C17
2	F	601	N0K	C18-C19-C20-N21
2	A	601	N0K	C17-C18-C19-C20
2	F	601	N0K	C16-C17-C18-C19
2	D	701	N0K	C16-C17-C18-C19
2	B	601	N0K	C3-C4-N7-C15
2	C	601	N0K	C3-C4-N7-C15
2	E	601	N0K	C3-C4-N7-C15
2	F	601	N0K	C3-C4-N7-C15
2	G	602	N0K	C3-C4-N7-C15
2	H	601	N0K	C3-C4-N7-C15
2	C	601	N0K	C20-N21-S1-O4
2	C	601	N0K	C17-C18-C19-C20
2	E	601	N0K	C16-C17-C18-C19
2	G	602	N0K	C15-C16-C17-C18
2	B	601	N0K	C16-C17-C18-C19
2	D	701	N0K	C15-C16-C17-C18
2	C	601	N0K	C15-C16-C17-C18

There are no ring outliers.

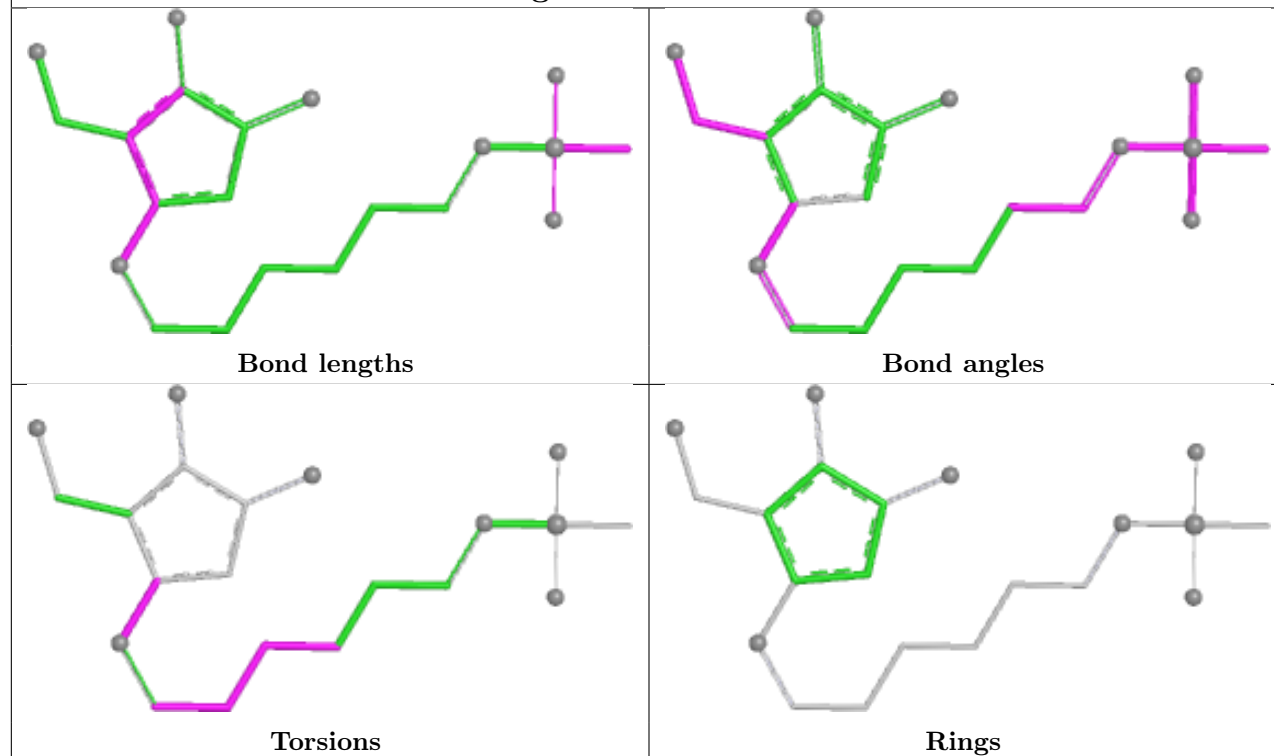
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	601	ACT	1	0

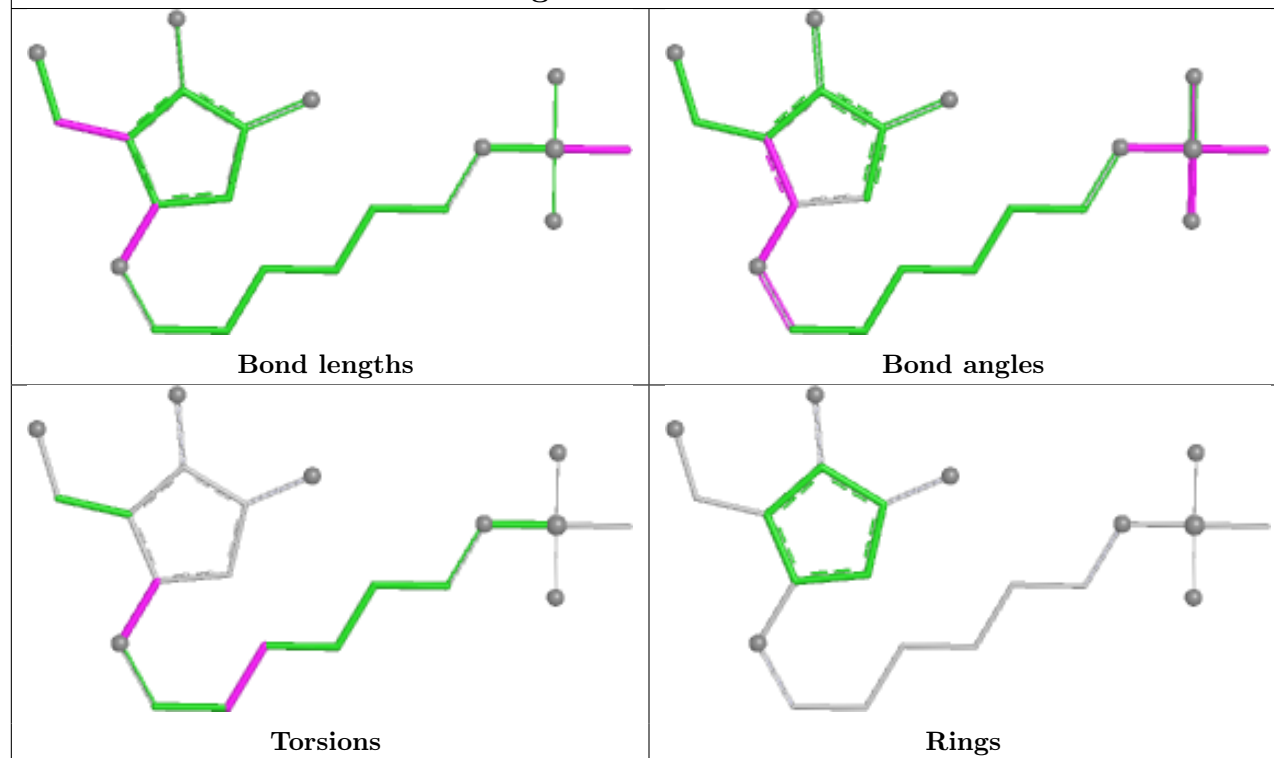
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



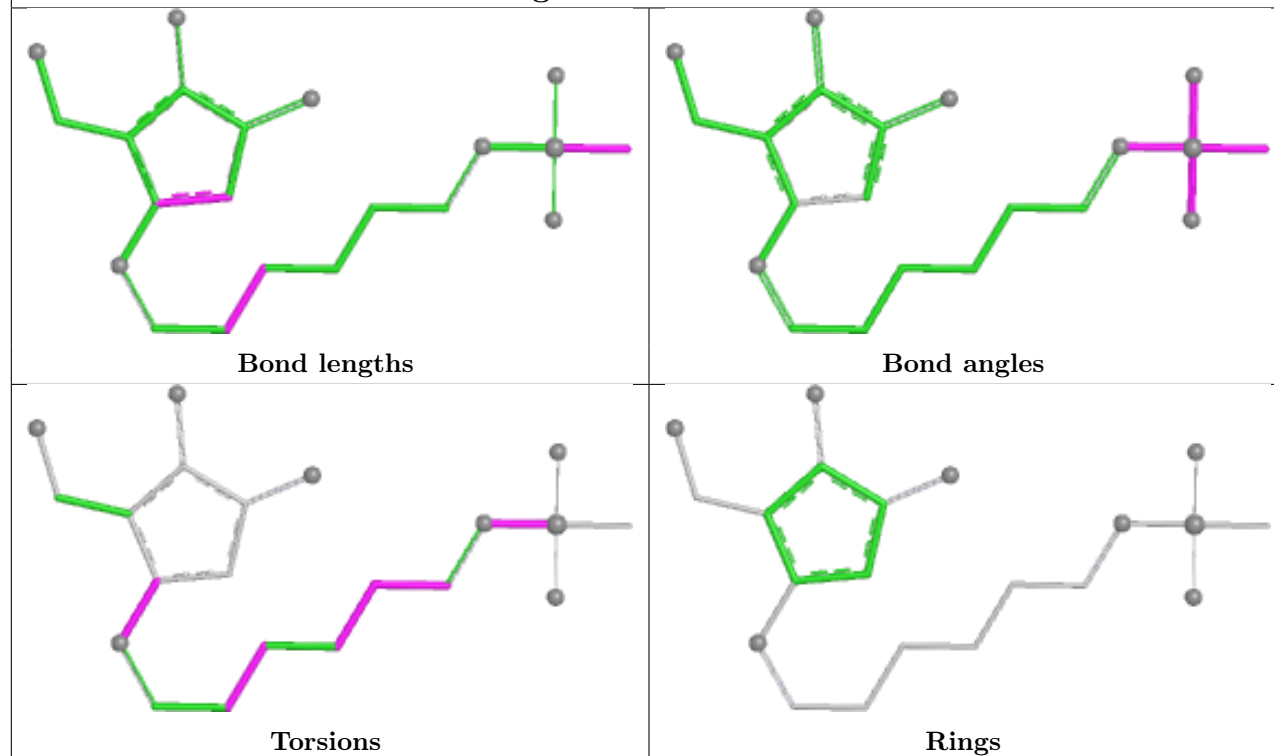
Ligand N0K D 701



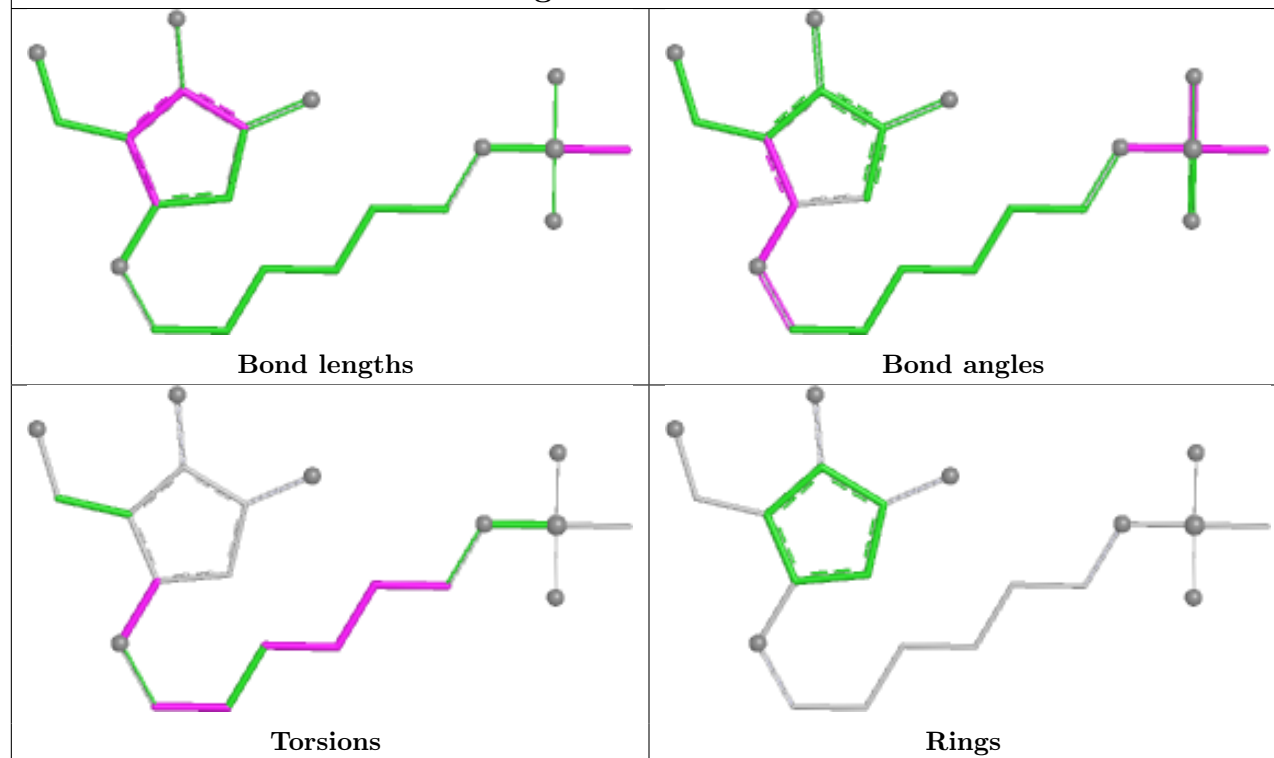
Ligand N0K G 602



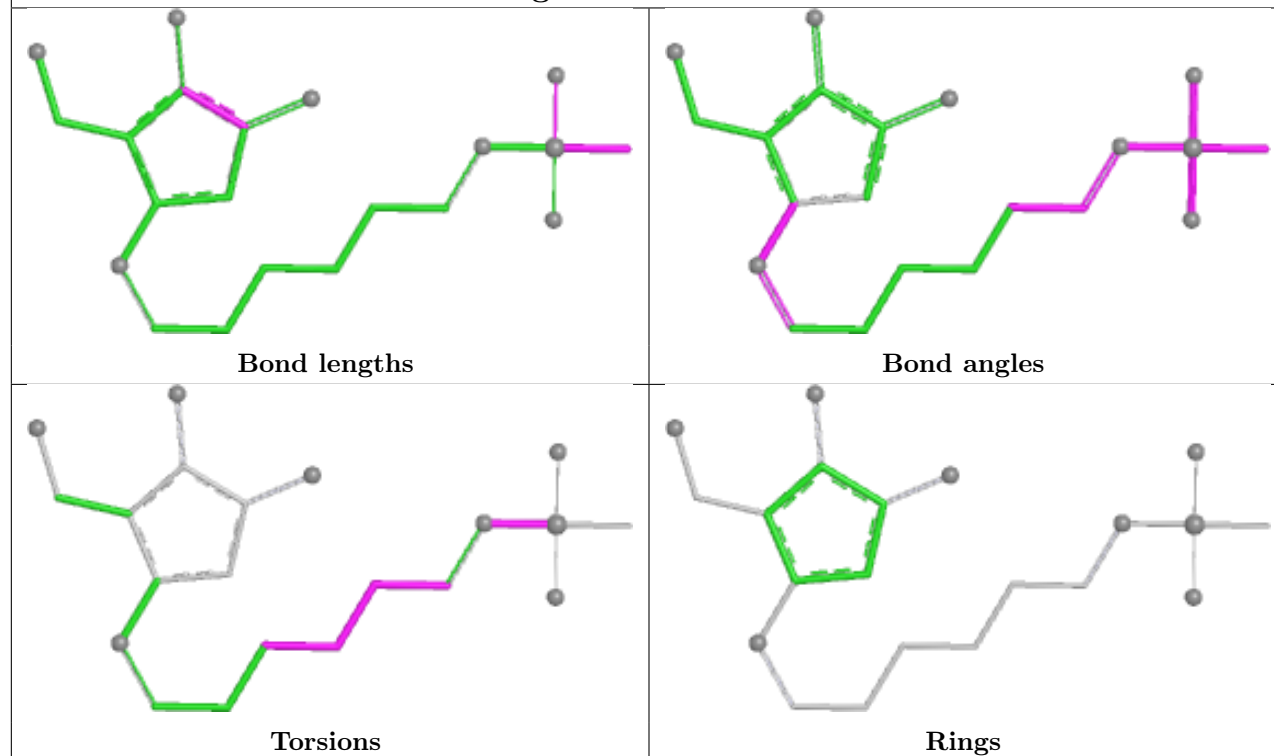
Ligand N0K C 601



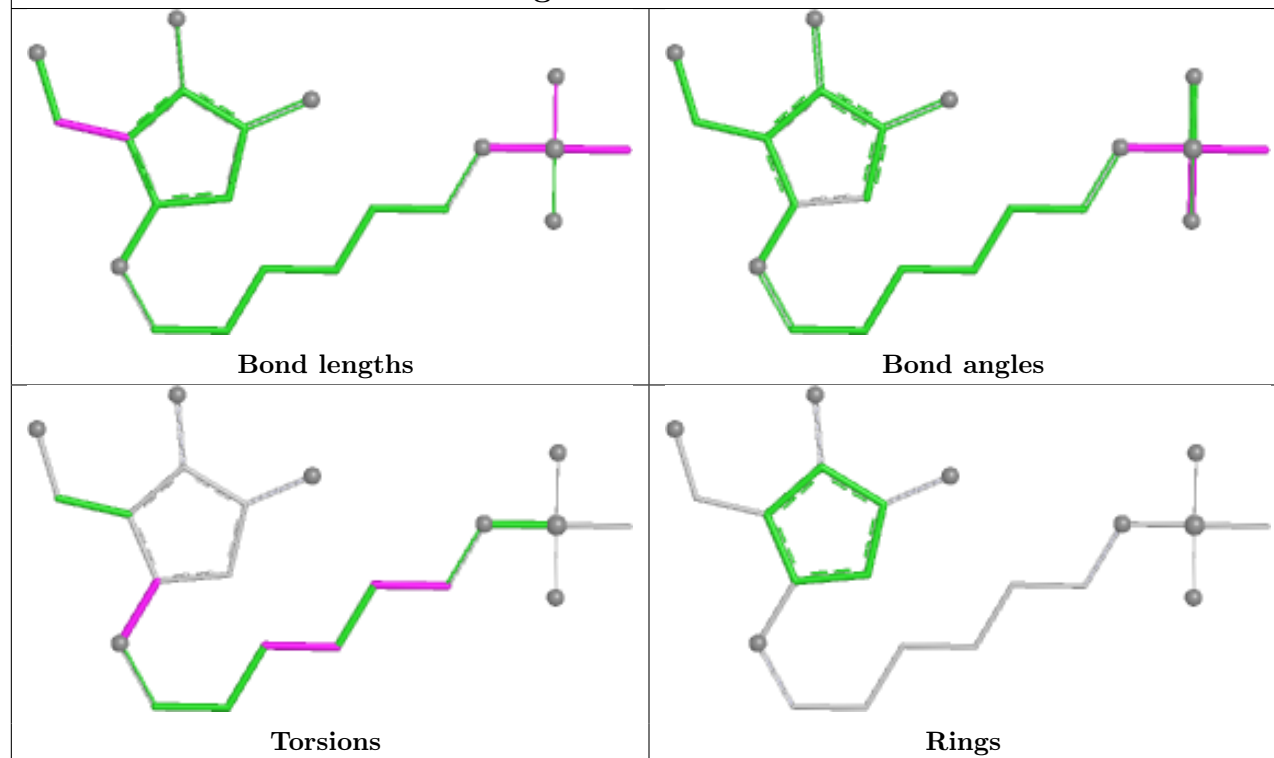
Ligand N0K F 601

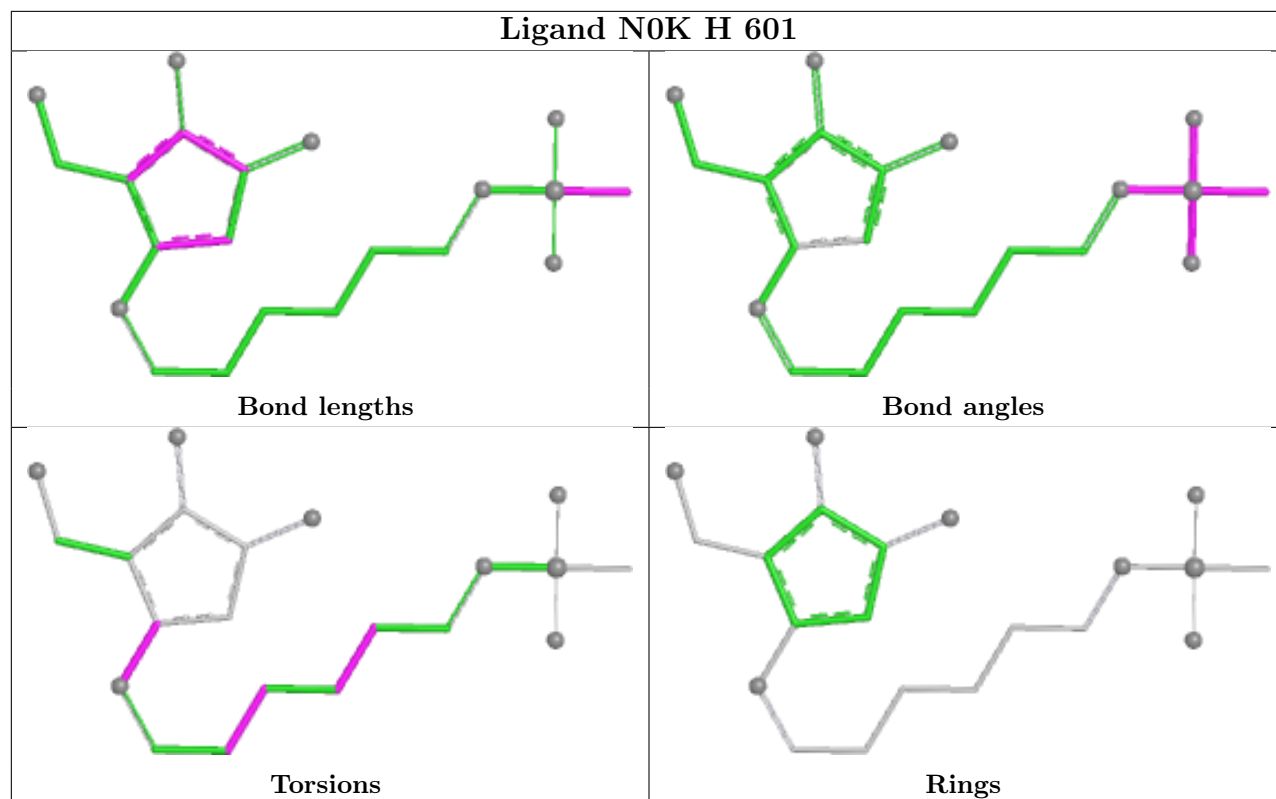


Ligand N0K A 601



Ligand N0K E 601





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	539/550 (98%)	-0.07	23 (4%)	40 44	10, 23, 39, 62	50 (9%)
1	B	530/550 (96%)	-0.26	11 (2%)	63 67	12, 22, 35, 55	25 (4%)
1	C	533/550 (96%)	-0.19	11 (2%)	63 67	9, 23, 38, 64	33 (6%)
1	D	539/550 (98%)	-0.46	7 (1%)	75 78	8, 19, 36, 66	33 (6%)
1	E	538/550 (97%)	-0.42	7 (1%)	75 78	8, 20, 37, 52	38 (7%)
1	F	536/550 (97%)	-0.39	9 (1%)	69 72	7, 20, 38, 55	42 (7%)
1	G	540/550 (98%)	-0.34	16 (2%)	52 56	8, 19, 34, 55	43 (7%)
1	H	534/550 (97%)	-0.08	15 (2%)	55 59	10, 25, 39, 75	52 (9%)
All	All	4289/4400 (97%)	-0.28	99 (2%)	61 65	7, 21, 37, 75	316 (7%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	438	ILE	12.0
1	C	441	ALA	11.0
1	C	433	THR	10.3
1	F	444	THR	10.0
1	G	438	ILE	9.6
1	A	36	ALA	9.5
1	H	444	THR	9.4
1	E	444	THR	9.3
1	G	435	THR	9.2
1	A	441	ALA	8.9
1	G	441	ALA	8.9
1	G	439	TRP	8.9
1	C	444	THR	8.7
1	C	443	ALA	8.4
1	F	438	ILE	8.4
1	C	445	PRO	7.8

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Mol	Chain	Res	Type	RSRZ
1	G	443	ALA	7.8
1	B	521	LEU	7.7
1	B	435	THR	7.5
1	B	36	ALA	7.5
1	F	439	TRP	7.3
1	E	443	ALA	7.2
1	B	522	ALA	7.2
1	G	36	ALA	7.0
1	B	437	LYS	7.0
1	C	36	ALA	6.7
1	G	444	THR	6.1
1	H	445	PRO	6.0
1	C	446	GLU	6.0
1	H	435	THR	5.9
1	A	435	THR	5.8
1	C	521	LEU	5.7
1	G	442	GLU	5.6
1	A	443	ALA	5.6
1	D	36	ALA	5.6
1	G	440	ASN	5.5
1	B	434	GLU	5.4
1	A	436	GLN	5.4
1	E	442	GLU	5.3
1	G	437	LYS	5.3
1	H	434	GLU	5.2
1	G	434	GLU	4.9
1	H	575	GLN	4.7
1	E	439	TRP	4.7
1	A	437	LYS	4.6
1	E	480	TRP	4.6
1	H	437	LYS	4.3
1	A	442	GLU	4.3
1	H	436	GLN	4.0
1	B	523	GLY	3.9
1	B	575	GLN	3.9
1	H	480	TRP	3.8
1	A	237	LEU	3.7
1	F	445	PRO	3.6
1	A	521	LEU	3.6
1	C	447	GLU	3.6
1	A	445	PRO	3.5
1	A	523	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	480	TRP	3.4
1	A	439	TRP	3.3
1	F	575	GLN	3.3
1	H	237	LEU	3.2
1	A	444	THR	3.1
1	D	445	PRO	3.1
1	C	522	ALA	3.1
1	E	438	ILE	3.0
1	D	480	TRP	3.0
1	F	480	TRP	3.0
1	B	448	LYS	2.9
1	G	480	TRP	2.8
1	B	436	GLN	2.8
1	A	434	GLU	2.7
1	H	521	LEU	2.7
1	G	523	GLY	2.6
1	A	433	THR	2.6
1	G	575	GLN	2.6
1	G	445	PRO	2.6
1	C	480	TRP	2.6
1	A	446	GLU	2.6
1	F	440	ASN	2.5
1	A	236	GLN	2.5
1	A	575	GLN	2.5
1	D	444	THR	2.5
1	A	480	TRP	2.4
1	A	224	ASN	2.4
1	D	435	THR	2.3
1	E	440	ASN	2.3
1	H	238	LYS	2.3
1	H	447	GLU	2.3
1	A	232	ILE	2.2
1	H	46	ASN	2.1
1	D	438	ILE	2.1
1	G	229[A]	ASP	2.1
1	D	439	TRP	2.1
1	H	523	GLY	2.1
1	A	46	ASN	2.1
1	A	239	PRO	2.1
1	F	435	THR	2.0
1	F	46	ASN	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	ACT	D	702	4/4	0.81	0.20	21,22,23,23	4
3	ACT	G	601	4/4	0.91	0.14	31,35,36,36	4
3	ACT	A	602	4/4	0.92	0.12	22,22,23,24	4
3	ACT	F	602	4/4	0.96	0.12	15,17,21,21	4
4	NA	C	602	1/1	0.96	0.12	37,37,37,37	0
2	N0K	B	601	21/33	0.97	0.08	18,20,34,35	7
2	N0K	C	601	21/33	0.97	0.09	18,21,33,34	10
2	N0K	D	701	21/33	0.97	0.09	15,17,30,36	7
2	N0K	G	602	21/33	0.97	0.08	15,18,33,41	7
4	NA	A	604	1/1	0.97	0.10	39,39,39,39	0
2	N0K	H	601	21/33	0.97	0.08	18,22,32,36	8
4	NA	F	603	1/1	0.97	0.10	31,31,31,31	0
4	NA	H	605	1/1	0.97	0.06	42,42,42,42	0
4	NA	B	603	1/1	0.98	0.09	29,29,29,29	0
2	N0K	E	601	21/33	0.98	0.07	15,18,32,34	8
4	NA	D	707	1/1	0.98	0.08	31,31,31,31	0
2	N0K	F	601	21/33	0.98	0.07	16,17,34,41	7
4	NA	G	603	1/1	0.98	0.14	34,34,34,34	0
4	NA	G	606	1/1	0.98	0.07	29,29,29,29	0
4	NA	H	603	1/1	0.98	0.06	36,36,36,36	0
2	N0K	A	601	21/33	0.98	0.07	17,20,31,33	8
4	NA	D	703	1/1	0.99	0.06	24,24,24,24	0
4	NA	D	706	1/1	0.99	0.07	25,25,25,25	0
4	NA	A	606	1/1	0.99	0.04	35,35,35,35	0
4	NA	E	605	1/1	0.99	0.08	24,24,24,24	0
4	NA	B	602	1/1	0.99	0.09	35,35,35,35	0
4	NA	F	604	1/1	0.99	0.04	29,29,29,29	0

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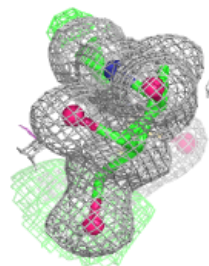
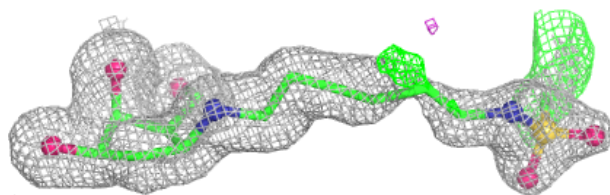
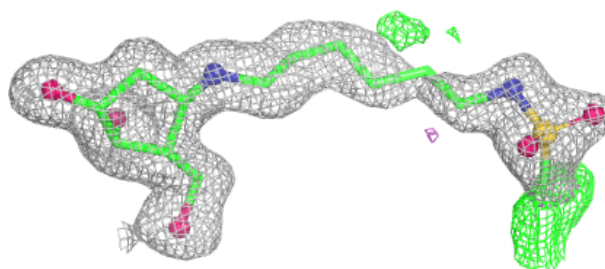
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	F	606	1/1	0.99	0.05	24,24,24,24	0
4	NA	F	607	1/1	0.99	0.03	32,32,32,32	0
4	NA	A	603	1/1	0.99	0.10	32,32,32,32	0
4	NA	A	605	1/1	0.99	0.04	28,28,28,28	0
4	NA	H	602	1/1	0.99	0.03	28,28,28,28	0
4	NA	C	604	1/1	0.99	0.06	31,31,31,31	0
4	NA	H	604	1/1	0.99	0.04	35,35,35,35	0
4	NA	C	605	1/1	0.99	0.09	42,42,42,42	0
4	NA	E	603	1/1	1.00	0.02	22,22,22,22	0
4	NA	E	604	1/1	1.00	0.03	25,25,25,25	0
4	NA	G	604	1/1	1.00	0.04	26,26,26,26	0
4	NA	G	605	1/1	1.00	0.06	24,24,24,24	0
4	NA	D	705	1/1	1.00	0.04	22,22,22,22	0
4	NA	C	603	1/1	1.00	0.06	26,26,26,26	0
4	NA	D	704	1/1	1.00	0.05	25,25,25,25	0
4	NA	F	605	1/1	1.00	0.06	23,23,23,23	0
4	NA	E	602	1/1	1.00	0.02	25,25,25,25	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.

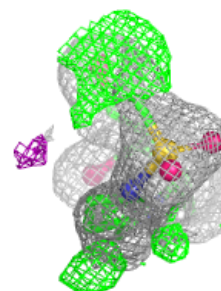
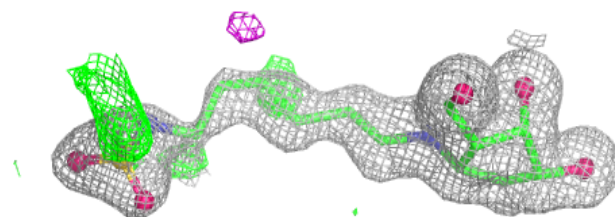
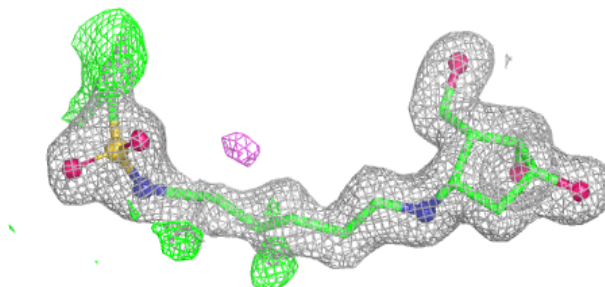
Electron density around N0K B 601:

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

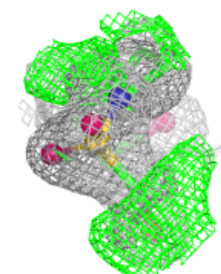
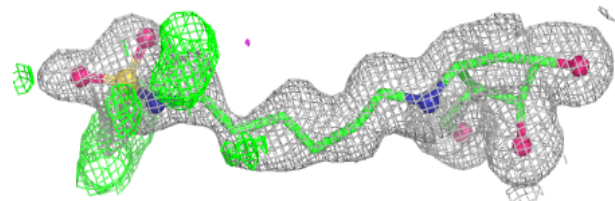
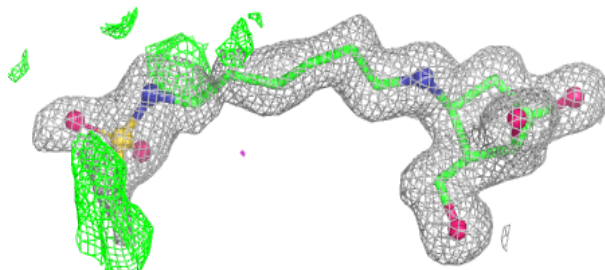


Electron density around N0K C 601:

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

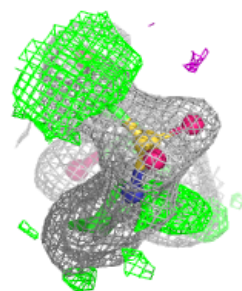
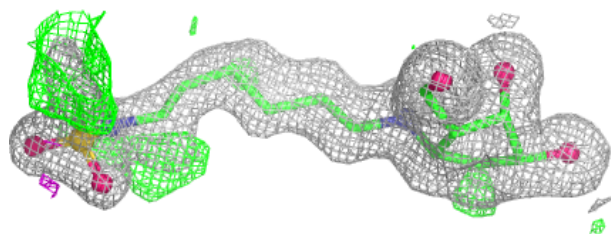
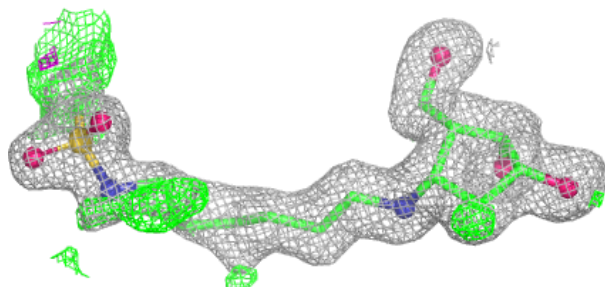
**Electron density around N0K D 701:**

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

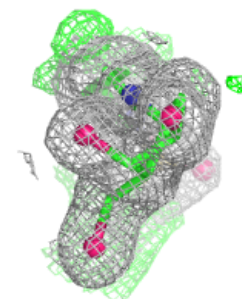
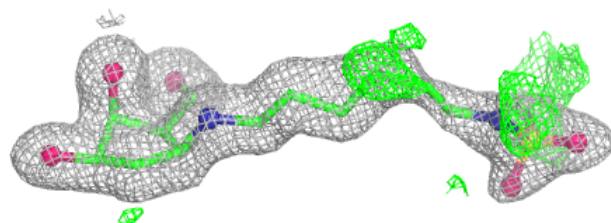
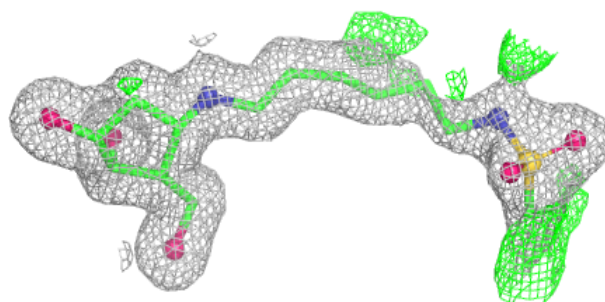


Electron density around N0K G 602:

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

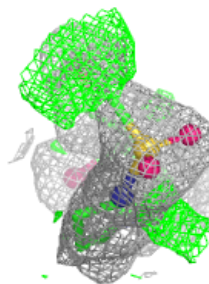
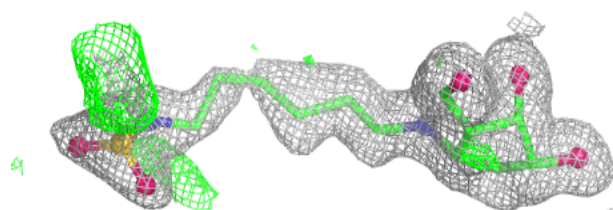
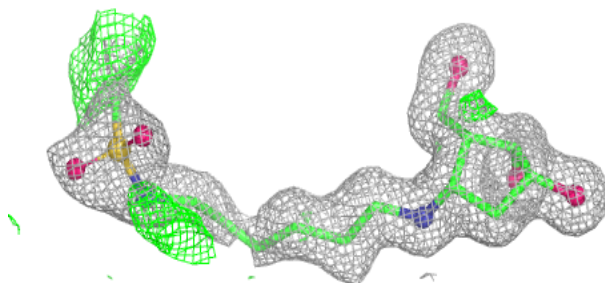
**Electron density around N0K H 601:**

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

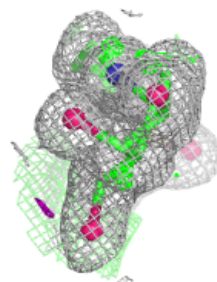
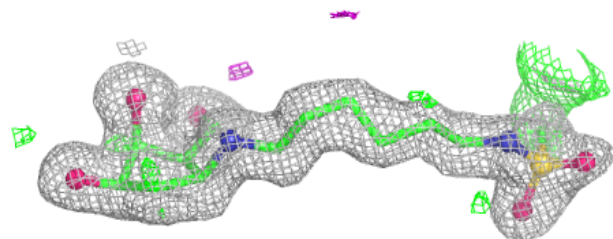
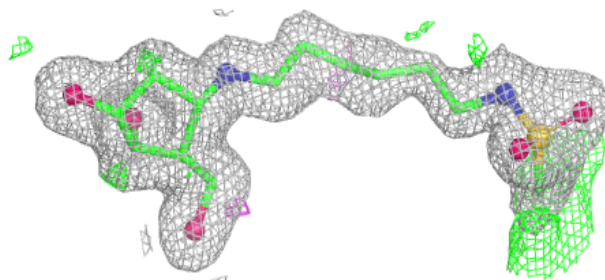


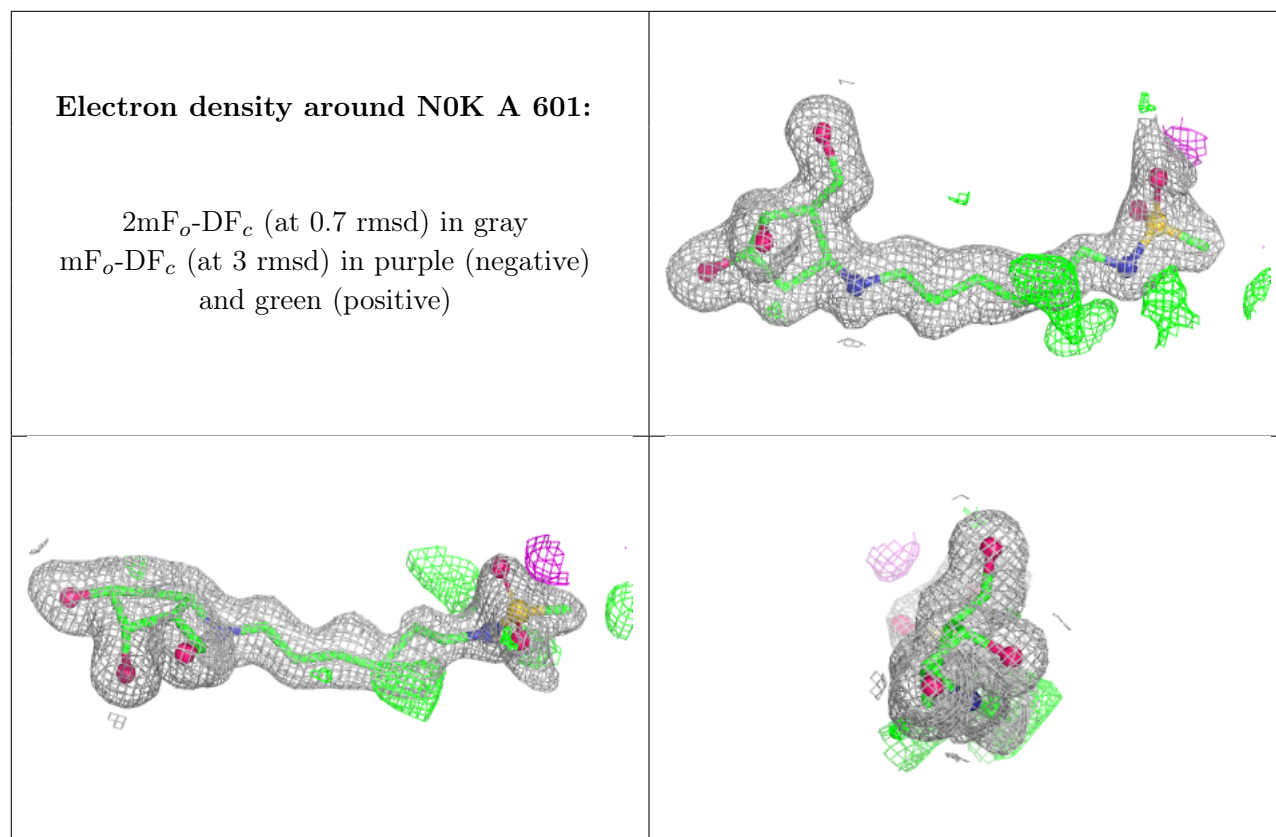
Electron density around N0K E 601:

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

**Electron density around N0K F 601:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.