



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:24 PM UTC

PDB ID : 9EU3 / pdb_00009eu3
Title : GH29A alpha-L-fucosidase
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Deposited on : 2024-03-27
Resolution : 2.28 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

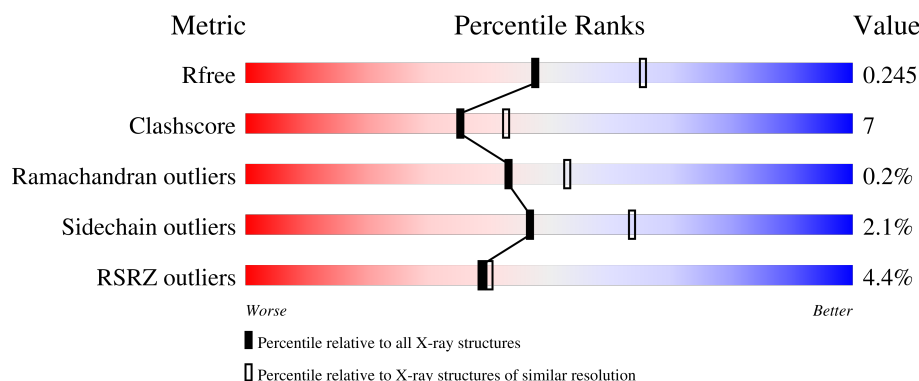
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	435	0% 86% 10% ..
1	B	435	3% 86% 10% ..
1	C	435	6% 77% 16% ...
1	D	435	7% 83% 11% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	A	503	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27486 atoms, of which 13334 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 Alpha-L-fucosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	422	Total	C	H	N	O	S	0	4	0
			6740	2182	3324	586	633	15			
1	B	422	Total	C	H	N	O	S	0	4	0
			6740	2182	3324	586	633	15			
1	C	422	Total	C	H	N	O	S	0	2	0
			6728	2179	3318	585	631	15			
1	D	422	Total	C	H	N	O	S	0	4	0
			6740	2182	3324	586	633	15			

There are 36 discrepancies between the modelled and reference sequences:

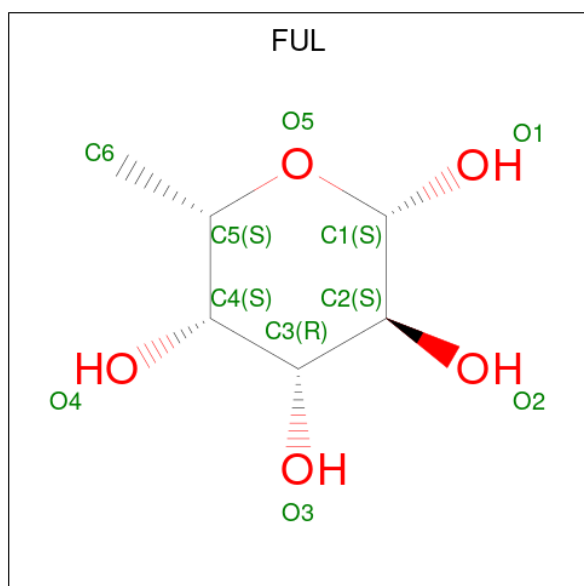
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP G8UMQ6
A	447	LEU	-	expression tag	UNP G8UMQ6
A	448	GLU	-	expression tag	UNP G8UMQ6
A	449	HIS	-	expression tag	UNP G8UMQ6
A	450	HIS	-	expression tag	UNP G8UMQ6
A	451	HIS	-	expression tag	UNP G8UMQ6
A	452	HIS	-	expression tag	UNP G8UMQ6
A	453	HIS	-	expression tag	UNP G8UMQ6
A	454	HIS	-	expression tag	UNP G8UMQ6
B	20	MET	-	initiating methionine	UNP G8UMQ6
B	447	LEU	-	expression tag	UNP G8UMQ6
B	448	GLU	-	expression tag	UNP G8UMQ6
B	449	HIS	-	expression tag	UNP G8UMQ6
B	450	HIS	-	expression tag	UNP G8UMQ6
B	451	HIS	-	expression tag	UNP G8UMQ6
B	452	HIS	-	expression tag	UNP G8UMQ6
B	453	HIS	-	expression tag	UNP G8UMQ6
B	454	HIS	-	expression tag	UNP G8UMQ6
C	20	MET	-	initiating methionine	UNP G8UMQ6
C	447	LEU	-	expression tag	UNP G8UMQ6
C	448	GLU	-	expression tag	UNP G8UMQ6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	449	HIS	-	expression tag	UNP G8UMQ6
C	450	HIS	-	expression tag	UNP G8UMQ6
C	451	HIS	-	expression tag	UNP G8UMQ6
C	452	HIS	-	expression tag	UNP G8UMQ6
C	453	HIS	-	expression tag	UNP G8UMQ6
C	454	HIS	-	expression tag	UNP G8UMQ6
D	20	MET	-	initiating methionine	UNP G8UMQ6
D	447	LEU	-	expression tag	UNP G8UMQ6
D	448	GLU	-	expression tag	UNP G8UMQ6
D	449	HIS	-	expression tag	UNP G8UMQ6
D	450	HIS	-	expression tag	UNP G8UMQ6
D	451	HIS	-	expression tag	UNP G8UMQ6
D	452	HIS	-	expression tag	UNP G8UMQ6
D	453	HIS	-	expression tag	UNP G8UMQ6
D	454	HIS	-	expression tag	UNP G8UMQ6

- Molecule 2 is beta-L-fucopyranose (CCD ID: FUL) (formula: C₆H₁₂O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			22	6	11	5		
2	B	1	Total	C	H	O	0	0
			22	6	11	5		
2	C	1	Total	C	H	O	0	0
			22	6	11	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	H	O	0	0
			22	6	11	5		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

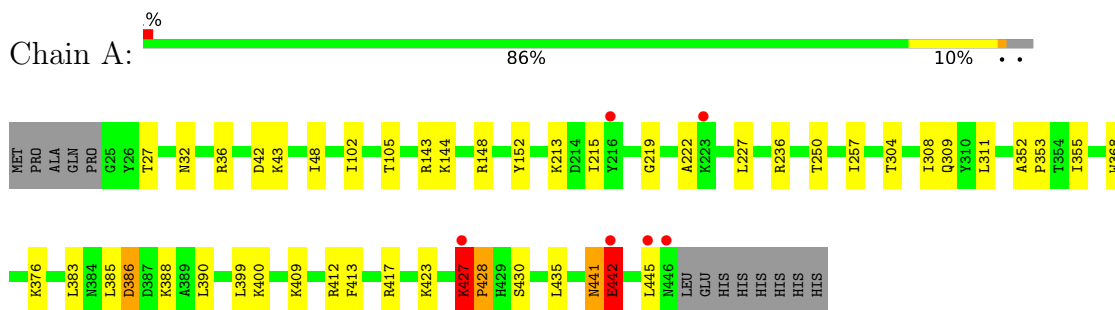
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	151	Total	O	0	0
			151	151		
5	B	80	Total	O	0	0
			80	80		
5	C	113	Total	O	0	0
			113	113		
5	D	103	Total	O	0	0
			103	103		

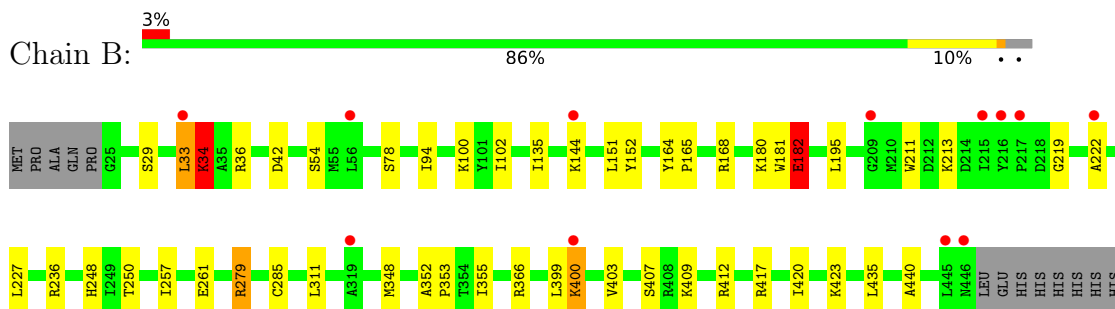
3 Residue-property plots [i](#)

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.

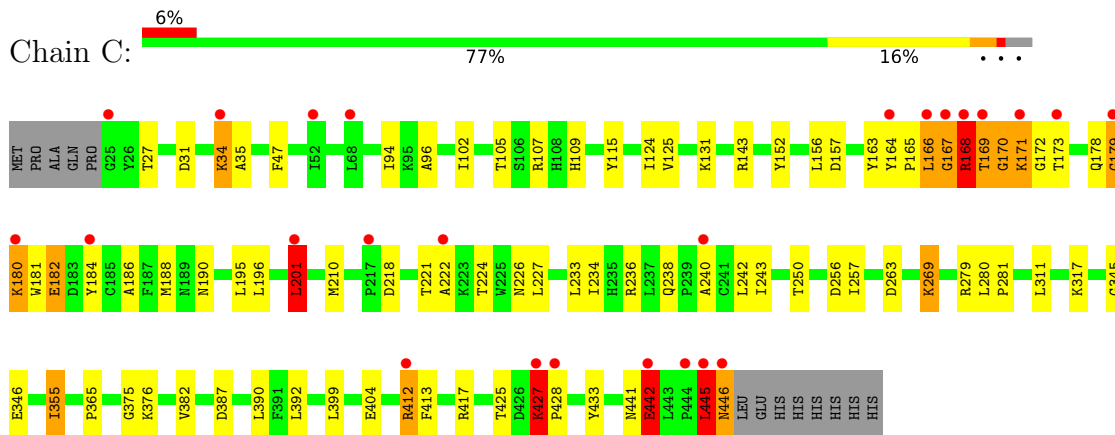
- Molecule 1: Alpha-L-fucosidase



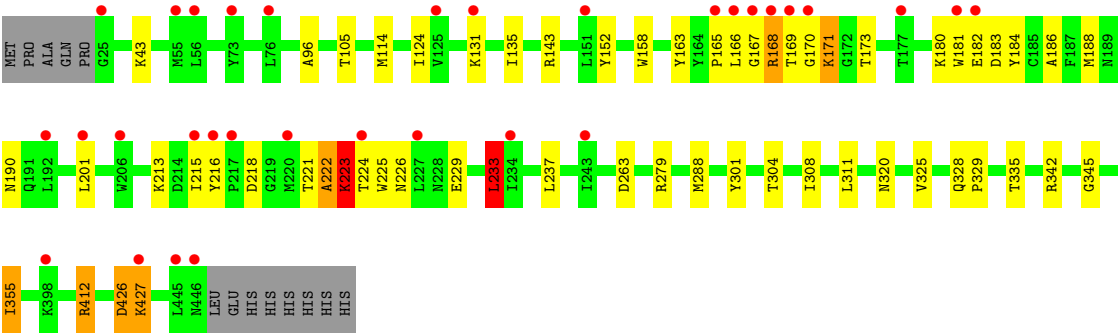
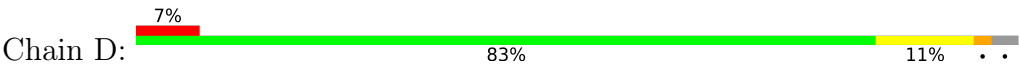
- Molecule 1: Alpha-L-fucosidase



- Molecule 1: Alpha-L-fucosidase



- Molecule 1: Alpha-L-fucosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.87Å 146.87Å 196.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	58.28 – 2.28 58.28 – 2.28	Depositor EDS
% Data completeness (in resolution range)	90.2 (58.28-2.28) 97.6 (58.28-2.28)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.212 , 0.243 0.214 , 0.245	Depositor DCC
R_{free} test set	5786 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	27486	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.35 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.5493e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: FUL, ZN, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.32	3/3524 (0.1%)	0.63	11/4779 (0.2%)
1	B	0.38	5/3524 (0.1%)	0.67	10/4779 (0.2%)
1	C	0.77	15/3510 (0.4%)	1.12	42/4761 (0.9%)
1	D	0.58	10/3524 (0.3%)	0.82	25/4779 (0.5%)
All	All	0.54	33/14082 (0.2%)	0.83	88/19098 (0.5%)

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	6
1	B	0	5
1	C	0	10
1	D	0	8
All	All	0	29

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	180	LYS	CE-NZ	20.85	2.12	1.49
1	C	180	LYS	CD-CE	15.69	1.99	1.52
1	D	426	ASP	C-N	-12.28	1.21	1.33
1	C	182	GLU	CD-OE2	11.85	1.47	1.25
1	D	182	GLU	CD-OE2	11.37	1.47	1.25
1	D	182	GLU	CD-OE1	9.82	1.44	1.25
1	C	201	LEU	CG-CD1	9.04	1.82	1.52
1	C	180	LYS	CB-CG	8.73	1.78	1.52
1	C	182	GLU	CD-OE1	8.25	1.41	1.25
1	C	201	LEU	CG-CD2	8.00	1.78	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	269	LYS	CE-NZ	7.94	1.73	1.49
1	C	180	LYS	CG-CD	7.89	1.76	1.52
1	B	34	LYS	CE-NZ	7.79	1.72	1.49
1	C	168	ARG	CB-CG	7.78	1.75	1.52
1	D	223	LYS	CD-CE	7.72	1.75	1.52
1	C	166	LEU	CG-CD2	7.51	1.77	1.52
1	D	131	LYS	CB-CG	7.31	1.74	1.52
1	C	171	LYS	CB-CG	6.91	1.73	1.52
1	D	131	LYS	CD-CE	6.82	1.73	1.52
1	A	427	LYS	CD-CE	6.67	1.72	1.52
1	C	166	LEU	CG-CD1	6.63	1.74	1.52
1	B	144	LYS	CD-CE	6.56	1.72	1.52
1	D	131	LYS	CG-CD	6.48	1.71	1.52
1	C	269	LYS	CB-CG	6.42	1.71	1.52
1	C	171	LYS	CE-NZ	6.33	1.68	1.49
1	A	215	ILE	C-N	6.33	1.51	1.33
1	B	182	GLU	CD-OE1	6.27	1.37	1.25
1	B	144	LYS	CB-CG	-5.67	1.35	1.52
1	D	182	GLU	CG-CD	5.41	1.65	1.52
1	A	427	LYS	CE-NZ	5.38	1.65	1.49
1	B	144	LYS	CE-NZ	5.35	1.65	1.49
1	D	223	LYS	CG-CD	5.32	1.68	1.52
1	D	171	LYS	CE-NZ	5.18	1.64	1.49

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	182	GLU	CG-CD-OE1	21.81	168.57	118.40
1	C	182	GLU	CG-CD-OE2	-21.77	68.33	118.40
1	B	34	LYS	CA-CB-CG	15.84	145.78	114.10
1	B	144	LYS	CA-CB-CG	15.52	145.14	114.10
1	C	180	LYS	CD-CE-NZ	15.01	159.94	111.90
1	C	182	GLU	CA-CB-CG	14.65	143.40	114.10
1	A	427	LYS	CA-CB-CG	14.29	142.67	114.10
1	D	182	GLU	N-CA-CB	14.24	134.03	110.39
1	C	180	LYS	CG-CD-CE	-14.09	78.89	111.30
1	C	445	LEU	CA-C-N	-13.26	97.83	121.70
1	C	445	LEU	C-N-CA	-13.26	97.83	121.70
1	D	427	LYS	CD-CE-NZ	12.59	152.19	111.90
1	C	180	LYS	CA-C-N	12.30	137.99	120.28
1	C	180	LYS	C-N-CA	12.30	137.99	120.28
1	C	168	ARG	CB-CG-CD	11.94	138.77	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	446	ASN	N-CA-CB	11.49	130.04	110.50
1	A	427	LYS	CD-CE-NZ	11.05	147.27	111.90
1	D	427	LYS	CA-CB-CG	10.99	136.07	114.10
1	A	427	LYS	CB-CG-CD	10.97	136.53	111.30
1	C	166	LEU	CB-CG-CD1	10.71	142.84	110.70
1	D	426	ASP	CA-C-N	10.06	136.42	122.74
1	D	426	ASP	C-N-CA	10.06	136.42	122.74
1	B	144	LYS	N-CA-CB	-9.94	94.32	110.42
1	C	412	ARG	CG-CD-NE	-9.84	90.36	112.00
1	D	427	LYS	CG-CD-CE	-9.53	89.38	111.30
1	D	223	LYS	CG-CD-CE	-9.26	90.00	111.30
1	C	182	GLU	OE1-CD-OE2	-9.25	100.71	122.90
1	D	182	GLU	CA-CB-CG	9.06	132.23	114.10
1	C	201	LEU	CD1-CG-CD2	9.02	130.63	110.80
1	C	427	LYS	CA-CB-CG	8.91	131.92	114.10
1	A	427	LYS	CG-CD-CE	-8.77	91.13	111.30
1	C	180	LYS	CB-CG-CD	8.46	130.76	111.30
1	C	427	LYS	CB-CG-CD	8.44	130.70	111.30
1	B	144	LYS	CB-CA-C	8.42	126.12	110.11
1	D	181	TRP	CA-C-N	-8.42	106.65	120.72
1	D	181	TRP	C-N-CA	-8.42	106.65	120.72
1	C	446	ASN	CA-C-O	-8.34	106.63	120.80
1	B	144	LYS	CG-CD-CE	-7.97	92.96	111.30
1	D	131	LYS	CA-CB-CG	7.94	129.99	114.10
1	D	171	LYS	CG-CD-CE	-7.81	93.34	111.30
1	C	417	ARG	CA-CB-CG	7.79	129.68	114.10
1	D	427	LYS	CB-CG-CD	7.53	128.61	111.30
1	B	34	LYS	CB-CG-CD	-7.49	94.07	111.30
1	C	34	LYS	CA-CB-CG	7.46	129.02	114.10
1	C	412	ARG	CA-CB-CG	7.45	129.00	114.10
1	C	201	LEU	CA-CB-CG	7.07	141.06	116.30
1	C	180	LYS	N-CA-CB	-6.99	98.90	110.23
1	D	168	ARG	CA-CB-CG	6.71	127.52	114.10
1	C	172	GLY	N-CA-C	-6.66	104.22	115.80
1	C	167	GLY	CA-C-N	-6.62	109.26	120.58
1	C	167	GLY	C-N-CA	-6.62	109.26	120.58
1	A	442	GLU	CA-CB-CG	6.56	127.22	114.10
1	C	170	GLY	CA-C-N	-6.38	110.23	122.61
1	C	170	GLY	C-N-CA	-6.38	110.23	122.61
1	D	171	LYS	CD-CE-NZ	6.32	132.13	111.90
1	A	428	PRO	N-CA-C	6.28	121.36	111.38
1	A	388	LYS	CA-CB-CG	6.26	126.62	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	442	GLU	CA-CB-CG	6.25	126.59	114.10
1	C	269	LYS	CB-CG-CD	6.22	125.60	111.30
1	D	233	LEU	CB-CG-CD1	-6.18	92.17	110.70
1	C	182	GLU	CB-CA-C	6.02	122.23	110.67
1	D	233	LEU	CB-CG-CD2	5.96	128.59	110.70
1	A	427	LYS	CB-CA-C	5.93	117.78	108.88
1	C	181	TRP	N-CA-CB	-5.89	101.15	110.22
1	D	233	LEU	N-CA-CB	5.73	118.64	110.16
1	C	169	THR	CA-CB-CG2	5.57	119.97	110.50
1	D	167	GLY	CA-C-N	-5.54	112.90	120.44
1	D	167	GLY	C-N-CA	-5.54	112.90	120.44
1	D	427	LYS	O-C-N	5.50	127.86	121.47
1	C	169	THR	N-CA-CB	5.50	119.14	110.56
1	C	179	GLY	N-CA-C	5.50	119.31	111.12
1	C	182	GLU	N-CA-C	-5.43	105.52	111.82
1	A	386	ASP	CA-C-N	-5.42	111.15	122.03
1	A	386	ASP	C-N-CA	-5.42	111.15	122.03
1	B	33	LEU	CA-C-N	-5.33	112.21	120.31
1	B	33	LEU	C-N-CA	-5.33	112.21	120.31
1	D	412	ARG	CA-CB-CG	5.32	124.73	114.10
1	C	168	ARG	N-CA-C	-5.29	105.18	111.69
1	B	279	ARG	CG-CD-NE	-5.25	100.45	112.00
1	D	223	LYS	CD-CE-NZ	5.23	128.65	111.90
1	D	168	ARG	N-CA-CB	5.22	117.64	110.07
1	C	34	LYS	CB-CG-CD	5.19	123.25	111.30
1	B	34	LYS	CG-CD-CE	5.16	123.17	111.30
1	D	182	GLU	CG-CD-OE2	-5.15	106.56	118.40
1	C	182	GLU	CA-C-N	-5.14	112.99	120.29
1	C	182	GLU	C-N-CA	-5.14	112.99	120.29
1	C	171	LYS	CG-CD-CE	5.07	122.97	111.30
1	A	409	LYS	CA-CB-CG	5.04	124.18	114.10

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	ARG	Sidechain
1	A	236	ARG	Sidechain
1	A	417	ARG	Sidechain
1	A	427	LYS	Peptide
1	A	441	ASN	Peptide
1	A	442	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	B	181	TRP	Peptide
1	B	236	ARG	Sidechain
1	B	279	ARG	Sidechain
1	B	400	LYS	Peptide
1	B	417	ARG	Sidechain
1	C	143	ARG	Sidechain
1	C	168	ARG	Peptide,Sidechain
1	C	201	LEU	Peptide
1	C	236	ARG	Sidechain
1	C	279	ARG	Sidechain
1	C	412	ARG	Sidechain
1	C	427	LYS	Peptide
1	C	442	GLU	Peptide
1	C	445	LEU	Peptide
1	D	143	ARG	Sidechain
1	D	168	ARG	Peptide
1	D	222	ALA	Peptide
1	D	279	ARG	Sidechain
1	D	342	ARG	Sidechain
1	D	412	ARG	Sidechain
1	D	426	ASP	Peptide
1	D	427	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	3324	3305	29	0
1	B	3416	3324	3305	24	0
1	C	3410	3318	3309	95	0
1	D	3416	3324	3304	54	0
2	A	11	11	11	0	0
2	B	11	11	11	0	0
2	C	11	11	11	0	0
2	D	11	11	11	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	1	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	151	0	0	2	0
5	B	80	0	0	1	0
5	C	113	0	0	0	0
5	D	103	0	0	0	1
All	All	14152	13334	13267	200	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 (200) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:LEU:CD2	1:C:166:LEU:CG	1.77	1.62
1:D:223:LYS:CD	1:D:223:LYS:CE	1.75	1.60
1:C:180:LYS:CB	1:C:180:LYS:CG	1.78	1.57
1:C:201:LEU:CD2	1:C:201:LEU:CG	1.79	1.56
1:C:168:ARG:CB	1:C:168:ARG:CG	1.75	1.56
1:C:180:LYS:CG	1:C:180:LYS:CD	1.76	1.54
1:C:201:LEU:CG	1:C:201:LEU:CD1	1.82	1.52
1:C:171:LYS:NZ	1:C:171:LYS:CE	1.68	1.50
1:C:269:LYS:CE	1:C:269:LYS:NZ	1.73	1.48
1:B:34:LYS:CE	1:B:34:LYS:NZ	1.72	1.47
1:C:180:LYS:CD	1:C:180:LYS:CE	1.99	1.39
1:C:180:LYS:CE	1:C:180:LYS:NZ	2.11	1.13
1:A:386:ASP:O	1:A:427:LYS:HD3	1.58	1.04
1:C:180:LYS:CG	1:C:180:LYS:CE	2.39	1.01
1:D:223:LYS:CE	1:D:223:LYS:CG	2.43	0.96
1:C:166:LEU:HD22	1:C:171:LYS:HB3	1.47	0.96
1:C:201:LEU:CD2	1:C:201:LEU:HG	2.02	0.90
1:C:376:LYS:HG2	1:C:442:GLU:HB3	1.54	0.87
1:C:168:ARG:CG	1:C:168:ARG:C	2.47	0.86
1:D:233:LEU:HD11	1:D:237:LEU:HD11	1.60	0.83
1:D:233:LEU:CD1	1:D:237:LEU:HD11	2.11	0.81
1:C:166:LEU:CD2	1:C:166:LEU:CB	2.57	0.81
1:C:166:LEU:CD2	1:C:171:LYS:HB3	2.13	0.79
1:D:233:LEU:HD12	1:D:233:LEU:O	1.83	0.78
1:C:180:LYS:HG3	1:C:180:LYS:HE2	1.65	0.77
1:C:168:ARG:HG2	1:C:169:THR:N	2.00	0.77
1:D:233:LEU:CD1	1:D:237:LEU:CD1	2.63	0.76
1:C:210:MET:HE1	1:C:227:LEU:HD11	1.68	0.76
1:C:180:LYS:CG	1:C:180:LYS:HE2	2.15	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:ARG:HG2	1:C:169:THR:CA	2.17	0.74
1:D:233:LEU:HD12	1:D:233:LEU:C	2.12	0.74
1:D:233:LEU:HD11	1:D:237:LEU:CD1	2.18	0.73
1:B:348:MET:HE1	1:B:355[A]:ILE:HD11	1.72	0.72
1:C:168:ARG:CG	1:C:168:ARG:CA	2.67	0.72
1:D:223:LYS:CE	1:D:223:LYS:HG2	2.17	0.72
1:C:168:ARG:HD2	1:C:169:THR:HG22	1.72	0.72
1:D:222:ALA:O	1:D:226:ASN:N	2.23	0.72
1:D:288:MET:HG2	1:D:301:TYR:HD1	1.54	0.71
1:C:201:LEU:CD1	1:C:201:LEU:HG	2.13	0.71
1:D:288:MET:HE3	1:D:325:VAL:HG12	1.73	0.70
1:D:158:TRP:NE1	1:D:169:THR:OG1	2.25	0.69
1:D:170:GLY:HA2	1:D:173:THR:HG23	1.75	0.69
1:D:165:PRO:O	1:D:213:LYS:NZ	2.26	0.68
1:D:180:LYS:HB2	1:D:183:ASP:OD2	1.94	0.68
1:C:201:LEU:HB2	1:C:238:GLN:OE1	1.94	0.67
1:D:165:PRO:HB2	1:D:216:TYR:OH	1.95	0.66
1:D:226:ASN:O	1:D:226:ASN:OD1	2.14	0.66
1:C:180:LYS:CG	1:C:180:LYS:CA	2.71	0.65
1:D:158:TRP:NE1	1:D:169:THR:HG1	1.95	0.65
1:C:171:LYS:NZ	1:C:171:LYS:CD	2.57	0.64
1:C:184:TYR:CE2	1:C:188:MET:HE2	2.32	0.63
1:C:168:ARG:C	1:C:168:ARG:HG3	2.23	0.62
1:D:218:ASP:O	1:D:224:THR:OG1	2.16	0.62
1:C:201:LEU:CD1	1:C:201:LEU:CB	2.75	0.62
1:B:412:ARG:HG3	1:B:423:LYS:HB2	1.82	0.61
1:C:257:ILE:HG22	1:C:281:PRO:HB2	1.83	0.61
1:C:168:ARG:CB	1:C:168:ARG:HG3	2.17	0.61
1:D:221:THR:OG1	1:D:223:LYS:HB3	2.01	0.61
1:C:125:VAL:O	1:C:131:LYS:HD3	2.00	0.61
1:D:215:ILE:HD12	1:D:216:TYR:N	2.15	0.60
1:A:385:LEU:O	1:A:428:PRO:HD2	2.01	0.60
1:A:441:ASN:O	1:A:442:GLU:O	2.20	0.60
1:A:304:THR:HG22	1:A:308:ILE:HD12	1.83	0.59
1:C:31:ASP:O	1:C:34:LYS:HB3	2.02	0.59
1:C:163:TYR:HE1	1:C:167:GLY:H	1.49	0.59
1:C:399:LEU:HD23	1:C:413:PHE:CD2	2.37	0.59
1:D:233:LEU:CD1	1:D:237:LEU:HD12	2.33	0.59
1:C:168:ARG:C	1:C:168:ARG:HG2	2.22	0.59
1:B:400:LYS:HE2	1:B:440:ALA:HB2	1.85	0.58
1:D:233:LEU:HD12	1:D:237:LEU:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:THR:CB	1:D:223:LYS:HB3	2.34	0.58
1:C:201:LEU:CD2	1:C:201:LEU:CB	2.78	0.57
1:C:168:ARG:CD	1:C:169:THR:HG22	2.34	0.56
1:D:158:TRP:CD1	1:D:169:THR:HG1	2.23	0.56
1:C:180:LYS:CG	1:C:180:LYS:HE3	2.34	0.56
1:A:400:LYS:NZ	5:A:604:HOH:O	2.39	0.56
1:D:311:LEU:HD21	1:D:355[A]:ILE:CD1	2.35	0.56
1:C:168:ARG:HG2	1:C:169:THR:HA	1.88	0.56
1:A:43:LYS:NZ	5:A:601:HOH:O	2.31	0.55
1:C:168:ARG:CB	1:C:168:ARG:HG2	2.17	0.55
1:C:31:ASP:HB3	1:C:240:ALA:HB2	1.88	0.55
1:C:180:LYS:CG	1:C:180:LYS:N	2.69	0.54
1:D:223:LYS:HG2	1:D:223:LYS:HE2	1.88	0.54
1:B:54[A]:SER:OG	5:B:601:HOH:O	2.18	0.54
1:A:48:ILE:HD12	1:A:102:ILE:HG23	1.88	0.54
1:C:218:ASP:O	1:C:224:THR:HG21	2.08	0.53
1:A:399:LEU:HD23	1:A:413:PHE:CD1	2.44	0.53
1:B:164:TYR:CD1	1:B:165:PRO:HA	2.44	0.53
1:C:168:ARG:HG3	1:C:168:ARG:O	2.09	0.53
1:D:186:ALA:O	1:D:190:ASN:ND2	2.41	0.53
1:C:222:ALA:HB1	1:C:227:LEU:HB2	1.91	0.52
1:D:226:ASN:OD1	1:D:229:GLU:HB3	2.09	0.52
1:C:404:GLU:OE2	1:C:433:TYR:OH	2.23	0.52
1:C:186:ALA:O	1:C:190:ASN:OD1	2.27	0.51
1:D:105:THR:HA	1:D:152:TYR:HB3	1.92	0.51
1:C:115:TYR:CE1	1:C:195:LEU:HD21	2.46	0.51
1:D:213:LYS:HE2	1:D:216:TYR:HE2	1.76	0.50
1:C:168:ARG:CD	1:C:169:THR:CG2	2.89	0.50
1:D:233:LEU:HD12	1:D:237:LEU:CD1	2.40	0.50
1:C:233:LEU:C	1:C:233:LEU:HD23	2.36	0.50
1:B:311:LEU:HD21	1:B:355[A]:ILE:CD1	2.42	0.50
1:A:32:ASN:O	1:A:36:ARG:HG3	2.12	0.49
1:B:34:LYS:NZ	1:B:34:LYS:CD	2.67	0.49
1:C:105:THR:HA	1:C:152:TYR:HB3	1.95	0.49
1:C:180:LYS:N	1:C:180:LYS:HG2	2.27	0.49
1:D:170:GLY:HA2	1:D:173:THR:CG2	2.42	0.49
1:B:151:LEU:HD13	1:B:195:LEU:HD22	1.95	0.48
1:B:407:SER:OG	1:B:409:LYS:HG3	2.13	0.48
1:D:221:THR:OG1	1:D:223:LYS:CG	2.62	0.48
1:A:311:LEU:HD21	1:A:355[A]:ILE:CD1	2.44	0.48
1:A:311:LEU:HD21	1:A:355[A]:ILE:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:LYS:HB2	1:B:182:GLU:HB2	1.95	0.48
1:C:375:GLY:C	1:C:442:GLU:HB2	2.39	0.48
1:A:43:LYS:HE3	4:A:503:CL:CL	2.51	0.48
1:B:168:ARG:NH2	1:B:211:TRP:O	2.47	0.48
1:C:109:HIS:CG	1:C:156:LEU:HD23	2.49	0.48
1:D:201:LEU:HD22	1:D:201:LEU:N	2.29	0.47
1:C:164:TYR:HB3	1:C:179:GLY:O	2.15	0.47
1:D:233:LEU:CD1	1:D:233:LEU:C	2.84	0.47
1:A:309:GLN:HG2	1:A:383:LEU:HD22	1.97	0.47
1:C:376:LYS:HG2	1:C:442:GLU:CB	2.36	0.47
1:D:171:LYS:H	1:D:171:LYS:HG2	1.55	0.47
1:A:144:LYS:HE3	1:A:144:LYS:HB2	1.62	0.47
1:A:412:ARG:NH1	1:A:423:LYS:HD3	2.29	0.47
1:C:196:LEU:HD11	1:C:234:ILE:HG12	1.97	0.46
1:A:105:THR:HA	1:A:152:TYR:HB3	1.98	0.46
1:B:94:ILE:HD13	1:B:102:ILE:HG12	1.98	0.46
1:A:213:LYS:O	1:A:219:GLY:HA3	2.16	0.46
1:A:304:THR:HG22	1:A:308:ILE:CD1	2.45	0.46
1:C:163:TYR:HD2	1:C:184:TYR:CE2	2.33	0.46
1:B:213:LYS:O	1:B:219:GLY:HA3	2.16	0.46
1:C:180:LYS:CD	1:C:180:LYS:HE2	2.30	0.46
1:A:400:LYS:HD3	1:C:346:GLU:OE1	2.16	0.45
1:A:376:LYS:HA	1:A:442:GLU:O	2.17	0.45
1:C:201:LEU:CD1	1:C:201:LEU:HB2	2.46	0.45
1:C:168:ARG:NE	1:C:169:THR:HG23	2.30	0.45
1:C:234:ILE:CG2	1:C:243:ILE:HD11	2.47	0.45
1:D:180:LYS:CB	1:D:183:ASP:OD2	2.63	0.45
1:C:376:LYS:HD3	1:C:441:ASN:C	2.42	0.45
1:A:43:LYS:CE	4:A:503:CL:CL	3.02	0.45
1:B:222:ALA:HA	1:B:227:LEU:HD12	1.99	0.45
1:D:222:ALA:O	1:D:225:TRP:N	2.50	0.45
1:A:48:ILE:HD12	1:A:102:ILE:CG2	2.47	0.45
1:B:399:LEU:HD22	1:B:420:ILE:HD13	1.99	0.45
1:D:213:LYS:HE2	1:D:216:TYR:CE2	2.52	0.45
1:C:107:ARG:NH2	1:C:157:ASP:OD2	2.41	0.44
1:A:42:ASP:OD2	1:A:148:ARG:NH1	2.38	0.44
1:C:234:ILE:HG21	1:C:243:ILE:HD11	1.99	0.44
1:D:163:TYR:O	1:D:166:LEU:HD23	2.17	0.44
1:D:328:GLN:HB3	1:D:329:PRO:HD2	2.00	0.44
1:D:96:ALA:O	1:D:345:GLY:HA3	2.18	0.43
1:D:152:TYR:CD1	1:D:152:TYR:C	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:LEU:HD21	1:C:355[A]:ILE:CD1	2.49	0.43
1:D:43:LYS:HA	1:D:320:ASN:CG	2.43	0.43
1:A:386:ASP:C	1:A:427:LYS:HD3	2.39	0.43
1:C:35:ALA:HB3	1:C:242:LEU:HD21	2.00	0.43
1:C:168:ARG:CZ	1:C:169:THR:CG2	2.96	0.43
1:A:222:ALA:HA	1:A:227:LEU:HD12	2.01	0.43
1:A:368:TRP:CE2	1:A:390:LEU:HD11	2.54	0.43
1:C:168:ARG:NE	1:C:169:THR:CG2	2.82	0.43
1:C:221:THR:OG1	1:C:224:THR:HG23	2.19	0.43
1:D:114:MET:O	1:D:135:ILE:HG12	2.19	0.43
1:B:42:ASP:HB3	1:B:100:LYS:HB2	2.01	0.42
1:C:317:LYS:HG2	1:C:365:PRO:HG2	1.99	0.42
1:C:222:ALA:O	1:C:226:ASN:N	2.52	0.42
1:D:213:LYS:HG3	1:D:225:TRP:CZ2	2.54	0.42
1:D:221:THR:C	1:D:223:LYS:HB3	2.44	0.42
1:D:165:PRO:HB2	1:D:216:TYR:HH	1.83	0.42
1:C:166:LEU:CD2	1:C:166:LEU:HB3	2.45	0.42
1:C:168:ARG:HG2	1:C:169:THR:CG2	2.50	0.42
1:C:390:LEU:HD21	1:C:392:LEU:HD21	2.02	0.42
1:C:170:GLY:O	1:C:173:THR:OG1	2.25	0.42
1:C:218:ASP:O	1:C:221:THR:HG23	2.18	0.42
1:B:33:LEU:HD23	1:B:36:ARG:HD2	2.02	0.41
1:C:168:ARG:CG	1:C:169:THR:HA	2.49	0.41
1:A:152:TYR:CD1	1:A:152:TYR:C	2.98	0.41
1:B:152:TYR:CD1	1:B:152:TYR:C	2.98	0.41
1:A:368:TRP:CD2	1:A:390:LEU:HD11	2.55	0.41
1:D:184:TYR:CE1	1:D:188:MET:HE2	2.55	0.41
1:D:304:THR:HG22	1:D:308:ILE:HD12	2.02	0.41
1:C:382:VAL:HB	1:C:433:TYR:HB3	2.02	0.41
1:A:352:ALA:N	1:A:353:PRO:CD	2.83	0.41
1:C:94:ILE:HD13	1:C:102:ILE:HG12	2.03	0.41
1:C:164:TYR:CD1	1:C:178:GLN:HG2	2.56	0.41
1:B:248:HIS:NE2	1:B:261:GLU:OE1	2.51	0.41
1:B:261:GLU:HA	1:B:285:CYS:SG	2.61	0.41
1:B:366:ARG:NH2	1:C:387:ASP:OD1	2.47	0.41
1:C:96:ALA:O	1:C:345:GLY:HA3	2.21	0.41
1:C:184:TYR:CZ	1:C:188:MET:HE2	2.55	0.41
1:C:201:LEU:CB	1:C:238:GLN:OE1	2.66	0.41
1:C:445:LEU:O	1:C:446:ASN:C	2.58	0.41
1:B:352:ALA:N	1:B:353:PRO:CD	2.84	0.40
1:C:256:ASP:O	1:C:280:LEU:HD22	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:THR:OG1	1:D:223:LYS:CB	2.68	0.40
1:C:427:LYS:HA	1:C:428:PRO:HD3	1.80	0.40
1:C:152:TYR:CD1	1:C:152:TYR:C	3.00	0.40
1:C:164:TYR:HA	1:C:165:PRO:C	2.46	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:D:684:HOH:O	5:D:684:HOH:O[5_555]	2.04	0.16

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	424/435 (98%)	410 (97%)	13 (3%)	1 (0%)	43	53
1	B	424/435 (98%)	408 (96%)	15 (4%)	1 (0%)	43	53
1	C	422/435 (97%)	408 (97%)	14 (3%)	0	100	100
1	D	424/435 (98%)	406 (96%)	17 (4%)	1 (0%)	43	53
All	All	1694/1740 (97%)	1632 (96%)	59 (4%)	3 (0%)	43	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	442	GLU
1	B	182	GLU
1	D	223	LYS

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	361/369 (98%)	355 (98%)	6 (2%)	53	70
1	B	361/369 (98%)	353 (98%)	8 (2%)	45	62
1	C	359/369 (97%)	347 (97%)	12 (3%)	33	47
1	D	361/369 (98%)	355 (98%)	6 (2%)	53	70
All	All	1442/1476 (98%)	1410 (98%)	32 (2%)	47	62

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	250	THR
1	A	257	ILE
1	A	430	SER
1	A	435	LEU
1	A	445	LEU
1	B	29	SER
1	B	34	LYS
1	B	78	SER
1	B	135	ILE
1	B	250	THR
1	B	257	ILE
1	B	403	VAL
1	B	435	LEU
1	C	27	THR
1	C	47	PHE
1	C	124	ILE
1	C	168	ARG
1	C	182	GLU
1	C	201	LEU
1	C	250	THR
1	C	263	ASP
1	C	355[A]	ILE
1	C	355[B]	ILE

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Mol	Chain	Res	Type
1	C	425	THR
1	C	427	LYS
1	D	124	ILE
1	D	233	LEU
1	D	263	ASP
1	D	335	THR
1	D	355[A]	ILE
1	D	355[B]	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	GLN
1	A	178	GLN
1	A	373	GLN
1	A	429	HIS
1	B	67	ASN
1	B	136	HIS
1	B	150	HIS
1	B	328	GLN
1	C	246	ASN
1	C	373	GLN
1	C	429	HIS
1	C	441	ASN
1	D	67	ASN
1	D	178	GLN
1	D	226	ASN
1	D	339	GLN

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 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	FUL	D	501	-	11,11,11	1.31	1 (9%)	16,16,16	0.79	0
2	FUL	B	501	-	11,11,11	1.31	1 (9%)	16,16,16	0.70	0
2	FUL	A	501	-	11,11,11	1.37	1 (9%)	16,16,16	1.04	0
2	FUL	C	501	-	11,11,11	1.29	1 (9%)	16,16,16	0.82	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FUL	D	501	-	-	-	0/1/1/1
2	FUL	B	501	-	-	-	0/1/1/1
2	FUL	A	501	-	-	-	0/1/1/1
2	FUL	C	501	-	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FUL	O5-C1	3.60	1.51	1.42
2	B	501	FUL	O5-C1	3.43	1.51	1.42
2	D	501	FUL	O5-C1	3.37	1.51	1.42
2	C	501	FUL	O5-C1	3.33	1.51	1.42

There are no bond angle outliers.

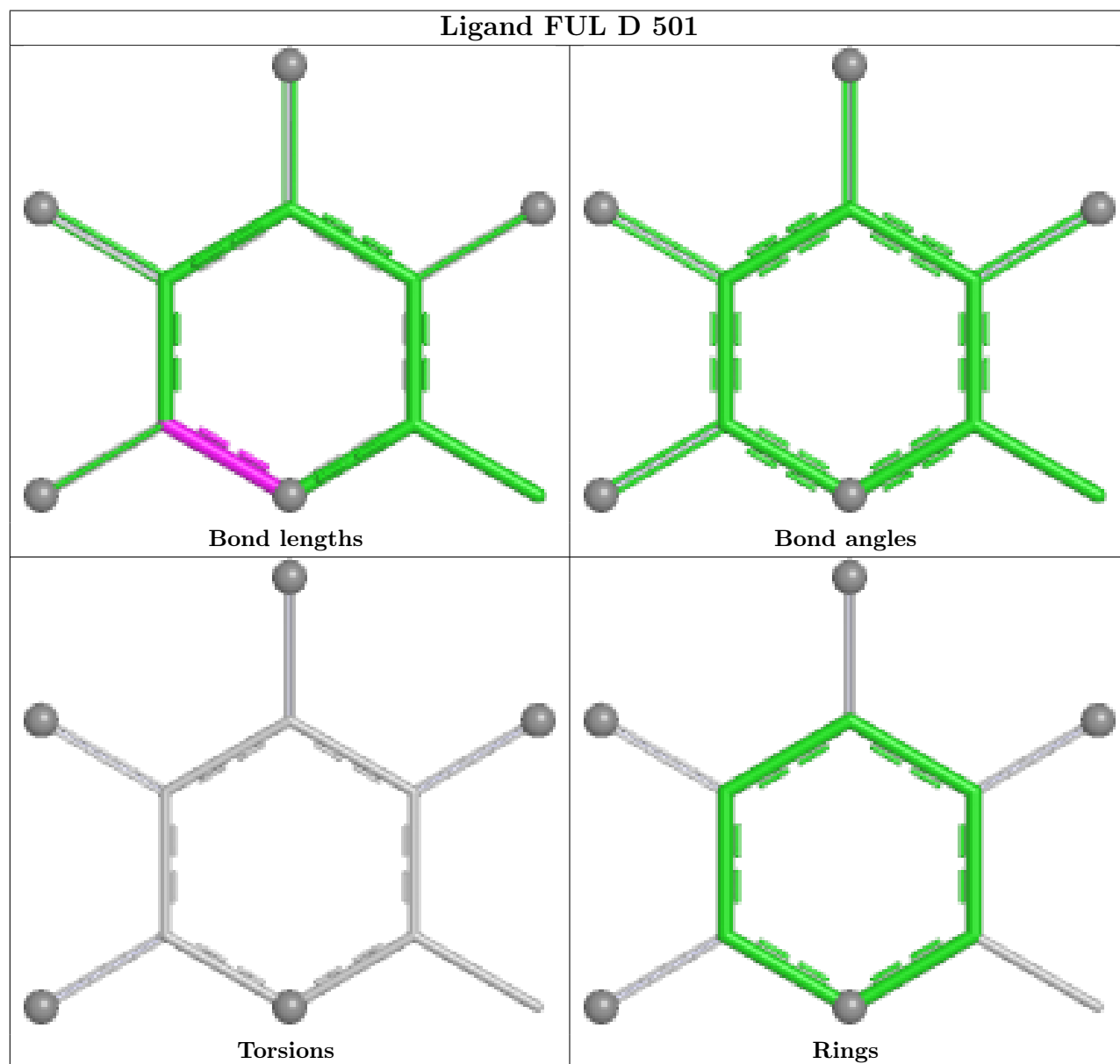
There are no chirality outliers.

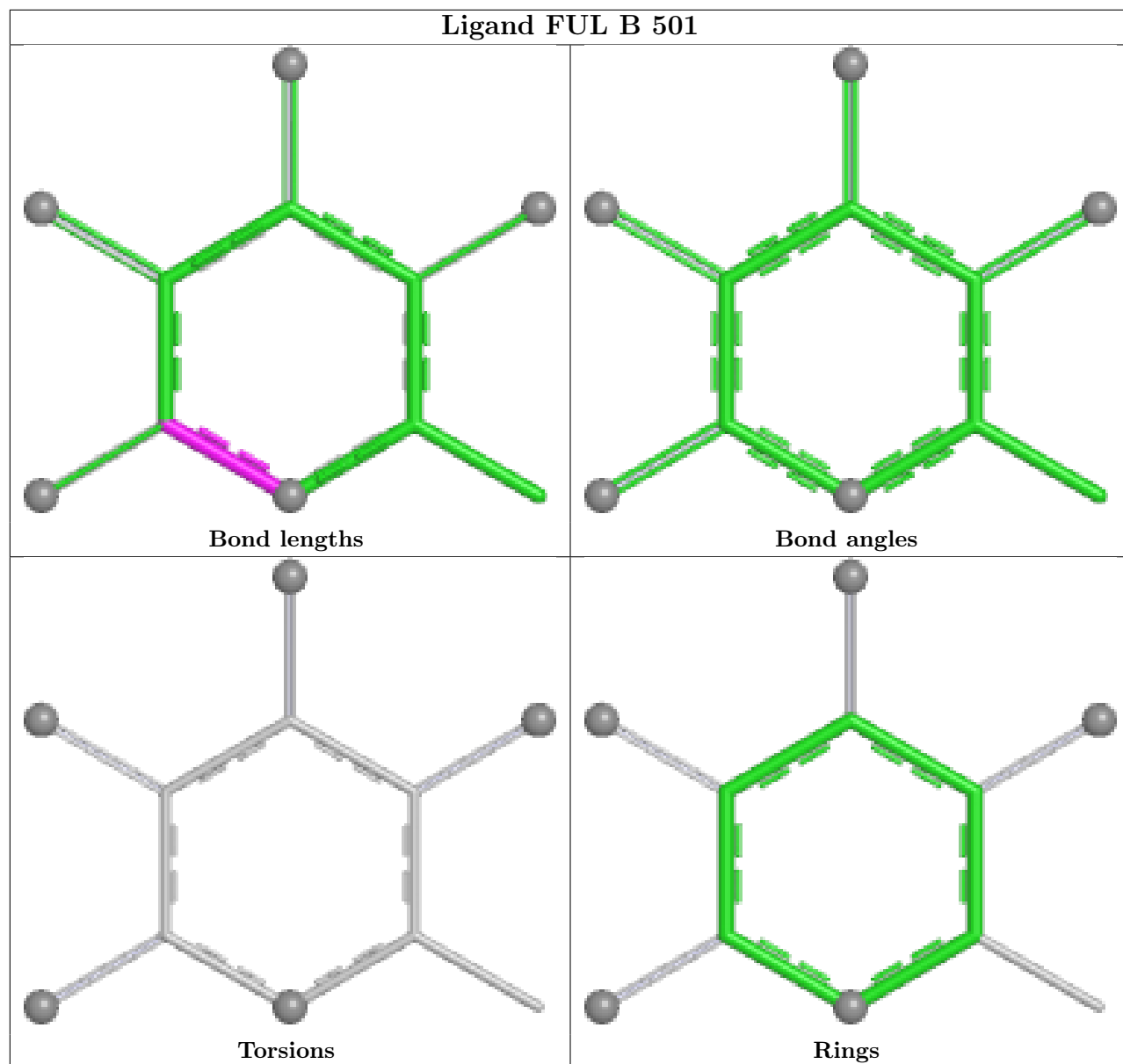
There are no torsion outliers.

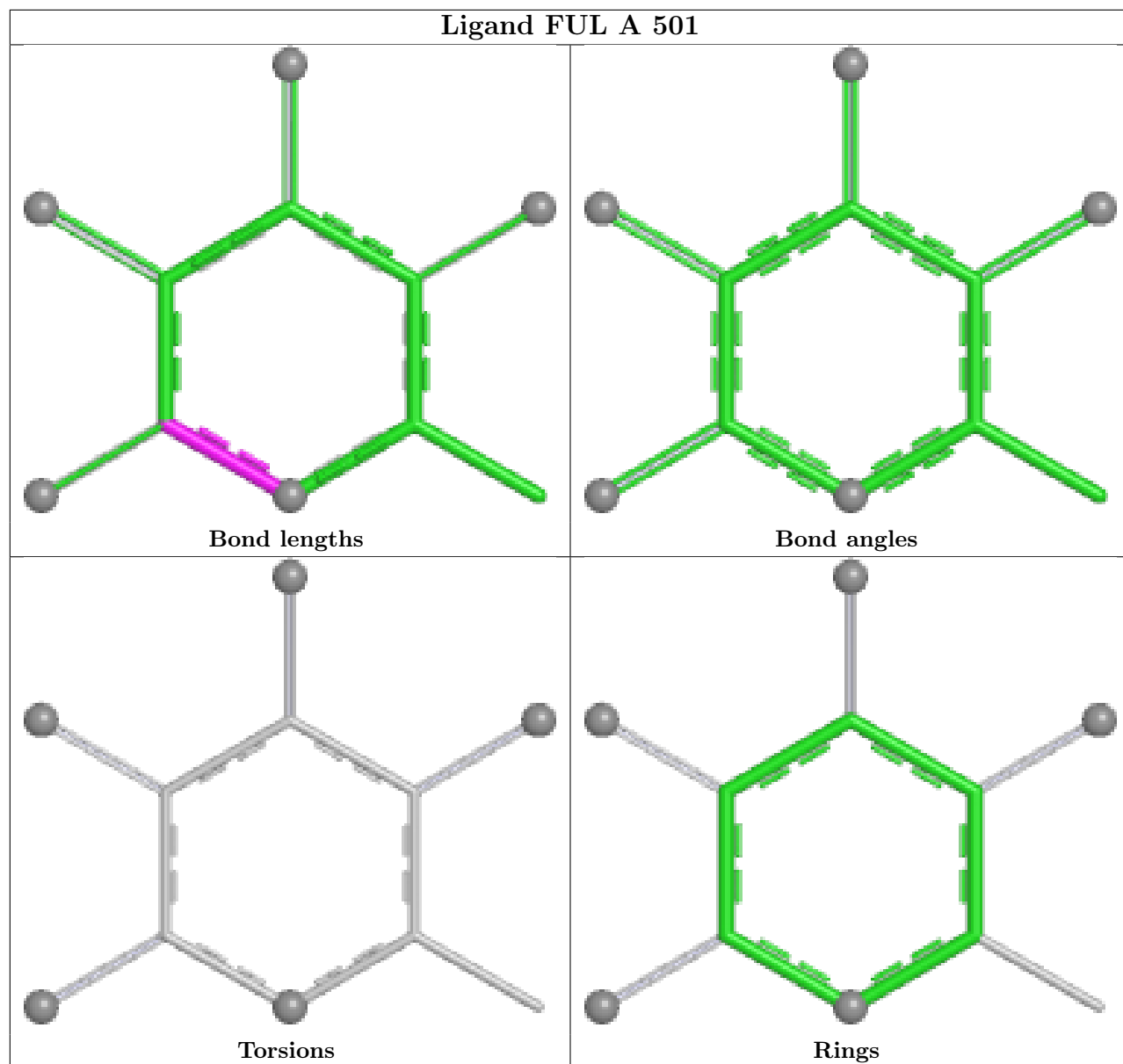
There are no ring outliers.

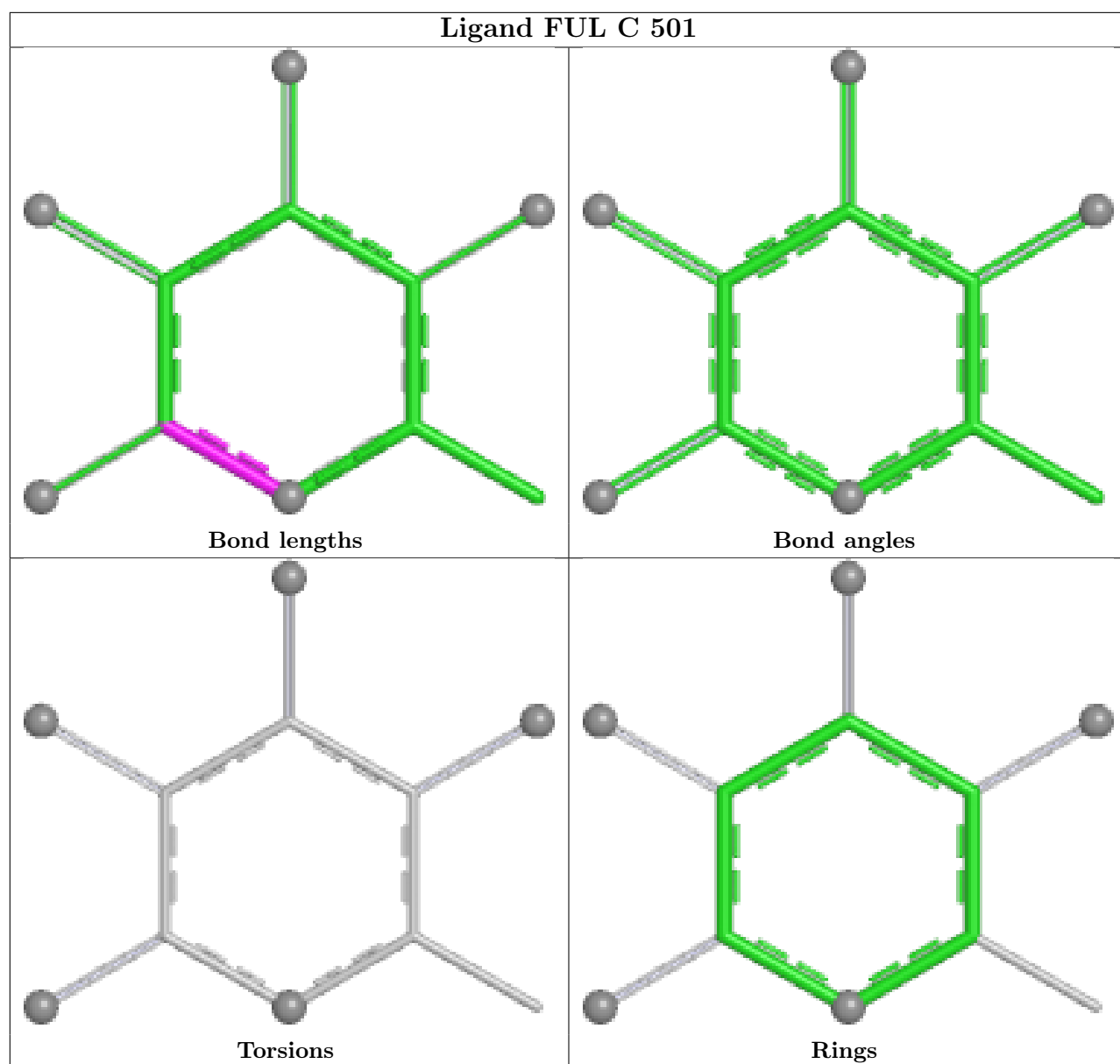
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	422/435 (97%)	0.08	6 (1%) 73 75	37, 68, 98, 145	2 (0%)
1	B	422/435 (97%)	0.42	12 (2%) 55 56	38, 84, 111, 167	2 (0%)
1	C	422/435 (97%)	0.45	25 (5%) 28 29	42, 82, 130, 169	1 (0%)
1	D	422/435 (97%)	0.57	32 (7%) 20 20	39, 85, 139, 187	2 (0%)
All	All	1688/1740 (97%)	0.38	75 (4%) 39 40	37, 80, 122, 187	7 (0%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	201	LEU	6.6
1	C	179	GLY	4.4
1	B	400	LYS	4.4
1	C	171	LYS	4.0
1	C	168	ARG	3.9
1	D	168	ARG	3.8
1	A	445	LEU	3.7
1	B	446	ASN	3.7
1	D	25	GLY	3.5
1	D	169	THR	3.5
1	D	445	LEU	3.4
1	C	217	PRO	3.3
1	A	427	LYS	3.3
1	C	427	LYS	3.3
1	B	215	ILE	3.3
1	B	445	LEU	3.1
1	C	180	LYS	3.1
1	D	131	LYS	3.1
1	D	217	PRO	3.1
1	B	217	PRO	3.0
1	A	442	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	216	TYR	3.0
1	C	169	THR	2.9
1	B	56	LEU	2.9
1	D	227	LEU	2.8
1	C	68	LEU	2.8
1	D	55[A]	MET	2.8
1	C	412	ARG	2.8
1	B	222	ALA	2.7
1	D	216	TYR	2.7
1	D	73	TYR	2.7
1	C	173	THR	2.7
1	C	52	ILE	2.6
1	D	181	TRP	2.6
1	C	446	ASN	2.6
1	B	33	LEU	2.6
1	D	56	LEU	2.6
1	B	216	TYR	2.6
1	C	445	LEU	2.6
1	D	76	LEU	2.5
1	D	427	LYS	2.5
1	D	446	ASN	2.5
1	D	167	GLY	2.5
1	C	166	LEU	2.5
1	D	166	LEU	2.5
1	C	25	GLY	2.5
1	D	224	THR	2.4
1	D	215	ILE	2.4
1	A	446	ASN	2.4
1	D	234	ILE	2.4
1	D	220	MET	2.3
1	D	243	ILE	2.3
1	D	151	LEU	2.3
1	C	167	GLY	2.3
1	C	222	ALA	2.3
1	D	201	LEU	2.2
1	C	442	GLU	2.2
1	D	125	VAL	2.2
1	D	177	THR	2.2
1	C	164	TYR	2.1
1	D	192	LEU	2.1
1	D	398	LYS	2.1
1	D	165	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	144	LYS	2.1
1	C	428	PRO	2.1
1	B	209	GLY	2.1
1	C	184	TYR	2.1
1	C	444	PRO	2.1
1	D	206	TRP	2.1
1	C	34	LYS	2.0
1	B	319	ALA	2.0
1	D	170	GLY	2.0
1	A	223	LYS	2.0
1	D	182	GLU	2.0
1	C	240	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

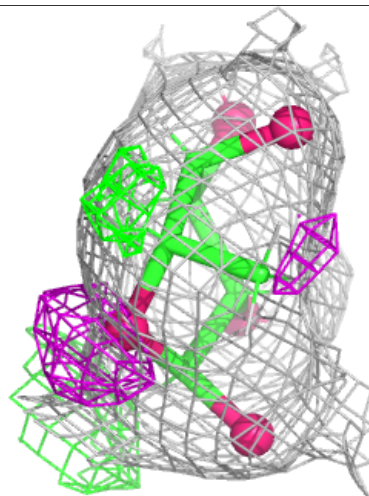
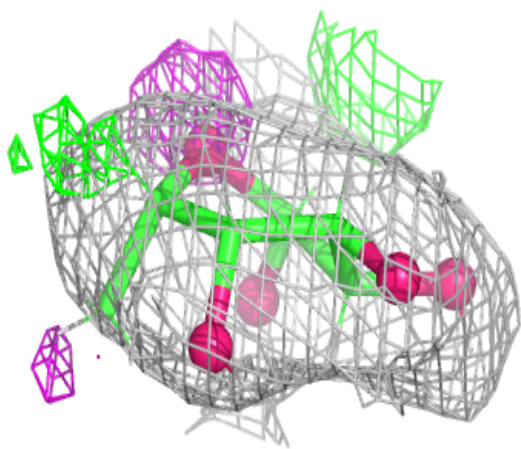
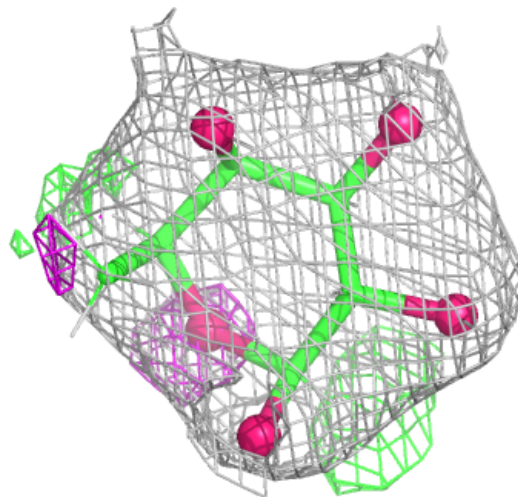
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZN	A	502	1/1	0.72	0.12	152,152,152,152	0
4	CL	A	503	1/1	0.81	0.44	77,77,77,77	0
2	FUL	A	501	11/11	0.91	0.10	55,59,70,71	0
2	FUL	C	501	11/11	0.92	0.09	65,73,83,85	0
2	FUL	B	501	11/11	0.93	0.12	66,72,85,86	0
2	FUL	D	501	11/11	0.94	0.09	72,81,91,97	0
3	ZN	C	502	1/1	0.99	0.04	79,79,79,79	1

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.

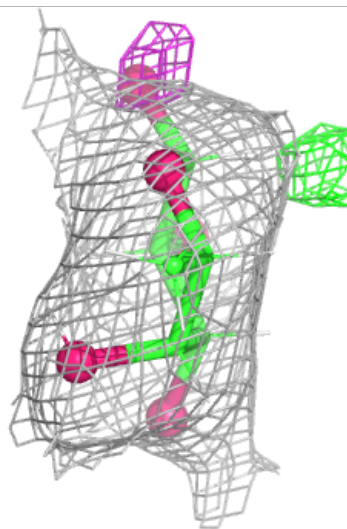
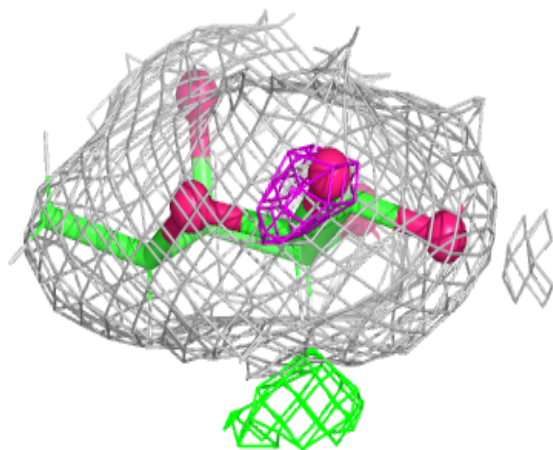
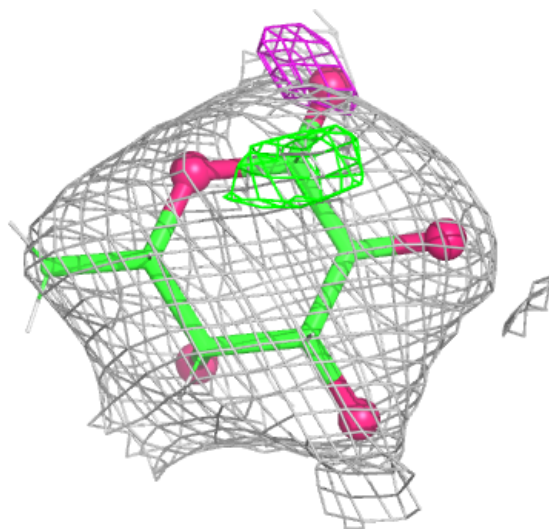
Electron density around FUL A 501:

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



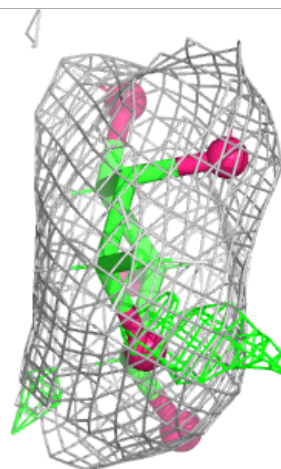
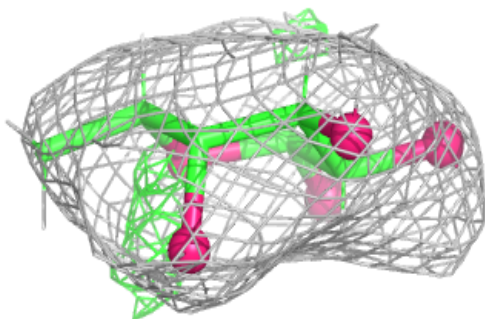
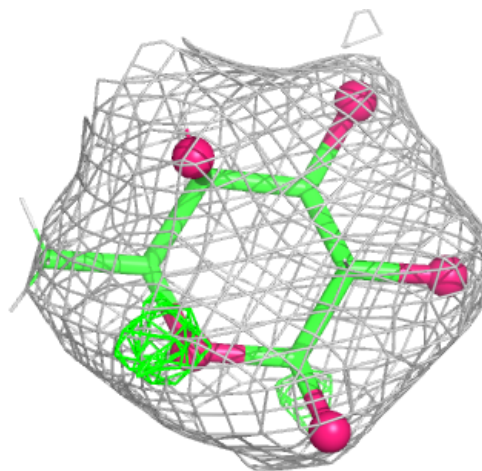
Electron density around FUL C 501:

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



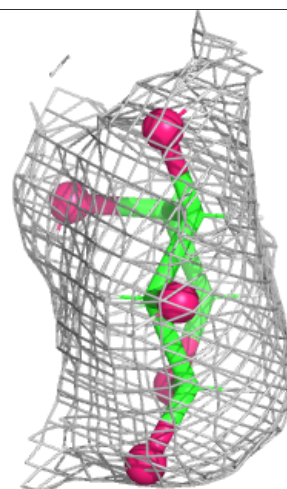
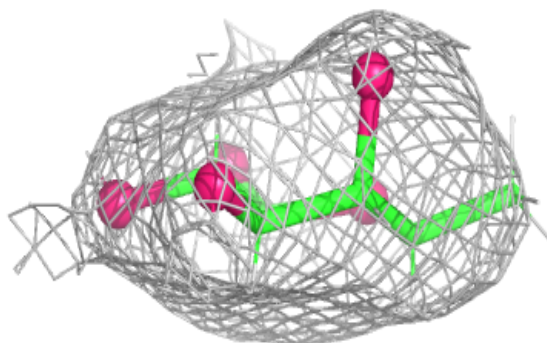
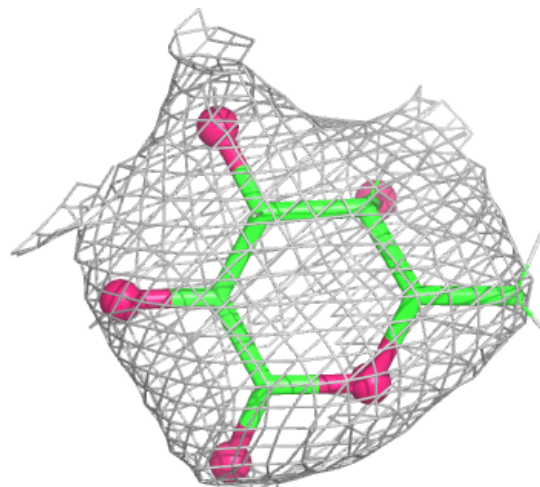
Electron density around FUL B 501:

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



Electron density around FUL D 501:

$2mF_o-DF_c$ (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.