



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 25, 2025 – 12:11 pm GMT

PDB ID : 9EU3  
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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41

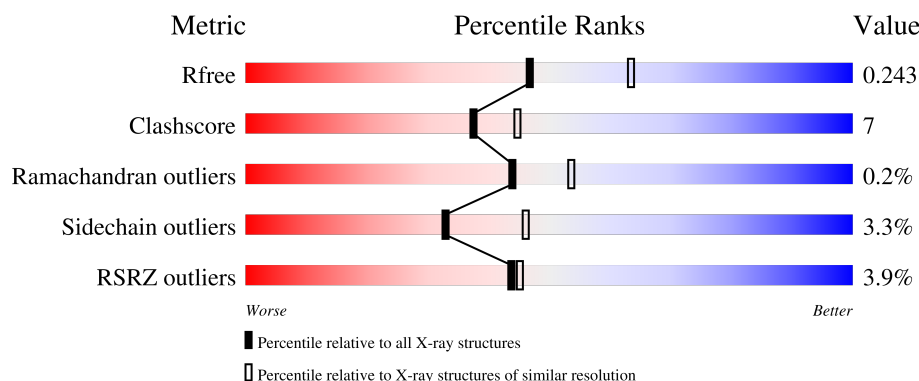
# 1 Overall quality at a glance

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))
$R_{free}$	164625	8487 (2.30-2.26)
Clashscore	180529	9437 (2.30-2.26)
Ramachandran outliers	177936	9341 (2.30-2.26)
Sidechain outliers	177891	9342 (2.30-2.26)
RSRZ outliers	164620	8487 (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  $\geq 3$ , 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	<div> <div>0%</div> <div>85%</div> <div>11%</div> <div>.</div> </div>
1	B	435	<div> <div>2%</div> <div>86%</div> <div>10%</div> <div>..</div> </div>
1	C	435	<div> <div>5%</div> <div>77%</div> <div>17%</div> <div>...</div> </div>
1	D	435	<div> <div>7%</div> <div>83%</div> <div>11%</div> <div>...</div> </div>

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:

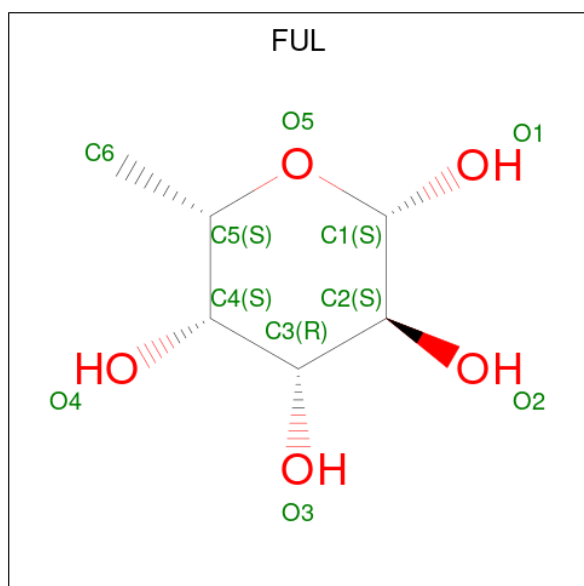
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP G8UMQ6
A	447	LEU	-	expression tag	UNP G8UMQ6
A	448	GLU	-	expression tag	UNP G8UMQ6
A	449	HIS	-	expression tag	UNP G8UMQ6
A	450	HIS	-	expression tag	UNP G8UMQ6
A	451	HIS	-	expression tag	UNP G8UMQ6
A	452	HIS	-	expression 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 (three-letter code: FUL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>) (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 (three-letter code: 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 (three-letter code: CL) (formula: Cl).

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

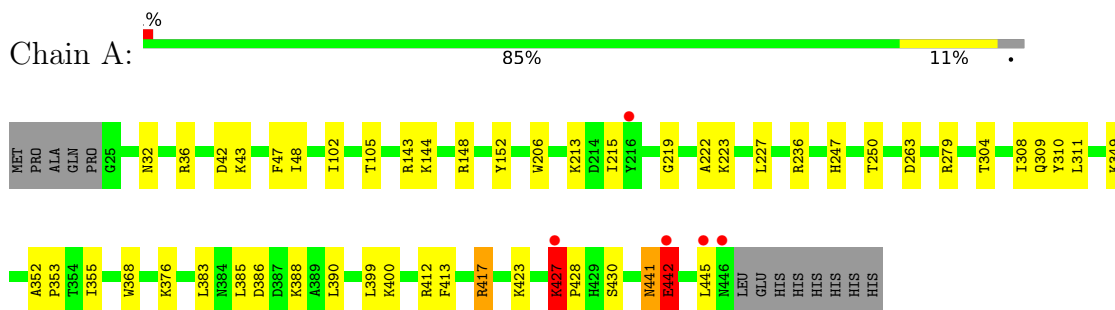
- Molecule 5 is water.

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		

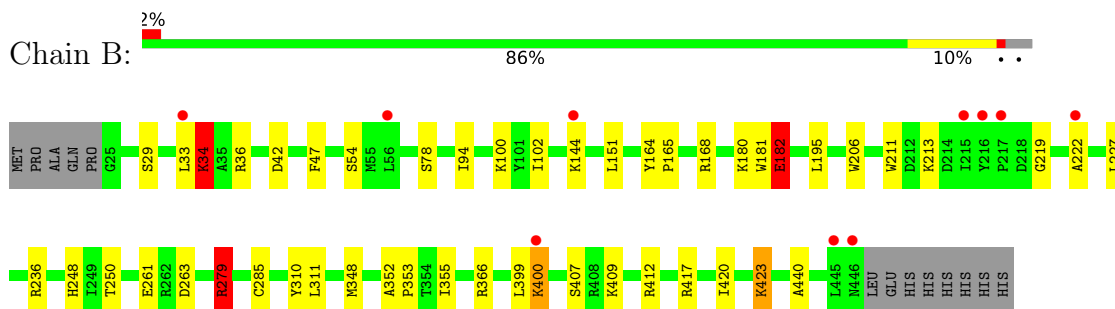
### 3 Residue-property plots [i](#)

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.

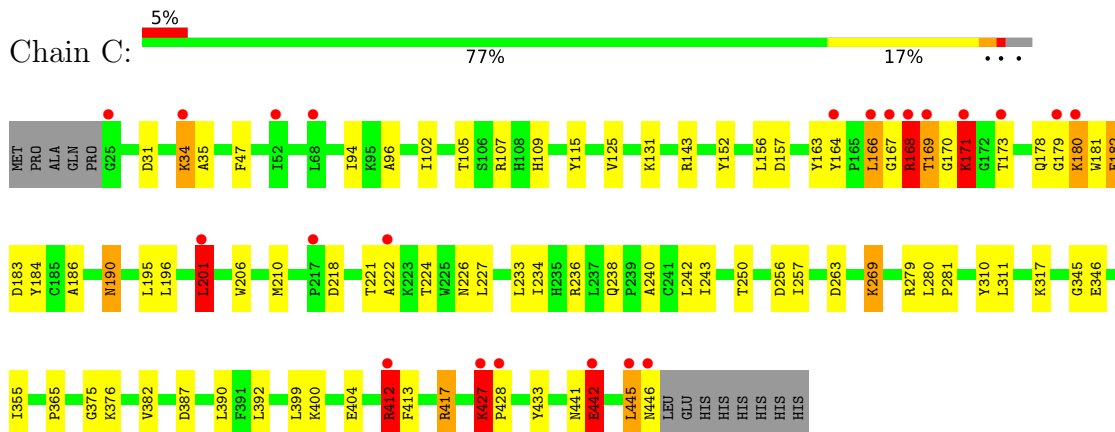
- Molecule 1: Alpha-L-fucosidase



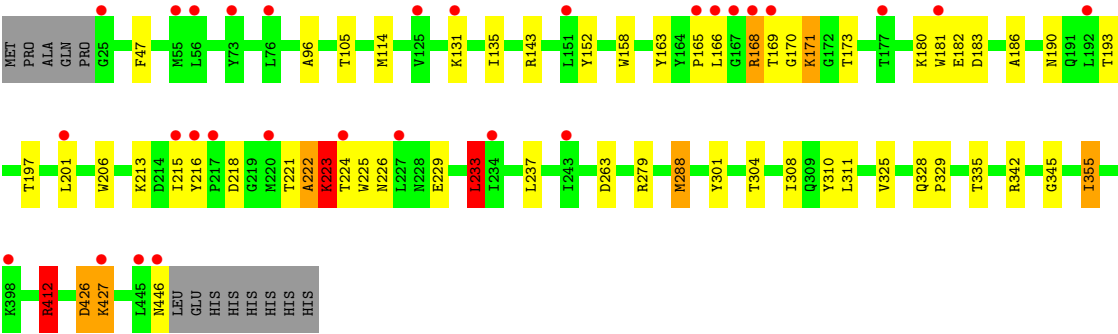
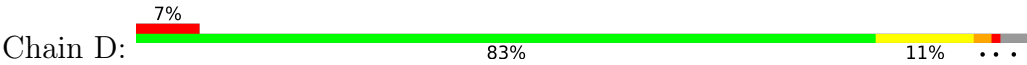
- Molecule 1: Alpha-L-fucosidase



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.212 , 0.243 0.213 , 0.243	Depositor DCC
$R_{free}$ test set	5808 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.7	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, CL, FUL

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	0.41	3/3524 (0.1%)	0.70	6/4779 (0.1%)
1	B	0.49	7/3524 (0.2%)	0.72	8/4779 (0.2%)
1	C	0.92	16/3510 (0.5%)	1.16	32/4761 (0.7%)
1	D	0.70	11/3524 (0.3%)	0.86	19/4779 (0.4%)
All	All	0.66	37/14082 (0.3%)	0.88	65/19098 (0.3%)

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 (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	180	LYS	CE-NZ	25.14	2.12	1.49
1	C	182	GLU	CD-OE2	20.20	1.47	1.25
1	D	182	GLU	CD-OE2	19.36	1.47	1.25
1	C	180	LYS	CD-CE	19.31	1.99	1.51
1	D	182	GLU	CD-OE1	16.70	1.44	1.25
1	C	182	GLU	CD-OE1	13.98	1.41	1.25
1	B	182	GLU	CD-OE1	10.56	1.37	1.25
1	D	223	LYS	CD-CE	9.75	1.75	1.51
1	C	180	LYS	CB-CG	9.66	1.78	1.52
1	C	269	LYS	CE-NZ	9.64	1.73	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	34	LYS	CE-NZ	9.46	1.72	1.49
1	D	182	GLU	CG-CD	9.07	1.65	1.51
1	D	131	LYS	CD-CE	8.67	1.73	1.51
1	C	168	ARG	CB-CG	8.61	1.75	1.52
1	A	427	LYS	CD-CE	8.48	1.72	1.51
1	B	144	LYS	CD-CE	8.35	1.72	1.51
1	C	201	LEU	CG-CD1	8.25	1.82	1.51
1	D	131	LYS	CB-CG	8.09	1.74	1.52
1	B	182	GLU	CG-CD	7.79	1.63	1.51
1	B	182	GLU	CD-OE2	7.74	1.34	1.25
1	C	171	LYS	CE-NZ	7.72	1.68	1.49
1	C	171	LYS	CB-CG	7.64	1.73	1.52
1	A	215	ILE	C-N	7.57	1.51	1.34
1	C	201	LEU	CG-CD2	7.33	1.78	1.51
1	C	269	LYS	CB-CG	7.09	1.71	1.52
1	C	180	LYS	CG-CD	6.96	1.76	1.52
1	C	166	LEU	CG-CD2	6.89	1.77	1.51
1	A	427	LYS	CE-NZ	6.57	1.65	1.49
1	B	144	LYS	CE-NZ	6.54	1.65	1.49
1	B	144	LYS	CB-CG	-6.34	1.35	1.52
1	D	427	LYS	CD-CE	6.34	1.67	1.51
1	D	171	LYS	CE-NZ	6.33	1.64	1.49
1	C	166	LEU	CG-CD1	6.10	1.74	1.51
1	C	168	ARG	CG-CD	5.85	1.66	1.51
1	D	131	LYS	CG-CD	5.72	1.71	1.52
1	D	426	ASP	C-N	-5.47	1.21	1.34
1	D	171	LYS	CD-CE	5.30	1.64	1.51

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	182	GLU	CG-CD-OE1	25.14	168.57	118.30
1	C	182	GLU	CG-CD-OE2	-24.98	68.33	118.30
1	C	180	LYS	CD-CE-NZ	20.97	159.94	111.70
1	C	182	GLU	OE1-CD-OE2	-18.83	100.71	123.30
1	C	166	LEU	CB-CG-CD1	18.73	142.84	111.00
1	D	427	LYS	CD-CE-NZ	17.60	152.19	111.70
1	A	427	LYS	CD-CE-NZ	15.46	147.27	111.70
1	B	34	LYS	CA-CB-CG	14.72	145.78	113.40
1	B	144	LYS	CA-CB-CG	14.43	145.14	113.40
1	C	182	GLU	CA-CB-CG	13.63	143.40	113.40
1	A	427	LYS	CA-CB-CG	13.30	142.67	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	182	GLU	N-CA-CB	13.02	134.03	110.60
1	C	201	LEU	CA-CB-CG	11.20	141.06	115.30
1	D	233	LEU	CB-CG-CD1	-11.07	92.17	111.00
1	C	180	LYS	CG-CD-CE	-11.00	78.89	111.90
1	C	446	ASN	N-CA-CB	10.80	130.04	110.60
1	C	168	ARG	CB-CG-CD	10.45	138.77	111.60
1	D	233	LEU	CB-CG-CD2	10.35	128.59	111.00
1	D	427	LYS	CA-CB-CG	10.30	136.07	113.40
1	C	412	ARG	CG-CD-NE	-10.21	90.36	111.80
1	A	427	LYS	CB-CG-CD	9.59	136.53	111.60
1	C	445	LEU	C-N-CA	-9.55	97.83	121.70
1	B	144	LYS	N-CA-CB	-9.04	94.32	110.60
1	D	171	LYS	CD-CE-NZ	8.88	132.13	111.70
1	D	182	GLU	CA-CB-CG	8.56	132.23	113.40
1	C	427	LYS	CA-CB-CG	8.42	131.92	113.40
1	B	144	LYS	CB-CA-C	7.86	126.12	110.40
1	D	182	GLU	OE1-CD-OE2	7.73	132.57	123.30
1	D	131	LYS	CA-CB-CG	7.54	129.99	113.40
1	D	427	LYS	CG-CD-CE	-7.51	89.38	111.90
1	C	417	ARG	CA-CB-CG	7.40	129.68	113.40
1	C	180	LYS	CB-CG-CD	7.37	130.76	111.60
1	D	223	LYS	CD-CE-NZ	7.37	128.65	111.70
1	C	427	LYS	CB-CG-CD	7.35	130.70	111.60
1	D	223	LYS	CG-CD-CE	-7.30	90.00	111.90
1	C	445	LEU	CB-CG-CD2	-7.19	98.78	111.00
1	C	34	LYS	CA-CB-CG	7.10	129.02	113.40
1	C	412	ARG	CA-CB-CG	7.09	129.00	113.40
1	A	427	LYS	CG-CD-CE	-6.92	91.13	111.90
1	B	34	LYS	CB-CG-CD	-6.74	94.07	111.60
1	C	201	LEU	CD1-CG-CD2	6.71	130.63	110.50
1	D	427	LYS	CB-CG-CD	6.54	128.61	111.60
1	C	180	LYS	C-N-CA	6.52	137.99	121.70
1	C	180	LYS	N-CA-CB	-6.50	98.90	110.60
1	D	168	ARG	CA-CB-CG	6.42	127.52	113.40
1	C	446	ASN	CA-C-O	-6.42	106.63	120.10
1	C	166	LEU	CA-CB-CG	-6.41	100.56	115.30
1	B	144	LYS	CG-CD-CE	-6.31	92.96	111.90
1	C	168	ARG	NE-CZ-NH2	-6.31	117.15	120.30
1	A	442	GLU	CA-CB-CG	6.28	127.22	113.40
1	D	171	LYS	CG-CD-CE	-6.19	93.34	111.90
1	C	183	ASP	CB-CG-OD2	6.02	123.72	118.30
1	D	181	TRP	C-N-CA	-6.02	106.65	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	LYS	CA-CB-CG	6.01	126.62	113.40
1	C	442	GLU	CA-CB-CG	6.00	126.59	113.40
1	C	182	GLU	CB-CA-C	5.91	122.23	110.40
1	D	426	ASP	C-N-CA	5.89	136.42	121.70
1	D	182	GLU	CG-CD-OE2	-5.87	106.56	118.30
1	B	182	GLU	OE1-CD-OE2	5.49	129.89	123.30
1	C	166	LEU	CB-CG-CD2	-5.44	101.76	111.00
1	C	169	THR	CA-CB-CG2	5.41	119.97	112.40
1	B	279	ARG	CG-CD-NE	-5.41	100.45	111.80
1	C	269	LYS	CB-CG-CD	5.38	125.60	111.60
1	C	181	TRP	N-CA-CB	-5.25	101.15	110.60
1	D	412	ARG	CA-CB-CG	5.15	124.73	113.40

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
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	Sidechain,Peptide
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

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Mol	Chain	Res	Type	Group
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	27	0
1	B	3416	3324	3305	23	0
1	C	3410	3318	3309	90	0
1	D	3416	3324	3304	48	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
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	186	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 (186) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:233:LEU:HD11	1:D:237:LEU:HD11	1.60	0.83
1:C:168:ARG:CG	1:C:168:ARG:C	2.47	0.82
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:180:LYS:CG	1:C:180:LYS:HE2	2.15	0.74
1:C:168:ARG:HG2	1:C:169:THR:CA	2.17	0.74
1:D:233:LEU:HD11	1:D:237:LEU:CD1	2.18	0.73
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:C:210:MET:HE1	1:C:227:LEU:HD11	1.72	0.70
1:D:170:GLY:HA2	1:D:173:THR:HG23	1.75	0.69
1:D:233:LEU:HD12	1:D:233:LEU:C	2.12	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:C:171:LYS:NZ	1:C:171:LYS:CD	2.57	0.64
1:D:165:PRO:O	1:D:213:LYS:NZ	2.26	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LYS:NZ	5:A:601:HOH:O	2.31	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:B:400:LYS:HE2	1:B:440:ALA:HB2	1.85	0.58
1:C:168:ARG:C	1:C:168:ARG:HG3	2.23	0.58
1:D:233:LEU:HD12	1:D:237:LEU:HD12	1.85	0.58
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:C:180:LYS:CG	1:C:180:LYS:HE3	2.34	0.56
1:D:158:TRP:NE1	1:D:169:THR:OG1	2.25	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: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:D:288:MET:HE3	1:D:325:VAL:HG12	1.89	0.54
1:C:168:ARG:C	1:C:168:ARG:HG2	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:ASN:OD1	1:D:229:GLU:HB3	2.09	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: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:C:170:GLY:O	1:C:173:THR:OG1	2.25	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:C:404:GLU:OE2	1:C:433:TYR:OH	2.23	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
1:B:180:LYS:HB2	1:B:182:GLU:HB2	1.95	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: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:C:233:LEU:C	1:C:233:LEU:HD23	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:233:LEU:CD1	1:D:233:LEU:C	2.84	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:C:311:LEU:HD21	1:C:355[A]:ILE:CD1	2.49	0.43
1:C:375:GLY:C	1:C:442:GLU:HB2	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:B:348:MET:CE	1:B:355[A]:ILE:HD11	2.50	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: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:368:TRP:CD2	1:A:390:LEU:HD11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:201:LEU:CB	1:C:238:GLN:OE1	2.66	0.41
1:B:352:ALA:N	1:B:353:PRO:CD	2.84	0.40
1:D:193:THR:O	1:D:197:THR:OG1	2.30	0.40
1:C:376:LYS:HD3	1:C:441:ASN:C	2.42	0.40
1:C:256:ASP:O	1:C:280:LEU:HD22	2.20	0.40
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

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%)	44	53
1	B	424/435 (98%)	408 (96%)	15 (4%)	1 (0%)	44	53
1	C	422/435 (97%)	408 (97%)	14 (3%)	0	100	100
1	D	424/435 (98%)	406 (96%)	17 (4%)	1 (0%)	44	53
All	All	1694/1740 (97%)	1632 (96%)	59 (4%)	3 (0%)	44	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%)	348 (96%)	13 (4%)	30	42
1	B	361/369 (98%)	351 (97%)	10 (3%)	38	52
1	C	359/369 (97%)	345 (96%)	14 (4%)	27	39
1	D	361/369 (98%)	350 (97%)	11 (3%)	36	50
All	All	1442/1476 (98%)	1394 (97%)	48 (3%)	33	46

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	PHE
1	A	206	TRP
1	A	223	LYS
1	A	247	HIS
1	A	250	THR
1	A	263	ASP
1	A	279	ARG
1	A	310	TYR
1	A	349	LYS
1	A	417	ARG
1	A	427	LYS
1	A	430	SER
1	A	445	LEU
1	B	29	SER
1	B	34	LYS
1	B	47	PHE
1	B	78	SER

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Mol	Chain	Res	Type
1	B	206	TRP
1	B	250	THR
1	B	263	ASP
1	B	279	ARG
1	B	310	TYR
1	B	423	LYS
1	C	47	PHE
1	C	168	ARG
1	C	171	LYS
1	C	182	GLU
1	C	190	ASN
1	C	201	LEU
1	C	206	TRP
1	C	250	THR
1	C	263	ASP
1	C	310	TYR
1	C	400	LYS
1	C	412	ARG
1	C	417	ARG
1	C	427	LYS
1	D	47	PHE
1	D	206	TRP
1	D	233	LEU
1	D	263	ASP
1	D	288	MET
1	D	310	TYR
1	D	335	THR
1	D	355[A]	ILE
1	D	355[B]	ILE
1	D	412	ARG
1	D	446	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	178	GLN
1	A	328	GLN
1	A	429	HIS
1	B	67	ASN
1	B	150	HIS
1	B	328	GLN

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Mol	Chain	Res	Type
1	C	373	GLN
1	C	429	HIS
1	D	178	GLN
1	D	226	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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	B	501	-	11,11,11	1.29	1 (9%)	15,16,16	0.72	0
2	FUL	C	501	-	11,11,11	1.28	1 (9%)	15,16,16	0.79	0
2	FUL	A	501	-	11,11,11	1.35	1 (9%)	15,16,16	1.03	0
2	FUL	D	501	-	11,11,11	1.29	1 (9%)	15,16,16	0.81	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	B	501	-	-	-	0/1/1/1
2	FUL	C	501	-	-	-	0/1/1/1
2	FUL	A	501	-	-	-	0/1/1/1
2	FUL	D	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	3.51	1.51	1.42
2	B	501	FUL	O5-C1	3.35	1.51	1.42
2	D	501	FUL	O5-C1	3.29	1.51	1.42
2	C	501	FUL	O5-C1	3.25	1.51	1.42

There are no bond angle outliers.

There are no chirality outliers.

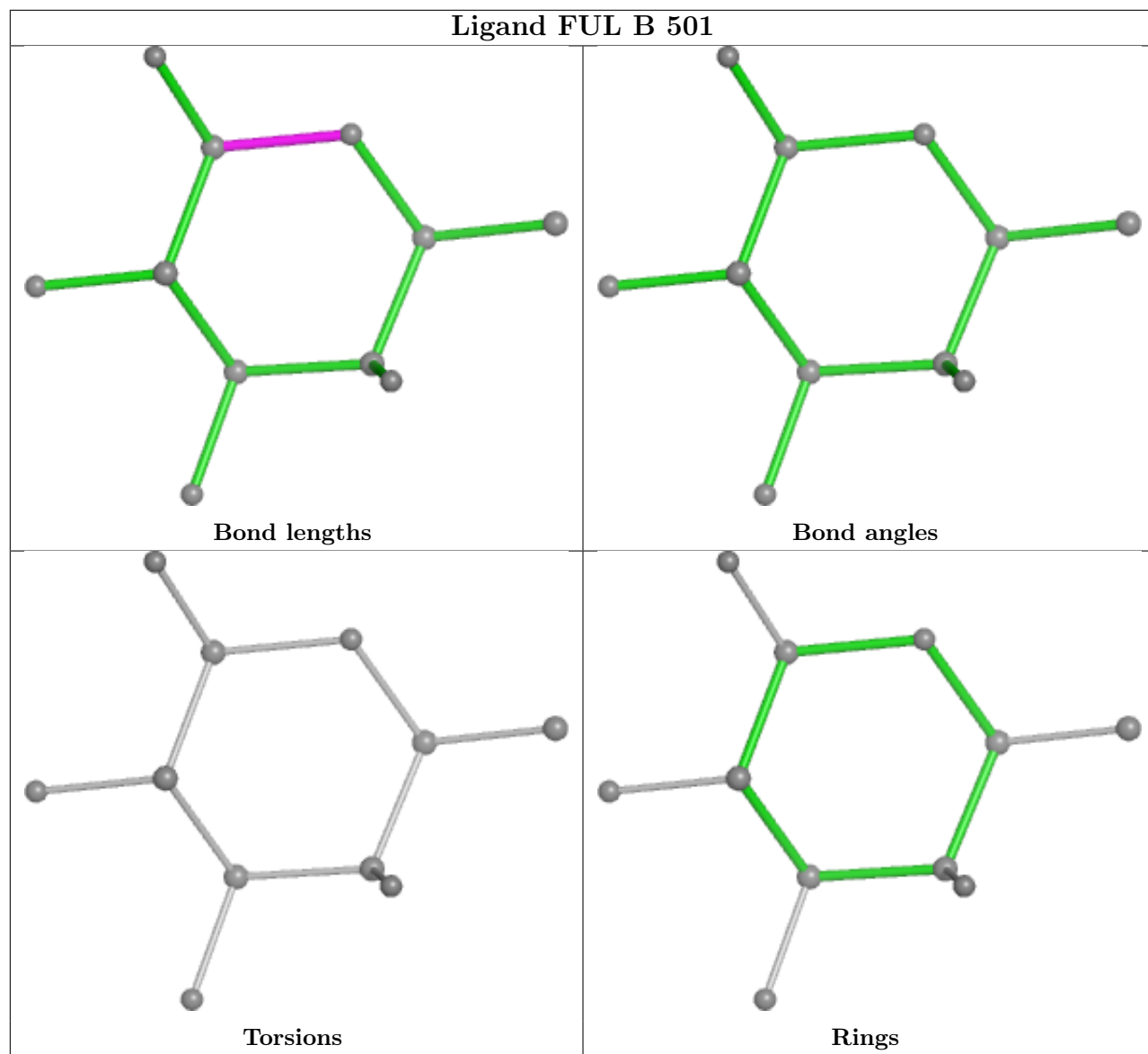
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

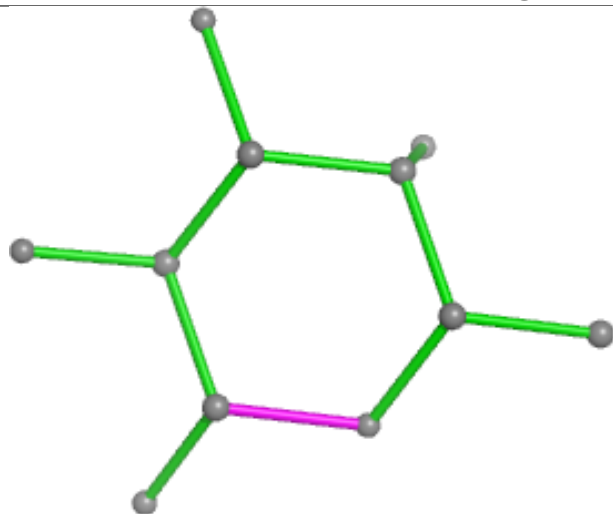
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

## Ligand FUL B 501

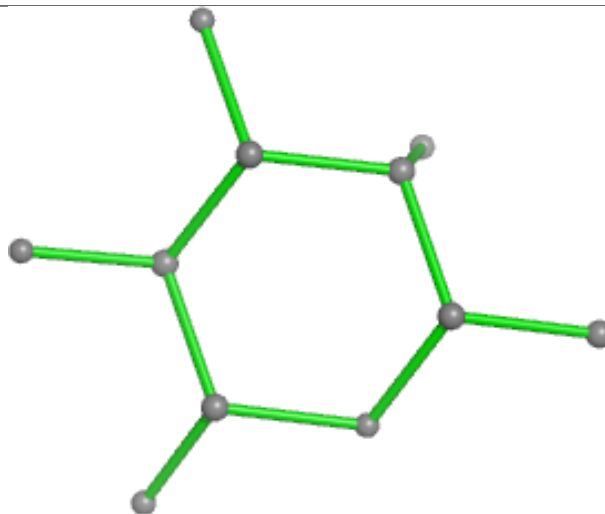




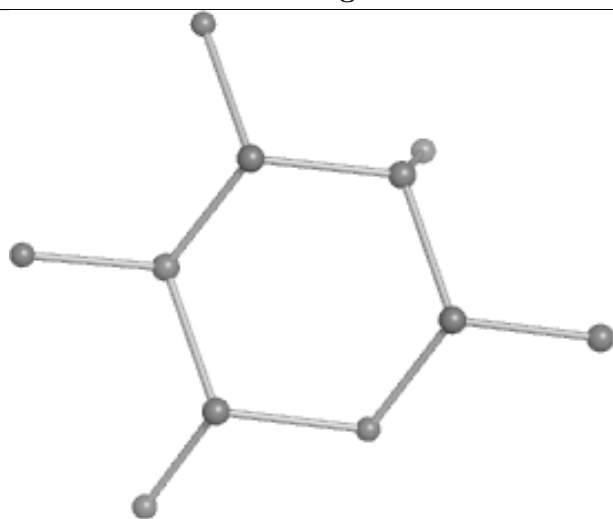
## Ligand FUL C 501



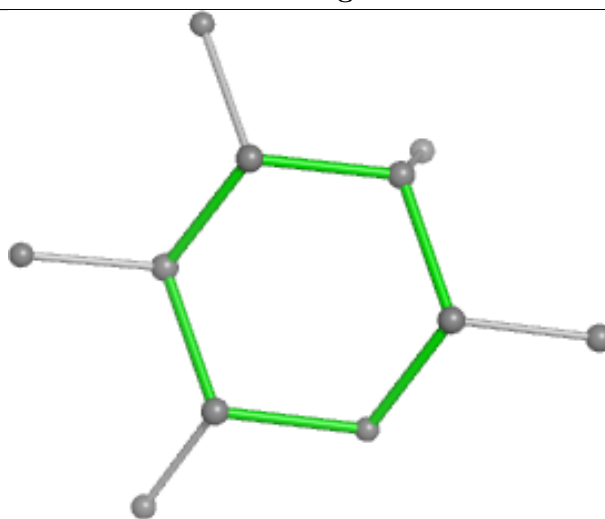
Bond lengths



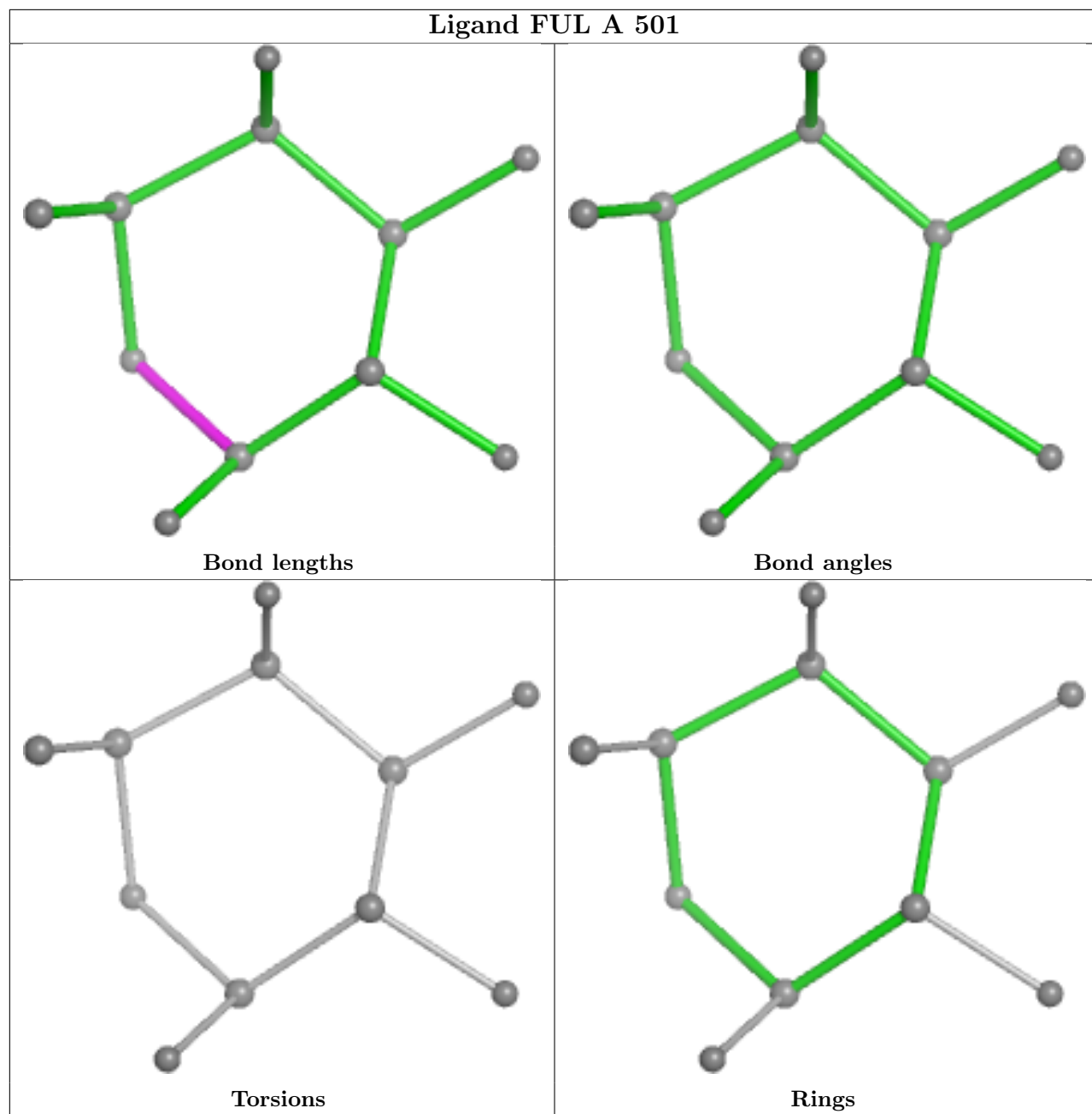
Bond angles

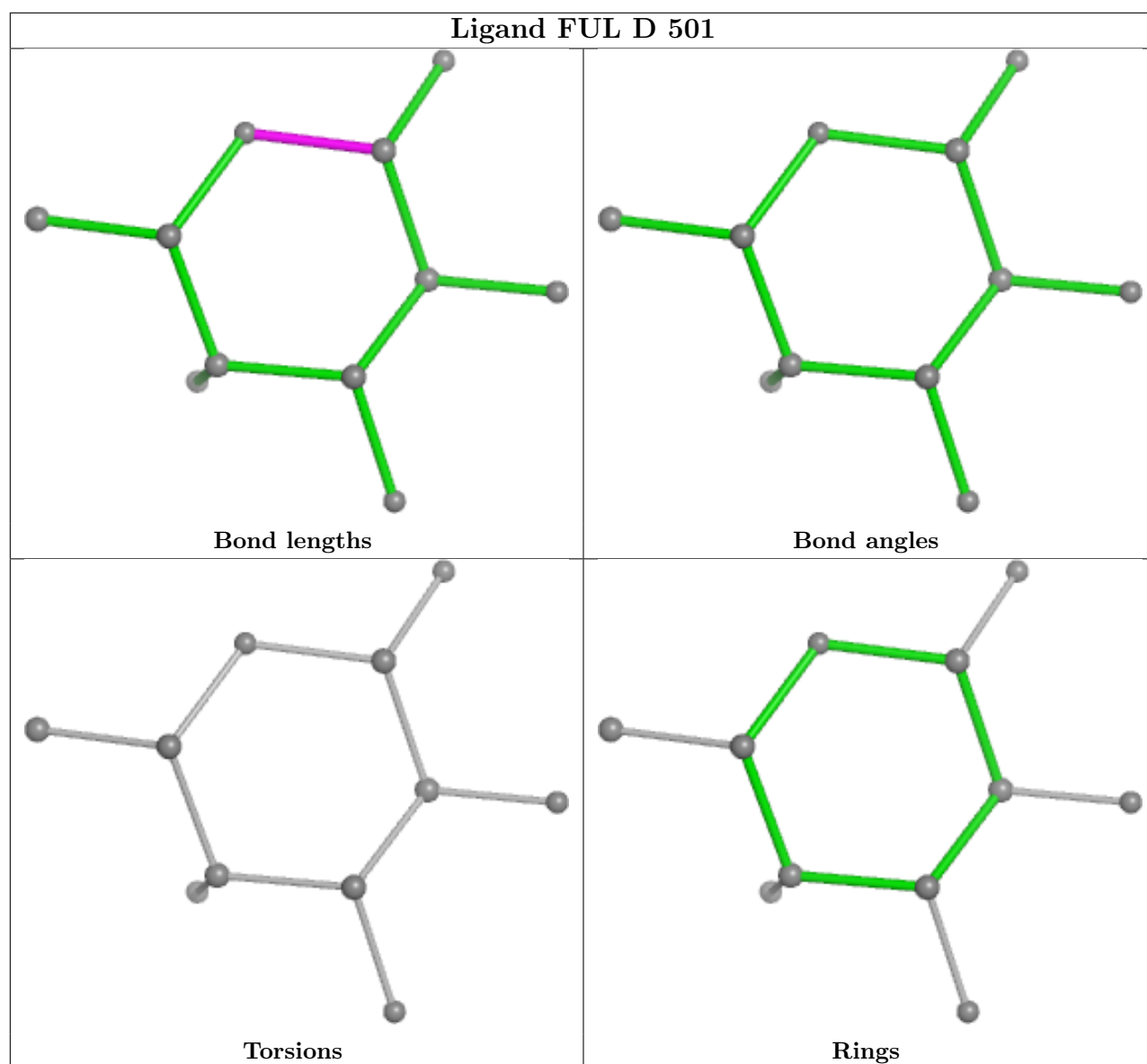


Torsions



Rings





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	422/435 (97%)	-0.02	5 (1%) 76 77	37, 68, 98, 145	2 (0%)
1	B	422/435 (97%)	0.31	10 (2%) 59 61	38, 84, 111, 167	2 (0%)
1	C	422/435 (97%)	0.35	22 (5%) 34 35	42, 82, 130, 169	1 (0%)
1	D	422/435 (97%)	0.47	29 (6%) 24 25	39, 85, 139, 187	2 (0%)
All	All	1688/1740 (97%)	0.28	66 (3%) 44 45	37, 80, 122, 187	7 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	201	LEU	6.5
1	B	400	LYS	4.4
1	C	179	GLY	4.3
1	C	171	LYS	4.0
1	C	168	ARG	3.9
1	D	168	ARG	3.8
1	B	446	ASN	3.6
1	A	445	LEU	3.6
1	D	169	THR	3.4
1	D	25	GLY	3.4
1	A	427	LYS	3.3
1	C	427	LYS	3.3
1	D	445	LEU	3.3
1	C	217	PRO	3.2
1	B	215	ILE	3.2
1	C	180	LYS	3.1
1	D	131	LYS	3.1
1	B	445	LEU	3.0
1	A	442	GLU	3.0
1	D	217	PRO	3.0
1	B	217	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	216	TYR	2.9
1	C	169	THR	2.8
1	B	56	LEU	2.8
1	D	227	LEU	2.7
1	C	412	ARG	2.7
1	C	68	LEU	2.7
1	D	55[A]	MET	2.7
1	B	222	ALA	2.6
1	C	173	THR	2.6
1	D	216	TYR	2.6
1	C	446	ASN	2.5
1	D	73	TYR	2.5
1	C	52	ILE	2.5
1	D	427	LYS	2.5
1	B	33	LEU	2.5
1	D	56	LEU	2.5
1	D	181	TRP	2.5
1	C	445	LEU	2.5
1	B	216	TYR	2.4
1	D	76	LEU	2.4
1	D	446	ASN	2.4
1	D	167	GLY	2.4
1	C	166	LEU	2.4
1	D	166	LEU	2.4
1	D	224	THR	2.3
1	D	215	ILE	2.3
1	C	25	GLY	2.3
1	A	446	ASN	2.3
1	D	234	ILE	2.3
1	D	220	MET	2.2
1	D	243	ILE	2.2
1	C	442	GLU	2.2
1	D	151	LEU	2.2
1	C	167	GLY	2.1
1	D	201	LEU	2.1
1	C	222	ALA	2.1
1	D	398	LYS	2.1
1	B	144	LYS	2.1
1	D	177	THR	2.1
1	D	125	VAL	2.0
1	D	165	PRO	2.0
1	D	192	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	164	TYR	2.0
1	C	34	LYS	2.0
1	C	428	PRO	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

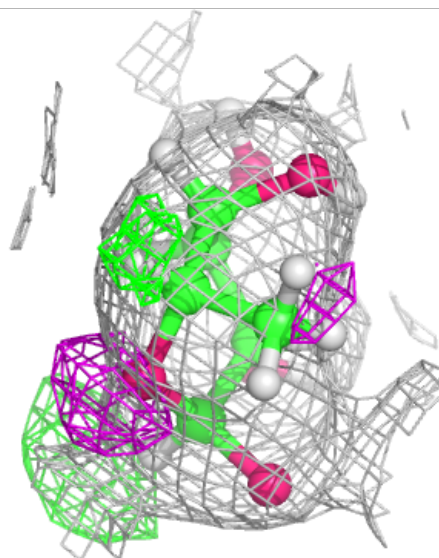
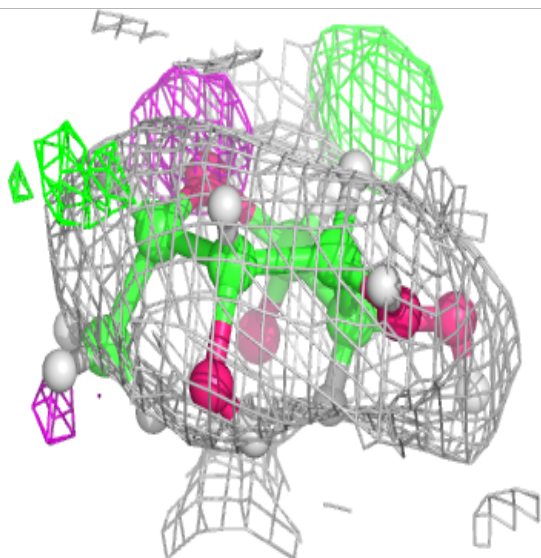
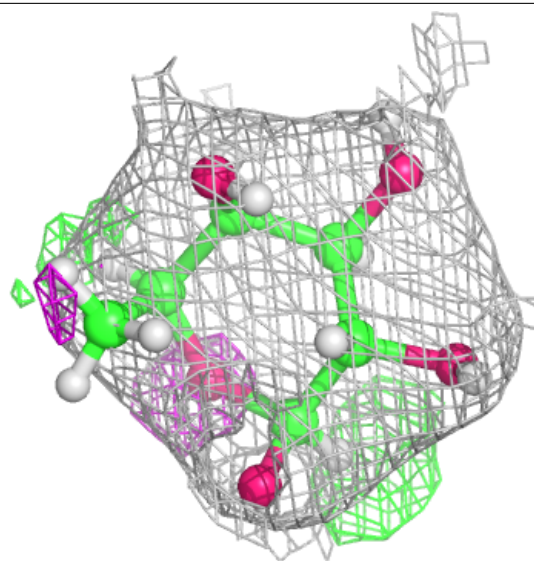
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	A	502	1/1	0.72	0.12	152,152,152,152	0
4	CL	A	503	1/1	0.80	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.

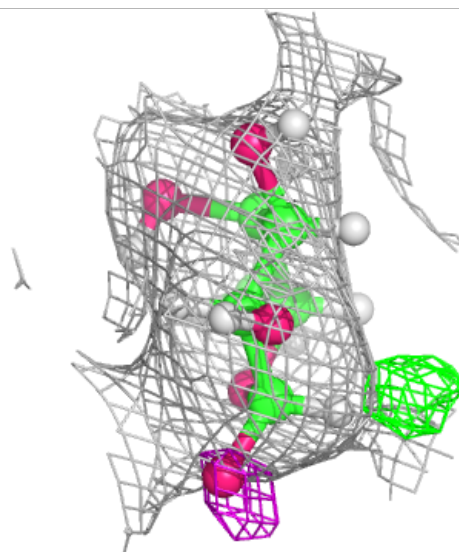
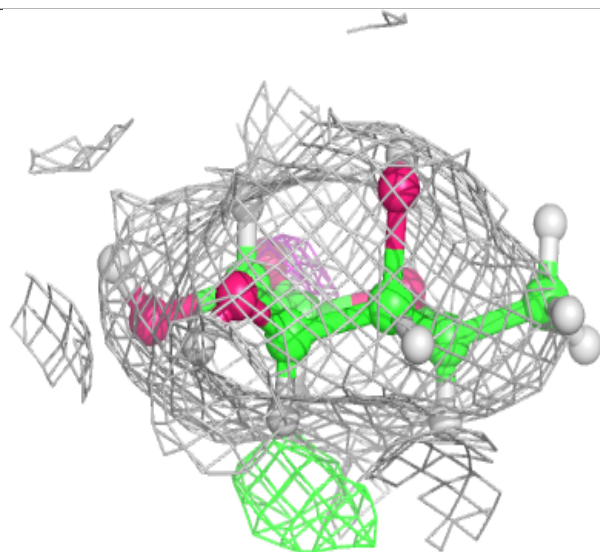
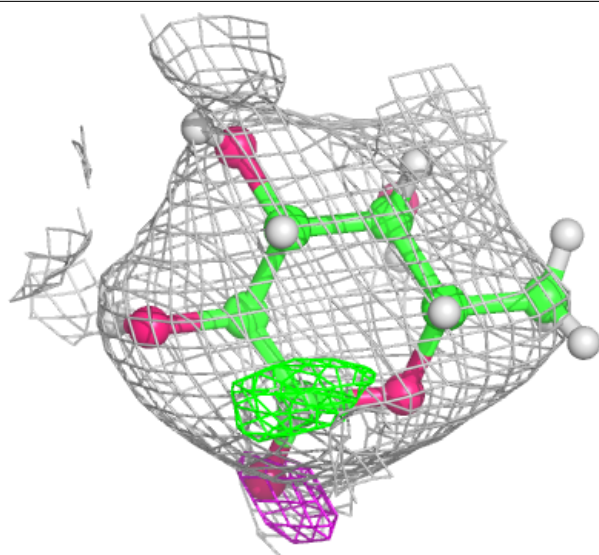
**Electron density around FUL A 501:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FUL C 501:**

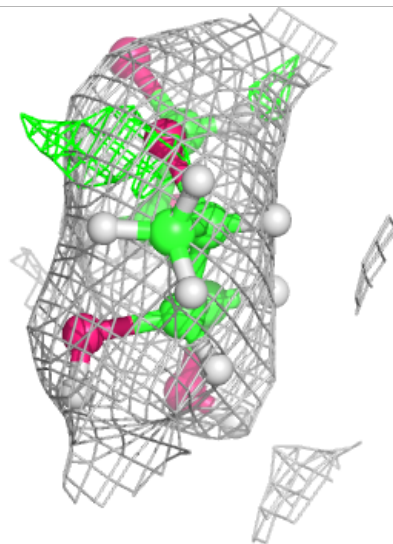
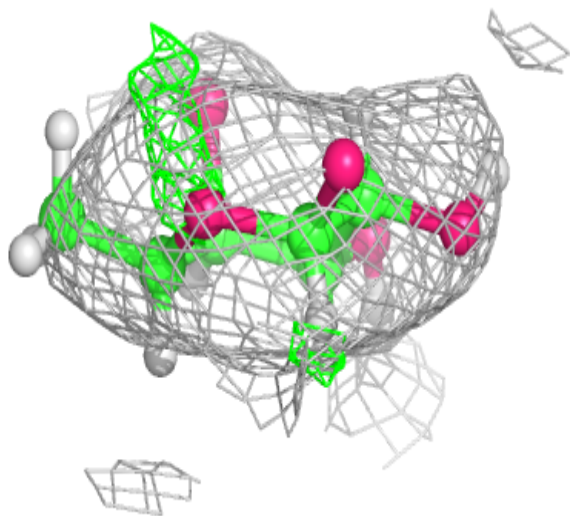
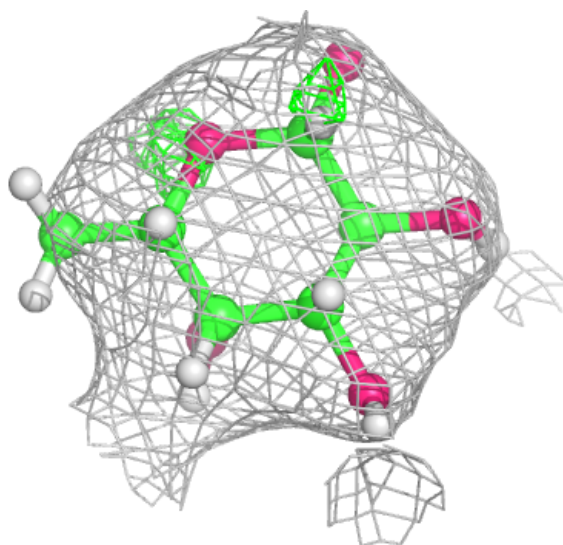
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





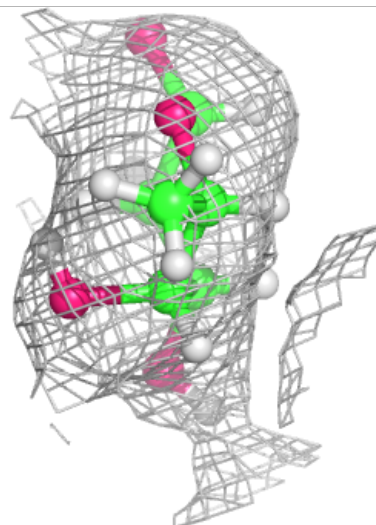
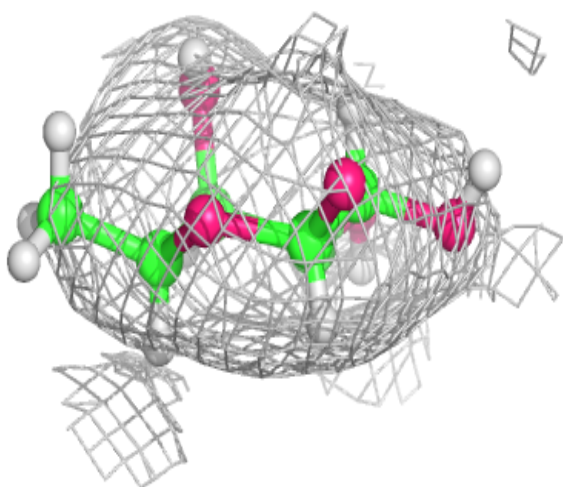
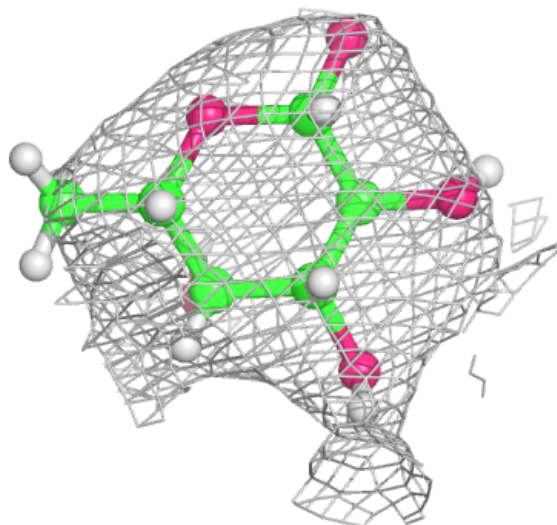
**Electron density around FUL B 501:**

$2mF_o-DF_c$  (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.