



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 02:07 PM BST

PDB ID : 5AWV  
Title : Crystal structure of glycopeptide hexose oxidase DBV29 complexed with te-  
icoplanin  
Authors : Liu, Y.C.; Li, T.L.  
Deposited on : 2015-07-09  
Resolution : 1.93 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

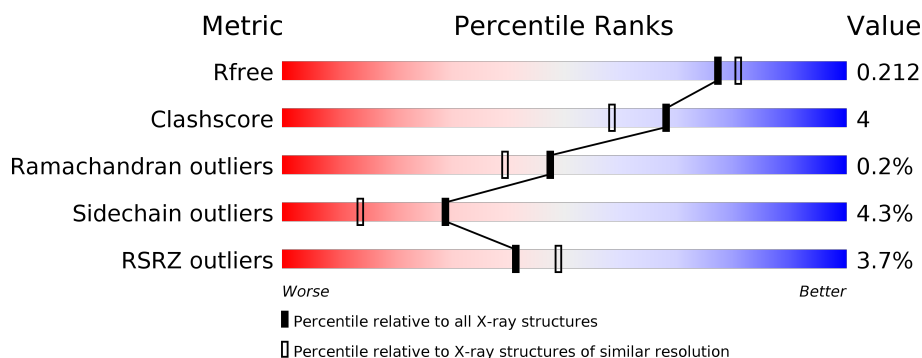
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.93 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))
$R_{free}$	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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 on 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	523	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>5%</div> </div> </div>
1	B	523	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>5%</div> </div> </div>
1	C	523	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>5%</div> </div> </div>
1	D	523	<div> <div>7%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>5%</div> </div> </div>
2	I	7	<div> <div></div> <div> <div>71%</div> <div>29%</div> </div> </div>
2	J	7	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	K	7	
2	L	7	
2	M	7	
2	N	7	
2	O	7	
2	P	7	

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
2	GHP	I	1	-	-	-	X
2	3FG	I	7	-	-	-	X
2	GHP	K	5	-	-	-	X
2	3FG	K	7	-	-	-	X
2	GHP	L	5	-	-	-	X
2	3FG	L	7	-	-	-	X
2	GHP	M	1	-	-	-	X
2	GHP	M	5	-	-	-	X
2	OMY	M	6	-	-	-	X
2	3FG	M	7	-	-	-	X
5	T55	B	602	-	-	-	X
5	T55	N	101	-	-	X	-
5	T55	O	101	-	-	-	X
6	MAN	I	101	-	-	-	X
6	MAN	K	102	-	-	-	X
6	MAN	L	101	-	-	-	X
6	MAN	M	102	-	-	-	X
7	NAG	I	102	-	-	-	X
7	NAG	J	102	-	-	-	X
7	NAG	K	103	-	-	-	X
7	NAG	L	102	-	-	-	X
7	NAG	M	103	-	-	-	X
7	NAG	O	103	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 18119 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.

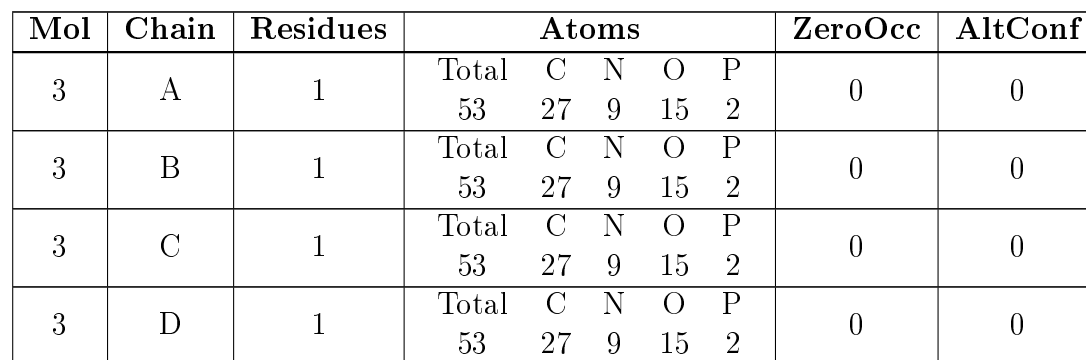
- Molecule 1 is a protein called Putative hexose oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			3856	2441	685	716	14			
1	B	498	Total	C	N	O	S	0	0	0
			3856	2441	685	716	14			
1	C	498	Total	C	N	O	S	0	0	0
			3856	2441	685	716	14			
1	D	498	Total	C	N	O	S	0	0	0
			3856	2441	685	716	14			

- Molecule 2 is a protein called TEICOPLANIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	7	Total	C	Cl	N	O	0	0	0
			85	58	2	7	18			
2	J	7	Total	C	Cl	N	O	0	0	0
			85	58	2	7	18			
2	K	7	Total	C	Cl	N	O	0	0	0
			85	58	2	7	18			
2	L	7	Total	C	Cl	N	O	0	0	0
			85	58	2	7	18			
2	M	7	Total	C	Cl	N	O	0	0	0
			85	58	2	7	18			
2	N	7	Total	C	Cl	N	O	0	0	0
			85	58	2	7	18			
2	O	7	Total	C	Cl	N	O	0	0	0
			85	58	2	7	18			
2	P	7	Total	C	Cl	N	O	0	0	0
			85	58	2	7	18			

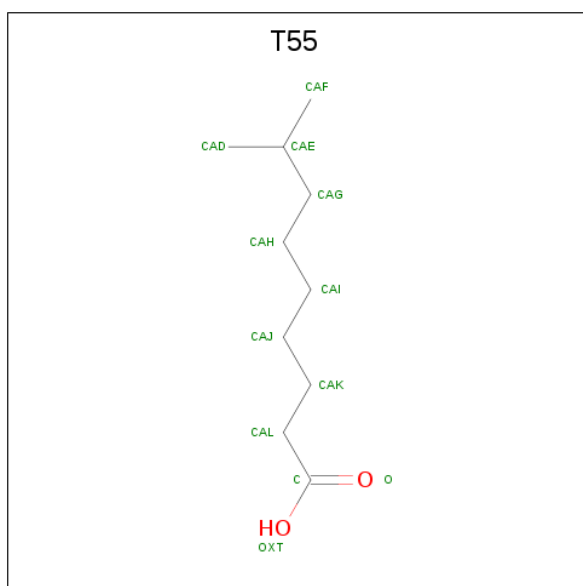
- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



- CIT
- 
- The chemical structure of Citric acid (CIT) is shown. It consists of a central carbon atom (C3) bonded to three hydroxyl groups (OH) and a carboxyl group (COOH). The carboxyl group is further bonded to a methylene group (CH2), which is in turn bonded to another carboxyl group (COOH). The atoms are labeled with green text: C1, C2, C3, C4, C5, C6, C7, O1, O2, O3, O4, O5, O6, O7. The hydroxyl groups are shown in red, and the carboxyl groups are shown in red. The methylene group is shown in green.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		
4	B	1	Total	C	O	0	0
			13	6	7		
4	C	1	Total	C	O	0	0
			13	6	7		
4	D	1	Total	C	O	0	0
			13	6	7		
4	O	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is 8-METHYLNONANOIC ACID (three-letter code: T55) (formula: C<sub>10</sub>H<sub>20</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			11	10	1		
5	K	1	Total	C	O	0	0
			11	10	1		
5	M	1	Total	C	O	0	0
			11	10	1		
5	N	1	Total	C	O	0	0
			11	10	1		
5	O	1	Total	C	O	0	0
			11	10	1		
5	P	1	Total	C	O	0	0
			11	10	1		

- Molecule 6 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	I	1	Total	C	O	0	0
			11	6	5		
6	J	1	Total	C	O	0	0
			11	6	5		
6	K	1	Total	C	O	0	0
			11	6	5		
6	L	1	Total	C	O	0	0
			11	6	5		
6	M	1	Total	C	O	0	0
			11	6	5		
6	N	1	Total	C	O	0	0
			11	6	5		
6	O	1	Total	C	O	0	0
			11	6	5		
6	P	1	Total	C	O	0	0
			11	6	5		

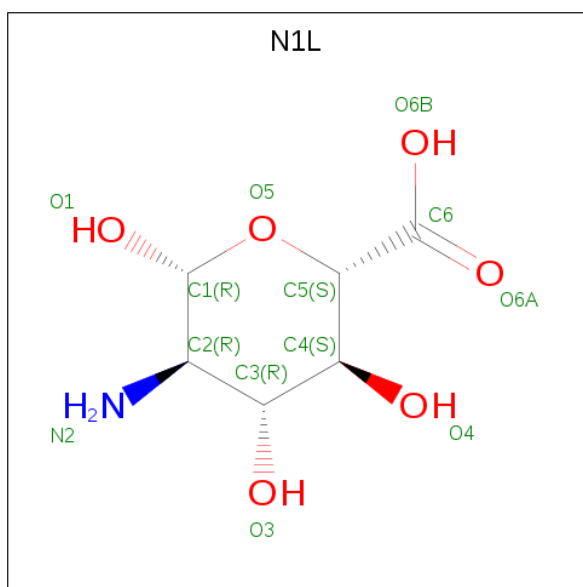
- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	I	1	Total	C	N	O	0	0
			14	8	1	5		
7	J	1	Total	C	N	O	0	0
			14	8	1	5		
7	K	1	Total	C	N	O	0	0
			14	8	1	5		
7	L	1	Total	C	N	O	0	0
			14	8	1	5		
7	M	1	Total	C	N	O	0	0
			14	8	1	5		
7	N	1	Total	C	N	O	0	0
			14	8	1	5		
7	O	1	Total	C	N	O	0	0
			14	8	1	5		
7	P	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is 2-amino-2-deoxy-beta-D-glucopyranuronic acid (three-letter code: N1L) (formula: C<sub>6</sub>H<sub>11</sub>NO<sub>6</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	K	1	Total	C	N	O	0	0
			12	6	1	5		
8	L	1	Total	C	N	O	0	0
			12	6	1	5		
8	M	1	Total	C	N	O	0	0
			12	6	1	5		
8	N	1	Total	C	N	O	0	0
			12	6	1	5		
8	O	1	Total	C	N	O	0	0
			12	6	1	5		
8	P	1	Total	C	N	O	0	0
			12	6	1	5		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	425	Total	O	0	0
			425	425		
9	B	379	Total	O	0	0
			379	379		
9	C	327	Total	O	0	0
			327	327		
9	D	217	Total	O	0	0
			217	217		
9	I	6	Total	O	0	0
			6	6		
9	J	5	Total	O	0	0
			5	5		

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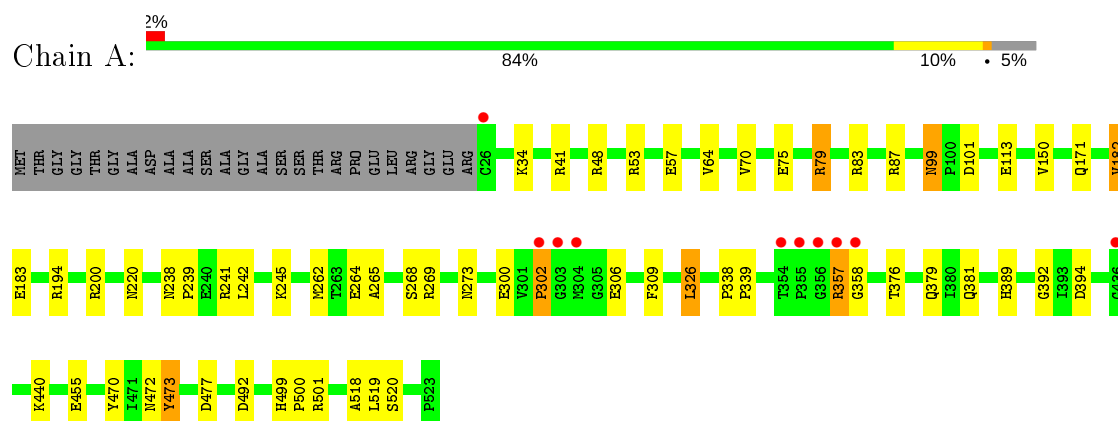
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	K	3	Total 3	O 3	0	0
9	L	1	Total 1	O 1	0	0
9	M	1	Total 1	O 1	0	0
9	N	12	Total 12	O 12	0	0
9	O	16	Total 16	O 16	0	0
9	P	8	Total 8	O 8	0	0

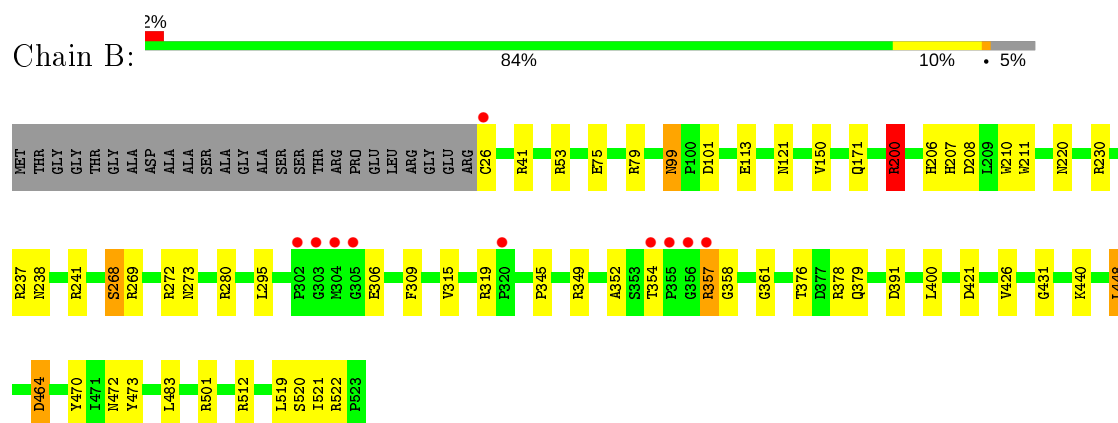
### 3 Residue-property plots [i](#)

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.

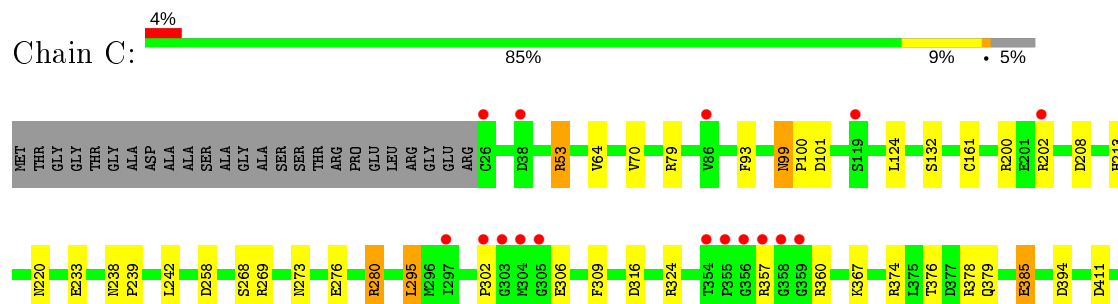
- Molecule 1: Putative hexose oxidase

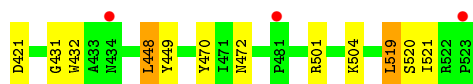


- Molecule 1: Putative hexose oxidase



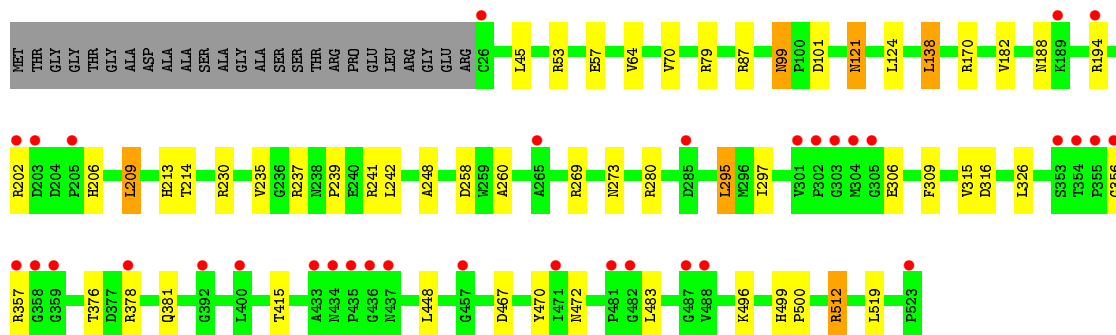
- Molecule 1: Putative hexose oxidase





- Molecule 1: Putative hexose oxidase

Chain D: 7% 85% 10% 5%



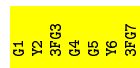
- Molecule 2: TEICOPLANIN

Chain I: 71% 29%



- Molecule 2: TEICOPLANIN

Chain J: 100%



- Molecule 2: TEICOPLANIN

Chain K: 86% 14%



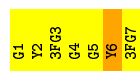
- Molecule 2: TEICOPLANIN

Chain L: 43% 57%

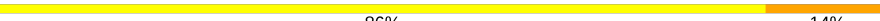


- Molecule 2: TEICOPLANIN

Chain M: 86% 14%




## ● Molecule 2: TEICOPLANIN

Chain N:  86% 14%

G1	Y2	3FG3	G4	G5	Y6	3FG7
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## ● Molecule 2: TEICOPLANIN

Chain O:  100%

G1	Y2	3FG3	G4	G5	Y6	3FG7
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## ● Molecule 2: TEICOPLANIN

Chain P:  100%

G1	Y2	3FG3	G4	G5	Y6	3FG7
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.79Å 150.78Å 124.85Å 90.00° 98.40° 90.00°	Depositor
Resolution (Å)	29.40 – 1.93 29.49 – 1.93	Depositor EDS
% Data completeness (in resolution range)	97.6 (29.40-1.93) 97.6 (29.49-1.93)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 1.93Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, $R_{free}$	0.156 , 0.205 0.167 , 0.212	Depositor DCC
$R_{free}$ test set	8214 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.9	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 50.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18119	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GHP, NAG, 3MY, T55, N1L, CIT, 3FG, OMY, FAD, MAN

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	1.07	3/3966 (0.1%)	1.04	16/5412 (0.3%)
1	B	1.02	1/3966 (0.0%)	1.03	14/5412 (0.3%)
1	C	0.95	0/3966	1.02	16/5412 (0.3%)
1	D	0.85	0/3966	0.94	9/5412 (0.2%)
All	All	0.98	4/15864 (0.0%)	1.01	55/21648 (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	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	75	GLU	CD-OE1	7.79	1.34	1.25
1	A	53	ARG	CZ-NH1	5.67	1.40	1.33
1	A	183	GLU	CD-OE2	-5.50	1.19	1.25
1	A	264	GLU	CD-OE2	5.15	1.31	1.25

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	53	ARG	NE-CZ-NH1	10.27	125.44	120.30
1	A	53	ARG	NE-CZ-NH2	-10.15	115.23	120.30
1	B	53	ARG	NE-CZ-NH1	10.02	125.31	120.30
1	C	53	ARG	NE-CZ-NH2	-9.61	115.50	120.30
1	C	448	LEU	CB-CG-CD2	8.79	125.94	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	357	ARG	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	3856	0	3743	38	0
1	B	3856	0	3743	29	0
1	C	3856	0	3744	27	0
1	D	3856	0	3744	21	0
2	I	85	0	35	2	0
2	J	85	0	36	0	0
2	K	85	0	32	1	0
2	L	85	0	34	3	0
2	M	85	0	34	1	0
2	N	85	0	34	5	0
2	O	85	0	36	0	0
2	P	85	0	34	0	0
3	A	53	0	29	0	0
3	B	53	0	29	0	0
3	C	53	0	29	0	0
3	D	53	0	29	0	0
4	A	13	0	5	0	0
4	B	13	0	5	0	0
4	C	13	0	5	0	0
4	D	13	0	5	0	0
4	O	13	0	5	0	0
5	B	11	0	19	1	0
5	K	11	0	19	1	0
5	M	11	0	19	4	0
5	N	11	0	19	14	0
5	O	11	0	19	0	0
5	P	11	0	19	0	1
6	I	11	0	10	0	0
6	J	11	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	11	0	10	0	0
6	L	11	0	10	0	0
6	M	11	0	10	0	0
6	N	11	0	10	0	0
6	O	11	0	9	0	0
6	P	11	0	10	0	0
7	I	14	0	13	0	0
7	J	14	0	13	0	0
7	K	14	0	13	0	0
7	L	14	0	13	3	0
7	M	14	0	13	0	0
7	N	14	0	13	0	0
7	O	14	0	13	0	0
7	P	14	0	13	0	0
8	K	12	0	7	1	0
8	L	12	0	7	2	0
8	M	12	0	7	1	0
8	N	12	0	6	0	0
8	O	12	0	7	0	0
8	P	12	0	7	0	0
9	A	425	0	0	10	4
9	B	379	0	0	7	1
9	C	327	0	0	7	1
9	D	217	0	0	5	0
9	I	6	0	0	0	0
9	J	5	0	0	0	0
9	K	3	0	0	0	0
9	L	1	0	0	0	0
9	M	1	0	0	0	0
9	N	12	0	0	0	0
9	O	16	0	0	1	0
9	P	8	0	0	0	0
All	All	18119	0	15728	123	4

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 4.

The worst 5 of 123 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ALA:HA	5:N:101:T55:CAD	1.84	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ALA:HA	5:N:101:T55:HAD1	1.51	0.92
1:D:269:ARG:HE	1:D:273:ASN:HD21	1.23	0.86
1:C:269:ARG:HE	1:C:273:ASN:HD21	1.23	0.86
1:A:519:LEU:N	9:A:701:HOH:O	1.59	0.81

All (4) 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)
9:A:800:HOH:O	9:C:948:HOH:O[1_655]	2.02	0.18
9:A:722:HOH:O	9:A:890:HOH:O[1_455]	2.02	0.18
5:P:101:T55:CAD	9:A:724:HOH:O[2_7413]	2.16	0.04
9:A:886:HOH:O	9:B:983:HOH:O[2_7513]	2.19	0.01

## 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	496/523 (95%)	479 (97%)	16 (3%)	1 (0%)	47	39
1	B	496/523 (95%)	478 (96%)	18 (4%)	0	100	100
1	C	496/523 (95%)	478 (96%)	17 (3%)	1 (0%)	47	39
1	D	496/523 (95%)	473 (95%)	21 (4%)	2 (0%)	34	24
All	All	1984/2092 (95%)	1908 (96%)	72 (4%)	4 (0%)	47	39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	PRO
1	D	356	GLY
1	D	376	THR

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Mol	Chain	Res	Type
1	C	302	PRO

### 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	404/419 (96%)	390 (96%)	14 (4%)	36	21
1	B	404/419 (96%)	386 (96%)	18 (4%)	27	12
1	C	404/419 (96%)	387 (96%)	17 (4%)	30	14
1	D	404/419 (96%)	383 (95%)	21 (5%)	23	9
All	All	1616/1676 (96%)	1546 (96%)	70 (4%)	29	14

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	483	LEU
1	C	268	SER
1	D	378	ARG
1	C	79	ARG
1	C	132	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	379	GLN
1	C	99	ASN
1	D	379	GLN
1	B	437	ASN
1	B	513	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

56 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	OMY	O	6	2,7	12,14,15	2.40	5 (41%)	17,19,21	1.63	2 (11%)
2	3FG	N	7	2,6	9,13,13	2.66	4 (44%)	13,18,18	1.37	2 (15%)
2	GHP	P	4	8,2	10,11,12	2.10	3 (30%)	11,14,16	1.86	4 (36%)
2	GHP	N	1	2	10,11,12	2.42	5 (50%)	11,14,16	1.16	0
2	GHP	L	4	8,2	10,11,12	3.17	4 (40%)	11,14,16	1.11	1 (9%)
2	GHP	M	4	8,2	10,11,12	2.94	3 (30%)	11,14,16	1.01	0
2	3FG	O	7	2,6	9,13,13	2.92	3 (33%)	13,18,18	1.76	2 (15%)
2	GHP	I	5	2	10,11,12	3.25	3 (30%)	11,14,16	2.18	4 (36%)
2	GHP	O	1	2	10,11,12	3.14	2 (20%)	11,14,16	0.84	0
2	3FG	O	3	2	11,12,13	1.73	3 (27%)	13,16,18	1.75	4 (30%)
2	GHP	M	5	2	10,11,12	3.56	3 (30%)	11,14,16	2.25	5 (45%)
2	3FG	I	7	2,6	9,13,13	2.94	3 (33%)	13,18,18	1.59	3 (23%)
2	GHP	O	5	2	10,11,12	3.16	6 (60%)	11,14,16	1.74	2 (18%)
2	OMY	I	6	2,7	12,14,15	2.94	7 (58%)	17,19,21	2.48	5 (29%)
2	3MY	P	2	2	12,13,14	2.05	6 (50%)	14,17,19	1.92	3 (21%)
2	GHP	N	5	2	10,11,12	3.05	2 (20%)	11,14,16	2.20	3 (27%)
2	3FG	J	3	2	11,12,13	2.53	6 (54%)	13,16,18	2.40	3 (23%)
2	OMY	K	6	2,7	12,14,15	2.42	5 (41%)	17,19,21	1.64	4 (23%)
2	OMY	M	6	2,7	12,14,15	2.62	4 (33%)	17,19,21	2.24	5 (29%)
2	3MY	K	2	2	12,13,14	3.36	3 (25%)	14,17,19	2.10	3 (21%)
2	3MY	O	2	2	12,13,14	2.05	3 (25%)	14,17,19	1.96	5 (35%)
2	3MY	L	2	2	12,13,14	2.64	4 (33%)	14,17,19	2.18	4 (28%)
2	GHP	I	4	2	10,11,12	2.74	3 (30%)	11,14,16	1.13	1 (9%)
2	3MY	N	2	2	12,13,14	2.76	2 (16%)	14,17,19	2.61	7 (50%)
2	GHP	J	5	2	10,11,12	2.61	2 (20%)	11,14,16	2.57	4 (36%)
2	3MY	J	2	2	12,13,14	2.90	3 (25%)	14,17,19	1.90	6 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	3FG	K	3	2	11,12,13	3.06	2 (18%)	13,16,18	1.81	3 (23%)
2	3FG	M	7	2,6	9,13,13	2.60	3 (33%)	13,18,18	2.30	2 (15%)
2	GHP	K	5	2	10,11,12	3.82	2 (20%)	11,14,16	1.68	3 (27%)
2	3FG	K	7	2,6	9,13,13	2.67	3 (33%)	13,18,18	1.50	2 (15%)
2	GHP	I	1	2	10,11,12	3.15	2 (20%)	11,14,16	0.86	0
2	GHP	K	1	2	10,11,12	3.34	2 (20%)	11,14,16	0.95	1 (9%)
2	3FG	P	3	2	11,12,13	2.30	4 (36%)	13,16,18	1.65	3 (23%)
2	GHP	J	1	2	10,11,12	2.87	3 (30%)	11,14,16	1.44	2 (18%)
2	OMY	N	6	2,7	12,14,15	2.37	7 (58%)	17,19,21	1.97	5 (29%)
2	3FG	N	3	2	11,12,13	2.43	3 (27%)	13,16,18	2.13	3 (23%)
2	GHP	O	4	8,2	10,11,12	3.03	3 (30%)	11,14,16	1.15	1 (9%)
2	3MY	I	2	2	12,13,14	2.20	3 (25%)	14,17,19	2.42	5 (35%)
2	OMY	L	6	2,7	12,14,15	2.62	4 (33%)	17,19,21	2.12	6 (35%)
2	3FG	I	3	2	11,12,13	3.43	2 (18%)	13,16,18	1.77	4 (30%)
2	GHP	K	4	8,2	10,11,12	2.14	3 (30%)	11,14,16	1.02	0
2	3MY	M	2	2	12,13,14	2.87	2 (16%)	14,17,19	2.77	3 (21%)
2	GHP	L	1	2	10,11,12	3.07	3 (30%)	11,14,16	0.62	0
2	3FG	L	7	2,6	9,13,13	3.22	2 (22%)	13,18,18	1.81	3 (23%)
2	GHP	L	5	2	10,11,12	3.21	2 (20%)	11,14,16	2.64	5 (45%)
2	3FG	J	7	2,6	9,13,13	3.38	6 (66%)	13,18,18	1.48	2 (15%)
2	GHP	P	5	2	10,11,12	3.39	3 (30%)	11,14,16	2.72	5 (45%)
2	GHP	J	4	2	10,11,12	3.24	5 (50%)	11,14,16	1.19	1 (9%)
2	OMY	P	6	2,7	12,14,15	2.11	2 (16%)	17,19,21	2.37	4 (23%)
2	GHP	P	1	2	10,11,12	3.62	7 (70%)	11,14,16	1.06	1 (9%)
2	GHP	N	4	8,2	10,11,12	3.73	2 (20%)	11,14,16	0.94	0
2	3FG	P	7	2,6	9,13,13	3.21	3 (33%)	13,18,18	1.50	3 (23%)
2	GHP	M	1	2	10,11,12	3.31	3 (30%)	11,14,16	1.21	1 (9%)
2	3FG	M	3	2	11,12,13	3.25	3 (27%)	13,16,18	1.47	2 (15%)
2	OMY	J	6	2,7	12,14,15	2.81	7 (58%)	17,19,21	2.61	5 (29%)
2	3FG	L	3	2	11,12,13	3.43	5 (45%)	13,16,18	1.63	3 (23%)

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	OMY	O	6	2,7	-	1/9/10/12	0/1/1/1
2	3FG	N	7	2,6	-	1/4/8/8	0/1/1/1
2	GHP	P	4	8,2	-	1/4/6/8	0/1/1/1
2	GHP	N	1	2	-	1/4/6/8	0/1/1/1
2	GHP	L	4	8,2	-	2/4/6/8	0/1/1/1
2	GHP	M	4	8,2	-	0/4/6/8	0/1/1/1
2	3FG	O	7	2,6	-	1/4/8/8	0/1/1/1
2	GHP	I	5	2	-	0/4/6/8	0/1/1/1
2	GHP	O	1	2	-	2/4/6/8	0/1/1/1
2	3FG	O	3	2	-	0/4/6/8	0/1/1/1
2	GHP	M	5	2	-	0/4/6/8	0/1/1/1
2	3FG	I	7	2,6	-	0/4/8/8	0/1/1/1
2	GHP	O	5	2	-	0/4/6/8	0/1/1/1
2	OMY	I	6	2,7	-	1/9/10/12	0/1/1/1
2	3MY	P	2	2	-	0/5/6/8	0/1/1/1
2	GHP	N	5	2	-	0/4/6/8	0/1/1/1
2	3FG	J	3	2	-	0/4/6/8	0/1/1/1
2	OMY	K	6	2,7	-	3/9/10/12	0/1/1/1
2	OMY	M	6	2,7	-	0/9/10/12	0/1/1/1
2	3MY	K	2	2	-	1/5/6/8	0/1/1/1
2	3MY	O	2	2	-	1/5/6/8	0/1/1/1
2	3MY	L	2	2	-	0/5/6/8	0/1/1/1
2	GHP	I	4	2	-	3/4/6/8	0/1/1/1
2	3MY	N	2	2	-	0/5/6/8	0/1/1/1
2	GHP	J	5	2	-	0/4/6/8	0/1/1/1
2	3MY	J	2	2	-	0/5/6/8	0/1/1/1
2	3FG	K	3	2	-	0/4/6/8	0/1/1/1
2	3FG	M	7	2,6	-	1/4/8/8	0/1/1/1
2	GHP	K	5	2	-	0/4/6/8	0/1/1/1
2	3FG	K	7	2,6	-	1/4/8/8	0/1/1/1
2	GHP	I	1	2	-	2/4/6/8	0/1/1/1
2	GHP	K	1	2	-	4/4/6/8	0/1/1/1
2	3FG	P	3	2	-	2/4/6/8	0/1/1/1
2	GHP	J	1	2	-	1/4/6/8	0/1/1/1
2	OMY	N	6	2,7	-	1/9/10/12	0/1/1/1
2	3FG	N	3	2	-	0/4/6/8	0/1/1/1
2	GHP	O	4	8,2	-	2/4/6/8	0/1/1/1
2	3MY	I	2	2	-	1/5/6/8	0/1/1/1
2	OMY	L	6	2,7	-	2/9/10/12	0/1/1/1
2	3FG	I	3	2	-	0/4/6/8	0/1/1/1
2	GHP	K	4	8,2	-	1/4/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3MY	M	2	2	-	1/5/6/8	0/1/1/1
2	GHP	L	1	2	-	4/4/6/8	0/1/1/1
2	3FG	L	7	2,6	-	1/4/8/8	0/1/1/1
2	GHP	L	5	2	-	0/4/6/8	0/1/1/1
2	3FG	J	7	2,6	-	1/4/8/8	0/1/1/1
2	GHP	P	5	2	-	0/4/6/8	0/1/1/1
2	GHP	J	4	2	-	2/4/6/8	0/1/1/1
2	OMY	P	6	2,7	-	1/9/10/12	0/1/1/1
2	GHP	P	1	2	-	0/4/6/8	0/1/1/1
2	GHP	N	4	8,2	-	2/4/6/8	0/1/1/1
2	3FG	P	7	2,6	-	2/4/8/8	0/1/1/1
2	GHP	M	1	2	-	4/4/6/8	0/1/1/1
2	3FG	M	3	2	-	0/4/6/8	0/1/1/1
2	OMY	J	6	2,7	-	1/9/10/12	0/1/1/1
2	3FG	L	3	2	-	0/4/6/8	0/1/1/1

The worst 5 of 198 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	5	GHP	C1-CA	-10.81	1.41	1.52
2	M	5	GHP	C1-CA	-9.96	1.42	1.52
2	N	4	GHP	C1-CA	-9.85	1.42	1.52
2	K	1	GHP	C1-CA	-9.62	1.42	1.52
2	I	3	3FG	CB-CA	-9.56	1.42	1.52

The worst 5 of 160 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	6	OMY	CG-CB-CA	-7.94	100.86	111.49
2	I	6	OMY	CG-CB-CA	-7.81	101.03	111.49
2	M	7	3FG	C-CA-CB	7.51	121.00	111.28
2	M	2	3MY	CD2-CE2-CZ	-7.48	116.58	120.91
2	P	6	OMY	CG-CB-CA	-6.92	102.22	111.49

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	6	OMY	O-C-CA-CB
2	K	6	OMY	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	K	6	OMY	C-CA-CB-ODE
2	N	6	OMY	O-C-CA-CB
2	L	6	OMY	O-C-CA-CB

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	6	OMY	1	0
2	K	2	3MY	1	0
2	L	2	3MY	1	0
2	N	2	3MY	5	0
2	I	1	GHP	1	0
2	L	6	OMY	1	0
2	I	3	3FG	2	0
2	L	1	GHP	1	0
2	L	3	3FG	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

37 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	NAG	N	103	2	14,14,15	1.31	1 (7%)	17,19,21	1.52	4 (23%)
4	CIT	D	602	-	3,12,12	1.04	0	3,17,17	0.93	0
5	T55	M	101	8	10,10,11	0.41	0	10,10,12	1.11	1 (10%)
5	T55	B	602	8	10,10,11	0.52	0	10,10,12	1.07	0
4	CIT	B	603	-	3,12,12	1.45	0	3,17,17	2.41	2 (66%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	T55	O	101	8	10,10,11	0.57	0	10,10,12	0.63	0
6	MAN	N	102	2	11,11,12	2.34	3 (27%)	15,15,17	1.73	4 (26%)
3	FAD	A	601	1	51,58,58	2.06	13 (25%)	60,89,89	2.13	14 (23%)
4	CIT	A	602	-	3,12,12	1.50	1 (33%)	3,17,17	1.54	1 (33%)
7	NAG	K	103	2	14,14,15	1.03	2 (14%)	17,19,21	1.72	7 (41%)
7	NAG	M	103	2	14,14,15	1.09	2 (14%)	17,19,21	1.55	5 (29%)
7	NAG	J	102	2	14,14,15	2.78	6 (42%)	17,19,21	3.71	9 (52%)
8	N1L	K	104	2,5	9,12,13	3.99	5 (55%)	9,17,19	1.24	1 (11%)
7	NAG	O	103	2	14,14,15	1.42	2 (14%)	17,19,21	1.63	3 (17%)
4	CIT	C	602	-	3,12,12	1.05	0	3,17,17	1.91	2 (66%)
6	MAN	K	102	2	11,11,12	1.27	1 (9%)	15,15,17	2.44	4 (26%)
4	CIT	O	105	-	3,12,12	1.98	1 (33%)	3,17,17	4.05	1 (33%)
7	NAG	I	102	2	14,14,15	1.93	5 (35%)	17,19,21	2.26	8 (47%)
6	MAN	P	102	2	11,11,12	1.71	3 (27%)	15,15,17	1.67	4 (26%)
8	N1L	P	104	2,5	9,12,13	3.99	6 (66%)	9,17,19	0.93	1 (11%)
5	T55	P	101	8	10,10,11	0.88	0	10,10,12	0.64	0
5	T55	N	101	8	10,10,11	0.55	0	10,10,12	1.57	3 (30%)
7	NAG	L	102	2	14,14,15	0.93	1 (7%)	17,19,21	1.75	4 (23%)
8	N1L	O	104	2,5	9,12,13	3.91	4 (44%)	9,17,19	1.94	3 (33%)
6	MAN	M	102	2	11,11,12	1.85	2 (18%)	15,15,17	1.93	4 (26%)
3	FAD	B	601	1	51,58,58	1.82	7 (13%)	60,89,89	2.52	15 (25%)
3	FAD	C	601	1	51,58,58	2.16	9 (17%)	60,89,89	2.51	19 (31%)
8	N1L	N	104	2,5	9,12,13	4.13	5 (55%)	9,17,19	1.27	1 (11%)
6	MAN	J	101	2	11,11,12	3.39	6 (54%)	15,15,17	2.23	1 (6%)
7	NAG	P	103	2	14,14,15	2.10	4 (28%)	17,19,21	1.40	2 (11%)
6	MAN	I	101	2	11,11,12	3.03	4 (36%)	15,15,17	3.19	4 (26%)
8	N1L	M	104	2,5	9,12,13	4.50	7 (77%)	9,17,19	2.93	6 (66%)
5	T55	K	101	8	10,10,11	0.48	0	10,10,12	0.84	0
6	MAN	O	102	2	11,11,12	2.48	4 (36%)	15,15,17	1.69	4 (26%)
8	N1L	L	103	2,5	9,12,13	3.30	4 (44%)	9,17,19	1.51	1 (11%)
6	MAN	L	101	2	11,11,12	0.78	0	15,15,17	1.25	1 (6%)
3	FAD	D	601	1	51,58,58	1.98	9 (17%)	60,89,89	2.52	15 (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
7	NAG	N	103	2	-	2/6/23/26	0/1/1/1
4	CIT	D	602	-	-	1/6/16/16	-
5	T55	M	101	8	-	0/7/8/9	-
5	T55	B	602	8	-	0/7/8/9	-
4	CIT	B	603	-	-	2/6/16/16	-
5	T55	O	101	8	-	1/7/8/9	-
6	MAN	N	102	2	-	2/2/19/22	0/1/1/1
3	FAD	A	601	1	-	4/30/50/50	0/6/6/6
4	CIT	A	602	-	-	1/6/16/16	-
7	NAG	K	103	2	-	2/6/23/26	0/1/1/1
7	NAG	M	103	2	-	3/6/23/26	0/1/1/1
7	NAG	J	102	2	-	2/6/23/26	0/1/1/1
8	N1L	K	104	2,5	-	0/0/21/24	0/1/1/1
7	NAG	O	103	2	-	4/6/23/26	0/1/1/1
4	CIT	C	602	-	-	1/6/16/16	-
6	MAN	K	102	2	-	2/2/19/22	0/1/1/1
4	CIT	O	105	-	-	4/6/16/16	-
7	NAG	I	102	2	-	4/6/23/26	0/1/1/1
6	MAN	P	102	2	-	0/2/19/22	0/1/1/1
8	N1L	P	104	2,5	-	0/0/21/24	0/1/1/1
5	T55	P	101	8	-	5/7/8/9	-
5	T55	N	101	8	-	0/7/8/9	-
7	NAG	L	102	2	-	4/6/23/26	0/1/1/1
8	N1L	O	104	2,5	-	0/0/21/24	0/1/1/1
6	MAN	M	102	2	-	0/2/19/22	1/1/1/1
3	FAD	B	601	1	-	4/30/50/50	0/6/6/6
3	FAD	C	601	1	-	4/30/50/50	0/6/6/6
8	N1L	N	104	2,5	-	0/0/21/24	0/1/1/1
6	MAN	J	101	2	-	2/2/19/22	0/1/1/1
7	NAG	P	103	2	-	2/6/23/26	0/1/1/1
6	MAN	I	101	2	-	0/2/19/22	0/1/1/1
8	N1L	M	104	2,5	-	0/0/21/24	0/1/1/1
5	T55	K	101	8	-	0/7/8/9	-
6	MAN	O	102	2	-	2/2/19/22	0/1/1/1
8	N1L	L	103	2,5	-	0/0/21/24	0/1/1/1
6	MAN	L	101	2	-	2/2/19/22	0/1/1/1
3	FAD	D	601	1	-	5/30/50/50	0/6/6/6

The worst 5 of 117 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	FAD	C4X-C10	10.74	1.49	1.38
8	M	104	N1L	C1-C2	8.62	1.62	1.52
8	N	104	N1L	C1-C2	8.26	1.62	1.52
8	P	104	N1L	C1-C2	8.20	1.62	1.52
6	J	101	MAN	O5-C1	7.79	1.56	1.43

The worst 5 of 154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	102	NAG	O5-C5-C6	13.11	127.75	107.20
3	B	601	FAD	C4-N3-C2	11.22	124.61	115.14
3	C	601	FAD	C4-N3-C2	10.32	123.86	115.14
3	D	601	FAD	C4-N3-C2	8.78	122.56	115.14
3	D	601	FAD	C4-C4X-C10	-8.30	114.46	119.95

There are no chirality outliers.

5 of 65 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	O	105	CIT	C2-C3-C4-C5
4	O	105	CIT	O7-C3-C4-C5
6	N	102	MAN	O5-C5-C6-O6
6	J	101	MAN	O5-C5-C6-O6
3	D	601	FAD	O3'-C3'-C4'-O4'

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	M	102	MAN	C1-C2-C3-C4-C5-O5

9 monomers are involved in 28 short contacts:

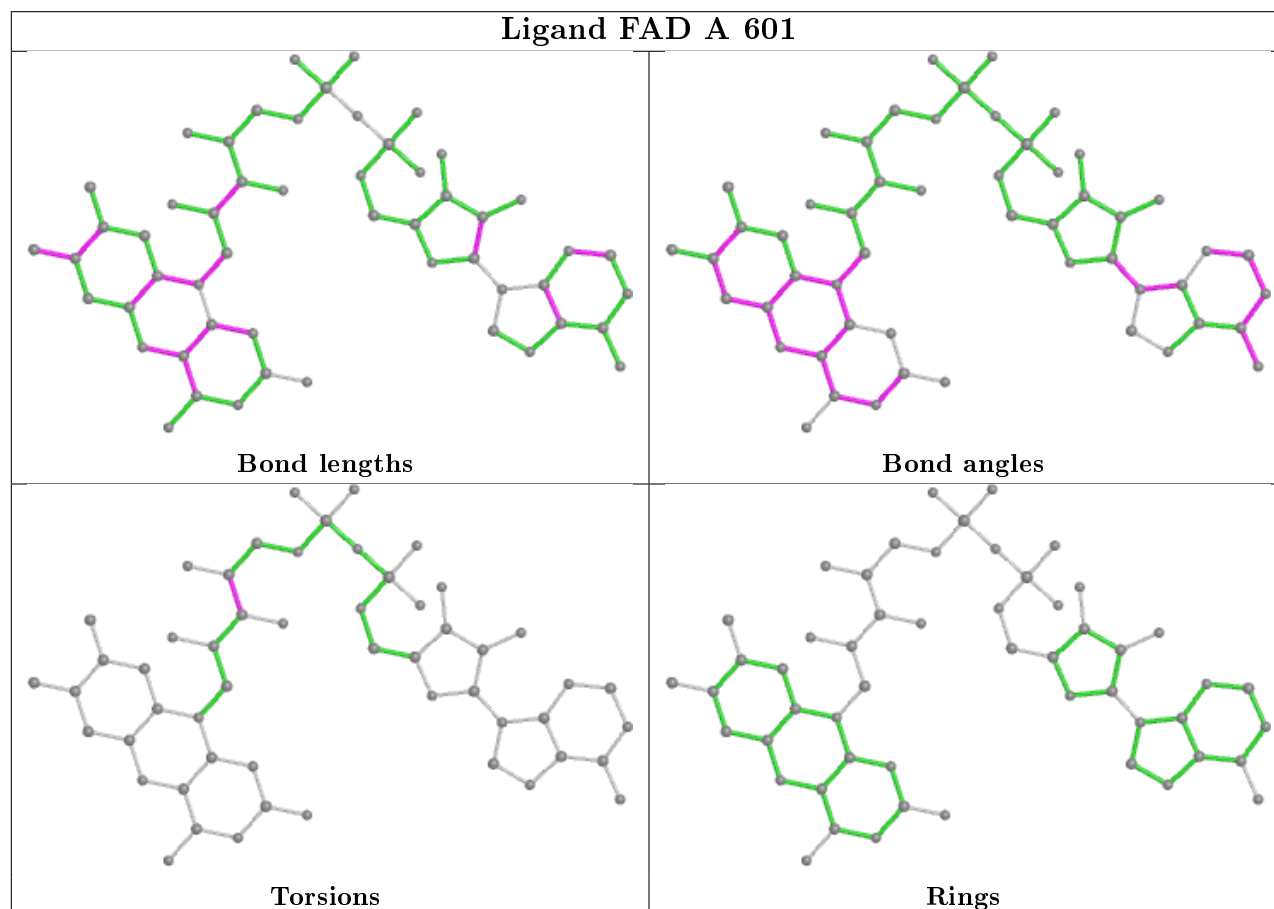
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	101	T55	4	0
5	B	602	T55	1	0
8	K	104	N1L	1	0
5	P	101	T55	0	1
5	N	101	T55	14	0
7	L	102	NAG	3	0
8	M	104	N1L	1	0
5	K	101	T55	1	0

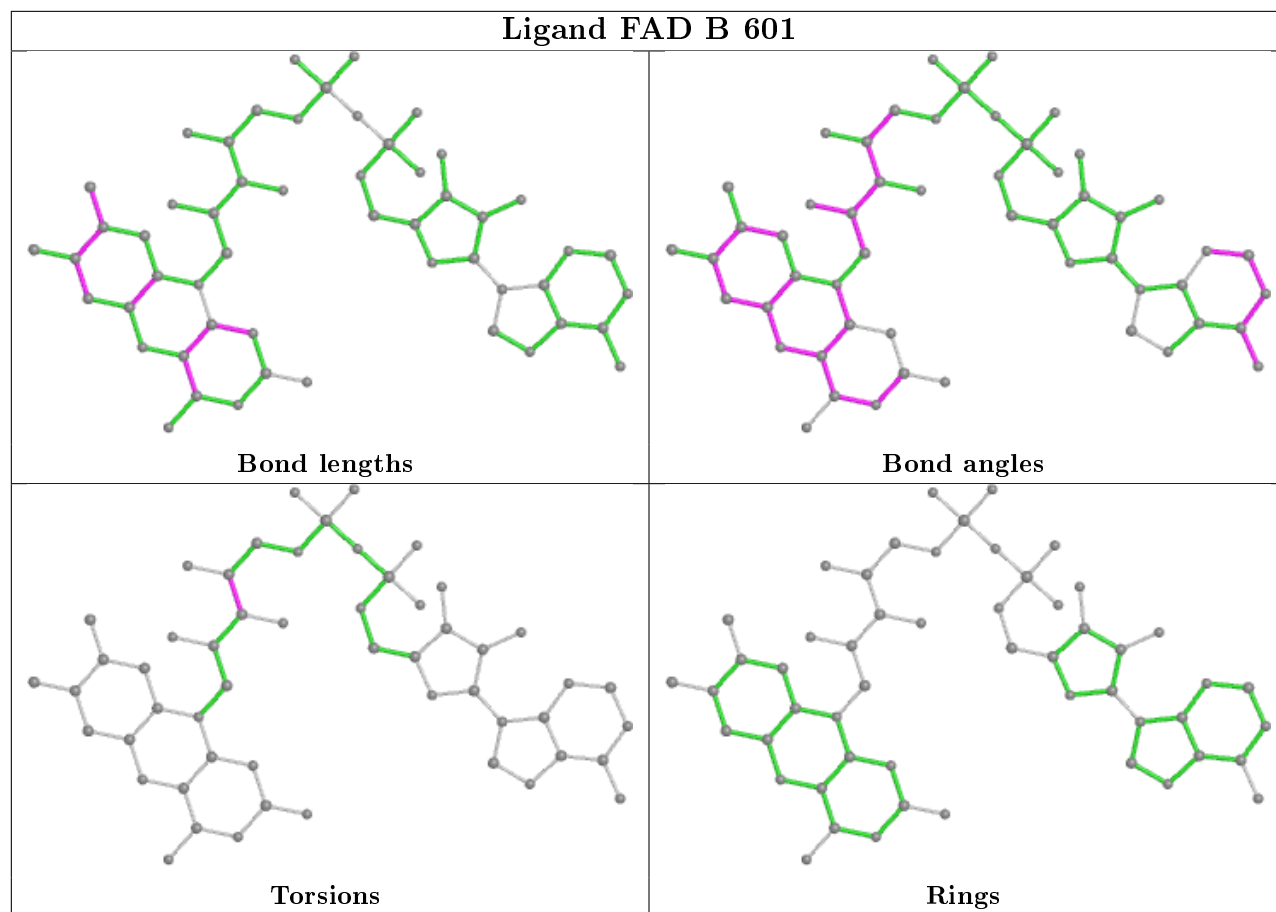
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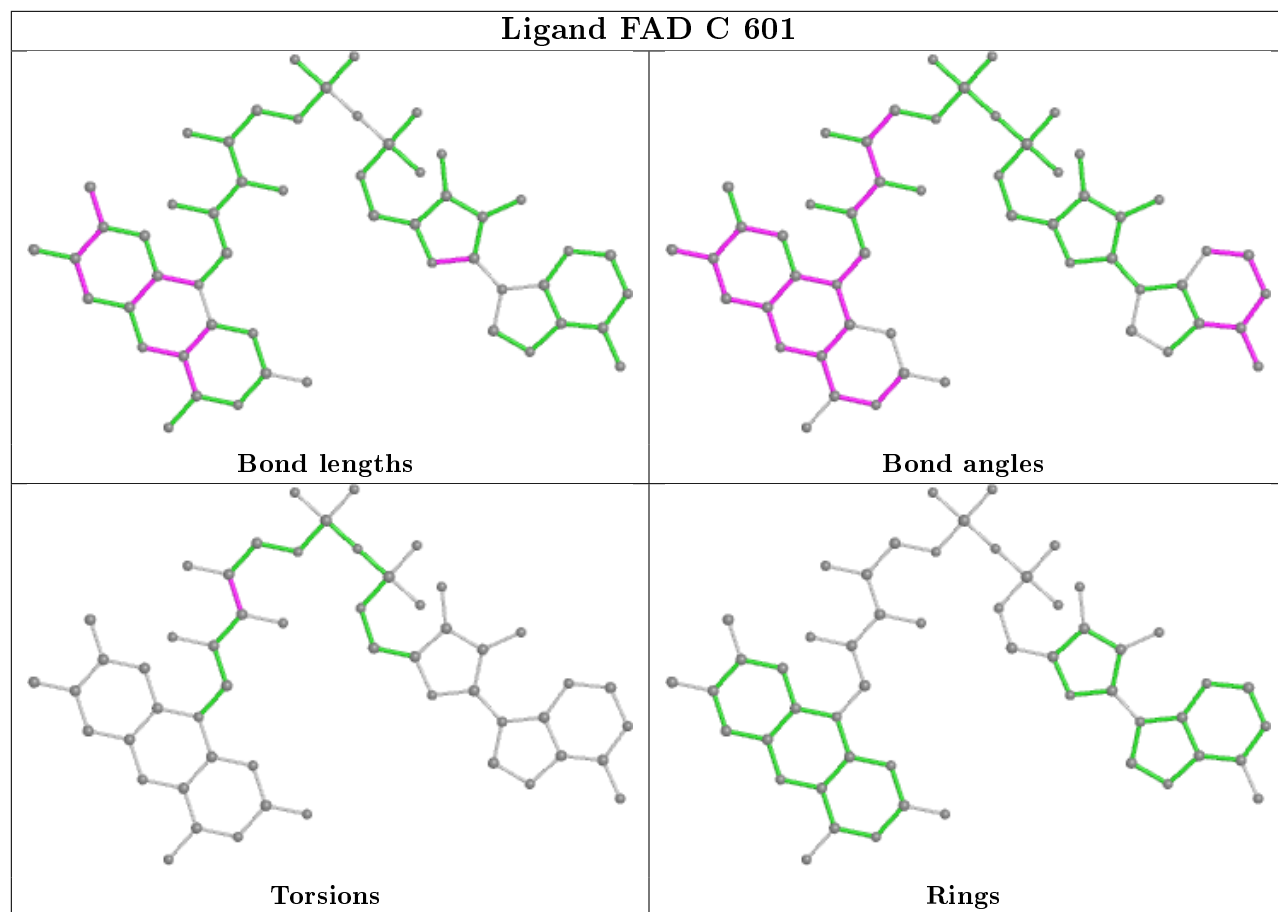
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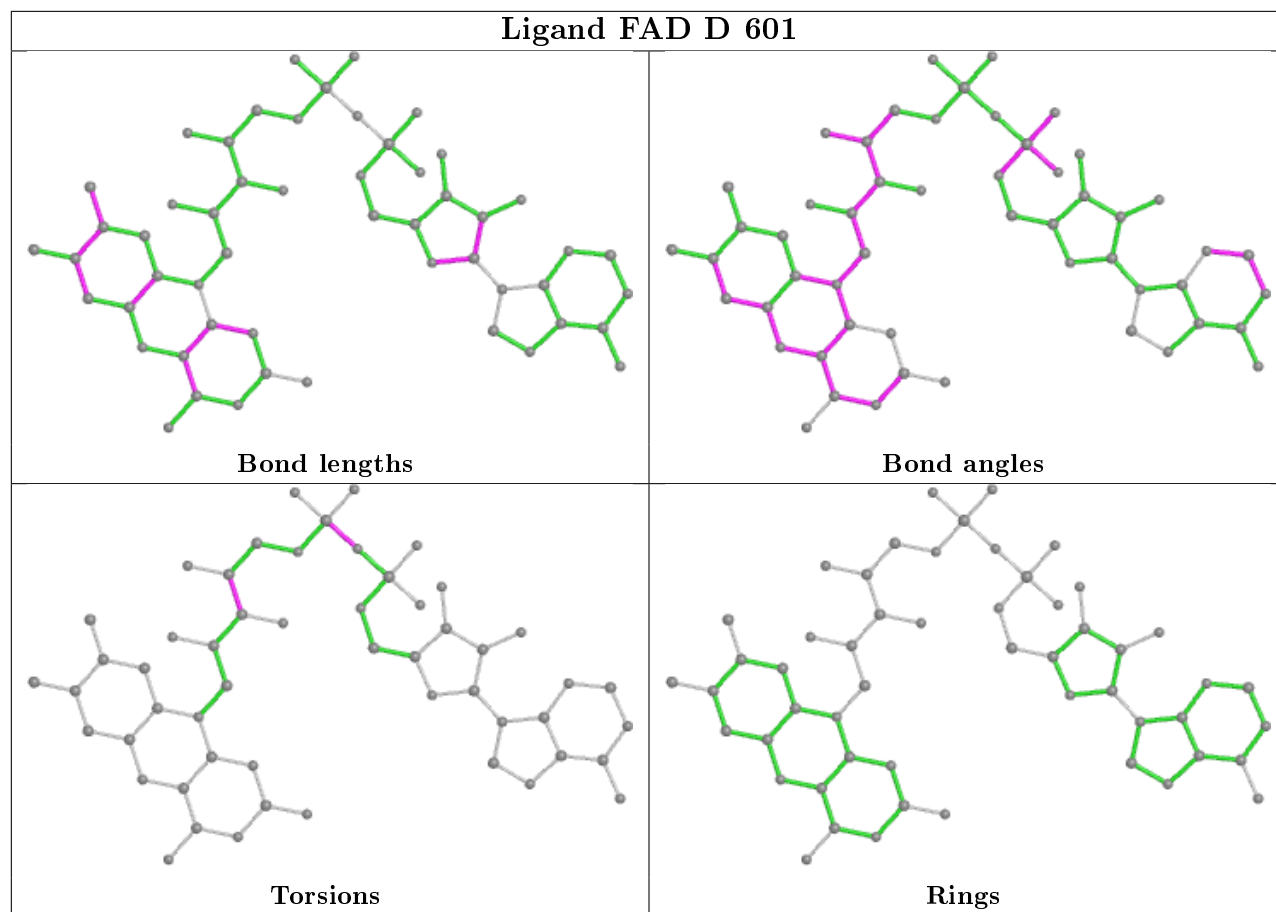
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	103	N1L	2	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	498/523 (95%)	-0.24	10 (2%) 65 71	12, 21, 42, 137	0
1	B	498/523 (95%)	-0.16	10 (2%) 65 71	14, 24, 48, 120	0
1	C	498/523 (95%)	-0.12	19 (3%) 40 48	17, 28, 52, 110	0
1	D	498/523 (95%)	0.28	35 (7%) 16 22	20, 39, 61, 109	0
2	I	0/7	-	-	-	-
2	J	0/7	-	-	-	-
2	K	0/7	-	-	-	-
2	L	0/7	-	-	-	-
2	M	0/7	-	-	-	-
2	N	0/7	-	-	-	-
2	O	0/7	-	-	-	-
2	P	0/7	-	-	-	-
All	All	1992/2148 (92%)	-0.06	74 (3%) 41 49	12, 27, 55, 137	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	358	GLY	9.2
1	D	357	ARG	8.3
1	D	302	PRO	8.3
1	B	356	GLY	7.3
1	D	356	GLY	6.8

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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( $\text{\AA}^2$ )	Q<0.9
2	3FG	L	7	13/13	0.10	0.70	101,144,162,174	0
2	3FG	M	7	13/13	0.15	0.79	116,143,162,171	0
2	GHP	M	5	11/12	0.34	0.62	112,143,167,185	0
2	GHP	K	5	11/12	0.41	0.54	108,137,152,169	0
2	3FG	K	7	13/13	0.42	0.70	107,144,168,176	0
2	3FG	I	7	13/13	0.51	0.43	69,100,119,129	0
2	OMY	K	6	14/15	0.54	0.36	91,123,147,148	0
2	GHP	L	5	11/12	0.55	0.49	102,132,149,172	0
2	GHP	M	1	11/12	0.57	0.46	80,89,97,99	0
2	OMY	M	6	14/15	0.62	0.42	88,128,160,170	0
2	GHP	I	1	11/12	0.63	0.48	102,108,111,117	0
2	GHP	K	4	11/12	0.70	0.15	60,66,78,85	0
2	GHP	I	5	11/12	0.70	0.32	58,76,103,104	0
2	OMY	L	6	14/15	0.72	0.31	84,114,150,151	0
2	GHP	M	4	11/12	0.74	0.21	59,80,94,105	0
2	GHP	L	4	11/12	0.75	0.12	54,66,75,78	0
2	3FG	I	3	12/13	0.75	0.36	53,89,99,104	0
2	GHP	J	4	11/12	0.75	0.28	40,55,61,63	0
2	GHP	K	1	11/12	0.75	0.18	50,59,70,71	0
2	GHP	L	1	11/12	0.76	0.25	54,62,72,72	0
2	3FG	L	3	12/13	0.79	0.25	66,75,83,87	0
2	3FG	M	3	12/13	0.80	0.25	69,77,84,85	0
2	OMY	J	6	14/15	0.80	0.33	52,66,72,85	0
2	OMY	I	6	14/15	0.80	0.36	57,70,75,79	0
2	3FG	J	7	13/13	0.81	0.31	40,50,56,59	0
2	3MY	M	2	13/14	0.81	0.23	74,77,97,132	0
2	3FG	O	7	13/13	0.81	0.26	40,45,52,54	0
2	3MY	K	2	13/14	0.83	0.16	50,56,66,112	0
2	3MY	I	2	13/14	0.84	0.35	49,83,94,99	0
2	3MY	J	2	13/14	0.84	0.34	44,55,65,77	0
2	3FG	K	3	12/13	0.85	0.19	58,72,78,80	0
2	GHP	J	1	11/12	0.85	0.24	44,49,51,52	0
2	GHP	I	4	11/12	0.86	0.21	41,50,55,55	0
2	3MY	L	2	13/14	0.87	0.16	52,62,72,104	0
2	GHP	J	5	11/12	0.88	0.25	45,50,56,60	0
2	3FG	J	3	12/13	0.90	0.29	43,50,53,66	0
2	GHP	P	1	11/12	0.90	0.18	32,34,38,38	0
2	3MY	O	2	13/14	0.90	0.22	29,33,35,43	0
2	OMY	O	6	14/15	0.91	0.23	34,40,48,56	0
2	3MY	N	2	13/14	0.91	0.20	25,33,40,58	0
2	GHP	P	5	11/12	0.91	0.12	26,31,40,41	0
2	OMY	P	6	14/15	0.92	0.13	30,39,40,68	0
2	GHP	O	5	11/12	0.92	0.17	27,34,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	3FG	N	7	13/13	0.93	0.27	34,41,47,51	0
2	3FG	P	7	13/13	0.93	0.17	35,42,47,50	0
2	GHP	O	1	11/12	0.94	0.15	28,31,36,37	0
2	GHP	O	4	11/12	0.94	0.14	25,30,32,33	0
2	3FG	O	3	12/13	0.94	0.16	27,31,32,36	0
2	3MY	P	2	13/14	0.94	0.21	28,31,35,46	0
2	GHP	N	5	11/12	0.94	0.21	29,32,36,38	0
2	3FG	P	3	12/13	0.95	0.20	31,38,40,42	0
2	GHP	N	1	11/12	0.95	0.21	25,30,33,34	0
2	GHP	N	4	11/12	0.95	0.16	25,29,36,40	0
2	OMY	N	6	14/15	0.95	0.22	32,36,39,60	0
2	3FG	N	3	12/13	0.96	0.20	28,31,34,34	0
2	GHP	P	4	11/12	0.97	0.10	27,30,31,34	0

## 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( $\text{\AA}^2$ )	Q<0.9
6	MAN	I	101	11/12	0.09	1.04	103,132,139,141	0
6	MAN	K	102	11/12	0.43	0.76	136,145,157,161	0
7	NAG	K	103	14/15	0.44	0.77	107,133,142,154	0
7	NAG	M	103	14/15	0.47	0.92	108,139,149,151	0
6	MAN	M	102	11/12	0.50	0.72	112,144,153,160	0
7	NAG	I	102	14/15	0.56	0.49	71,83,106,107	0
6	MAN	L	101	11/12	0.56	0.73	128,153,162,166	0
7	NAG	J	102	14/15	0.63	0.42	81,93,113,114	0
5	T55	N	101	11/12	0.67	0.27	40,45,56,73	0
7	NAG	L	102	14/15	0.69	0.62	107,135,149,153	0
7	NAG	O	103	14/15	0.71	0.42	66,77,92,94	0
8	N1L	M	104	12/13	0.72	0.30	52,59,75,78	0
5	T55	M	101	11/12	0.73	0.39	53,56,87,94	0
5	T55	B	602	11/12	0.75	0.43	48,50,65,72	0

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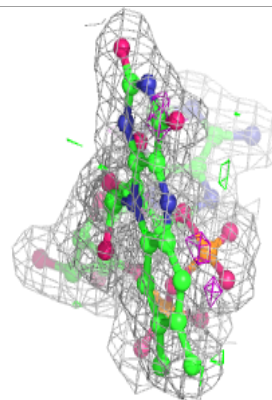
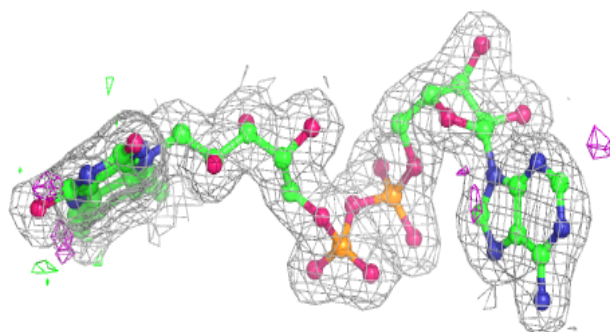
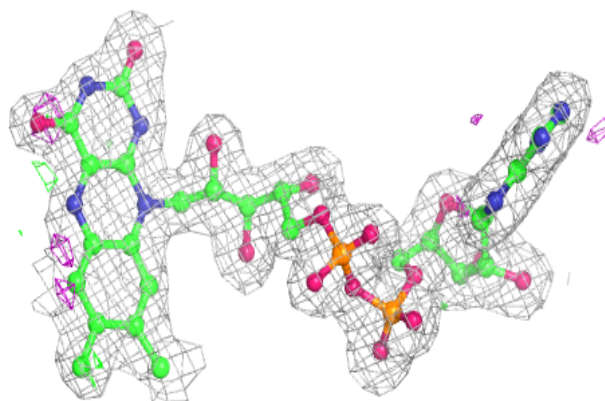
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	T55	P	101	11/12	0.75	0.36	33,41,78,79	0
5	T55	O	101	11/12	0.76	0.52	43,51,75,78	0
8	N1L	L	103	12/13	0.78	0.24	40,54,66,66	0
5	T55	K	101	11/12	0.78	0.30	51,56,62,71	0
6	MAN	J	101	11/12	0.79	0.27	52,62,67,77	0
8	N1L	K	104	12/13	0.83	0.20	36,56,70,73	0
4	CIT	A	602	13/13	0.85	0.19	37,46,55,59	0
7	NAG	P	103	14/15	0.86	0.16	40,45,48,54	0
8	N1L	N	104	12/13	0.88	0.30	40,42,50,50	0
4	CIT	O	105	13/13	0.88	0.21	31,40,50,51	0
8	N1L	O	104	12/13	0.88	0.24	33,40,48,55	0
4	CIT	B	603	13/13	0.88	0.20	38,56,71,78	0
4	CIT	C	602	13/13	0.91	0.27	45,55,62,67	0
6	MAN	O	102	11/12	0.92	0.10	34,40,45,49	0
6	MAN	P	102	11/12	0.92	0.20	28,39,50,57	0
6	MAN	N	102	11/12	0.92	0.21	38,45,53,54	0
4	CIT	D	602	13/13	0.93	0.23	39,43,51,54	0
8	N1L	P	104	12/13	0.93	0.22	29,32,37,51	0
7	NAG	N	103	14/15	0.94	0.15	30,40,45,48	0
3	FAD	C	601	53/53	0.97	0.13	19,22,28,32	0
3	FAD	D	601	53/53	0.97	0.11	20,26,38,43	0
3	FAD	B	601	53/53	0.98	0.10	10,14,24,29	0
3	FAD	A	601	53/53	0.99	0.10	11,15,22,26	0

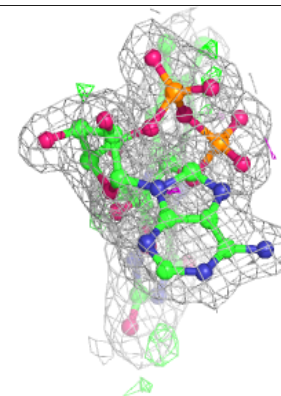
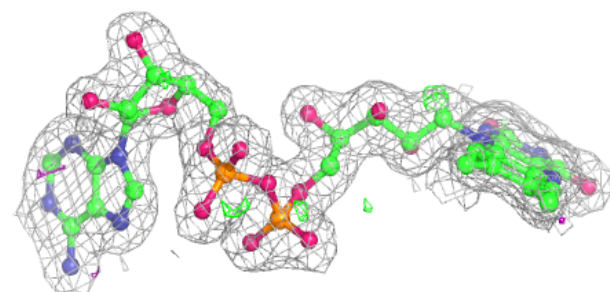
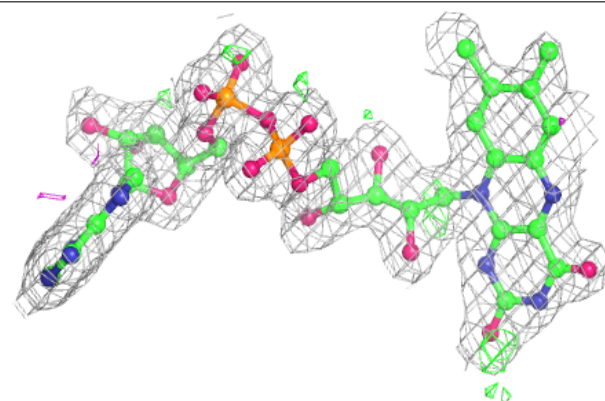
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around FAD 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)

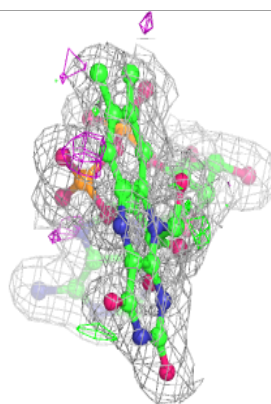
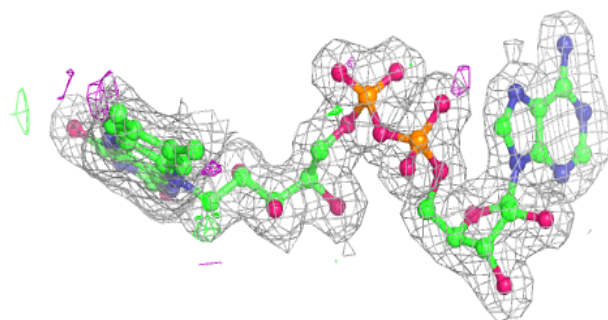
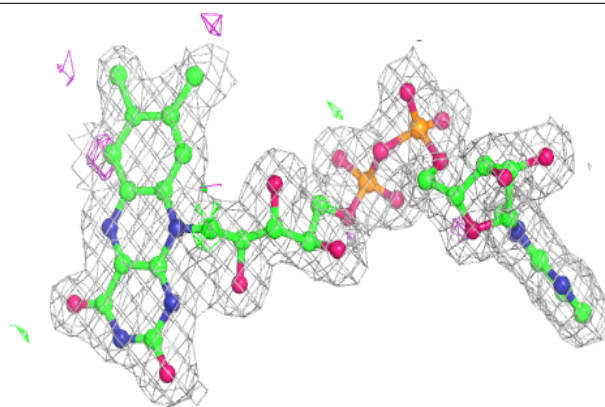
**Electron density around FAD D 601:**

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

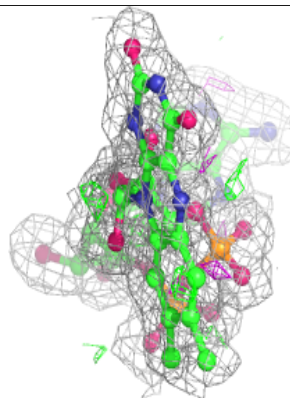
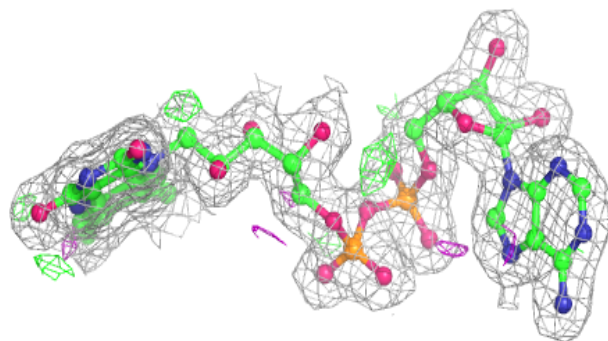
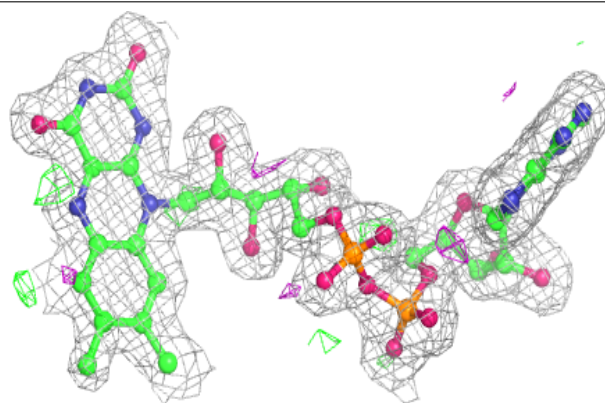


**Electron density around FAD B 601:**

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

**Electron density around FAD A 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 [i](#)

There are no such residues in this entry.