



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2021 – 08:07 PM EDT

PDB ID : 3IUE  
Title : Crystal structure of pantothenate synthetase in complex with 2-(5-methoxy-2-(5-Methylpyridin-2-ylsulfonylcarbamoyl)-1H-indol-1-yl) acetic acid  
Authors : Silvestre, H.L.; Wen, S.; Hung, A.W.; Ciulli, A.; Blundell, T.L.; Abell, C.  
Deposited on : 2009-08-31  
Resolution : 1.73 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.

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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 : 2.23.2  
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) : 2.23.2

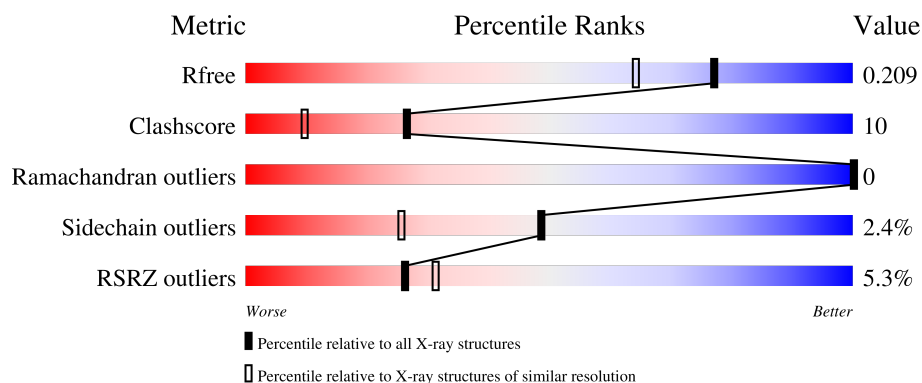
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 1.73 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	301	
1	B	301	

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
3	GOL	B	709	-	-	X	-
3	GOL	B	713	-	-	X	-
4	EDO	B	714	-	-	X	-
4	EDO	B	718	-	-	X	-
5	EOH	A	721	-	-	X	-
5	EOH	A	722	-	-	X	-
5	EOH	A	726	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5024 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.

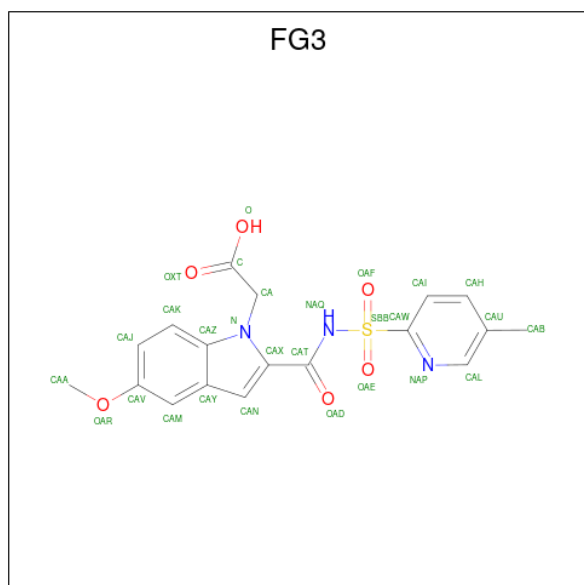
- Molecule 1 is a protein called Pantothenate synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	7	0
			2138	1354	383	395	6			
1	B	278	Total	C	N	O	S	0	10	0
			2116	1341	384	383	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	THR	engineered mutation	UNP P0A5R0
A	77	GLY	GLU	engineered mutation	UNP P0A5R0
B	2	ALA	THR	engineered mutation	UNP P0A5R0
B	77	GLY	GLU	engineered mutation	UNP P0A5R0

- Molecule 2 is (5-methoxy-2-[[[(5-methylpyridin-2-yl)sulfonyl]carbamoyl]-1H-indol-1-yl)acetic acid (three-letter code: FG3) (formula: C<sub>18</sub>H<sub>17</sub>N<sub>3</sub>O<sub>6</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			28	18	3	6	1		
2	A	1	Total	C	N	O	S	0	0
			28	18	3	6	1		
2	B	1	Total	C	N	O	S	0	1
			56	36	6	12	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



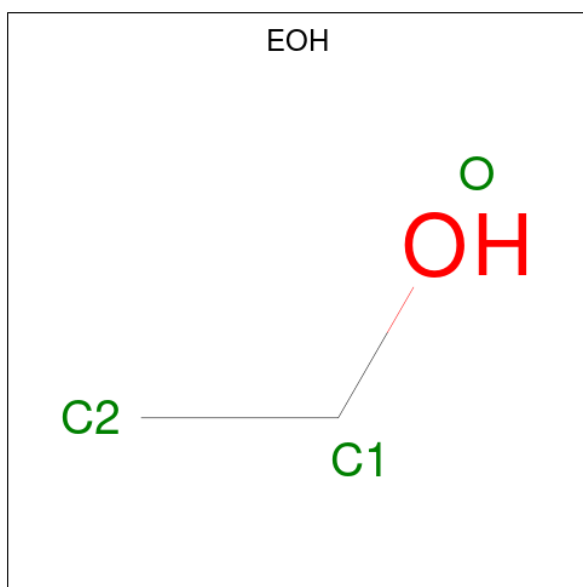
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is ETHANOL (three-letter code: EOH) (formula: C<sub>2</sub>H<sub>6</sub>O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 3 2 1	0	0
5	A	1	Total C O 3 2 1	0	0
5	A	1	Total C O 3 2 1	0	0
5	A	1	Total C O 3 2 1	0	0
5	A	1	Total C O 3 2 1	0	0
5	A	1	Total C O 3 2 1	0	0

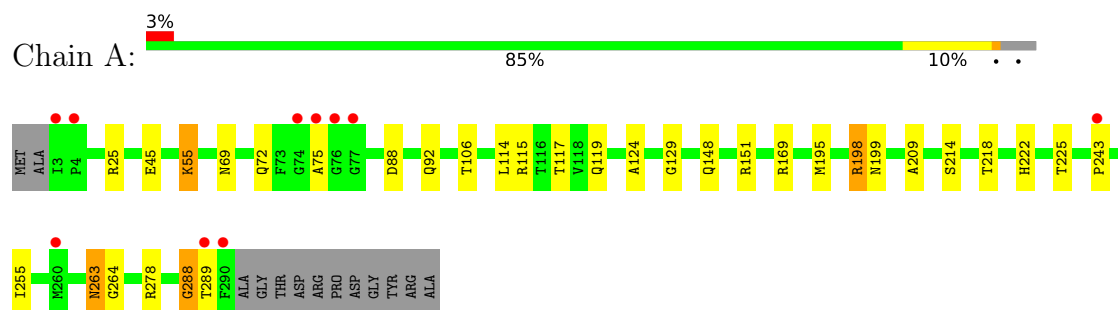
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	280	Total O 280 280	0	0
6	B	290	Total O 290 290	0	0

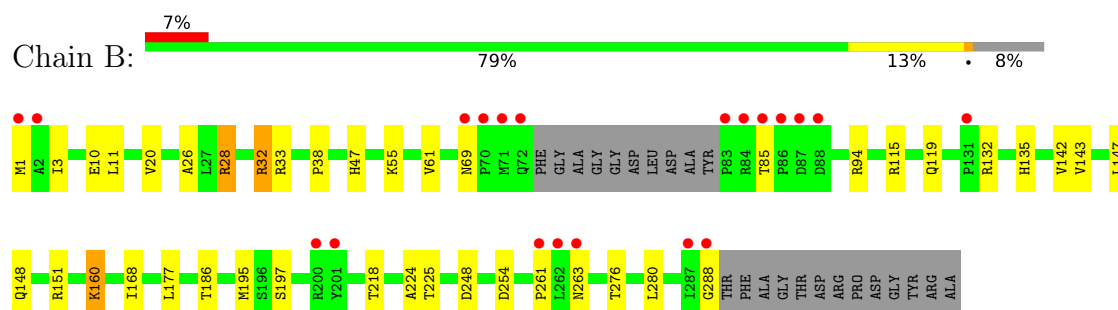
### 3 Residue-property plots [i](#)

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: Pantothenate synthetase



#### • Molecule 1: Pantothenate synthetase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.55Å 70.71Å 81.84Å 90.00° 99.37° 90.00°	Depositor
Resolution (Å)	27.68 – 1.73 27.68 – 1.73	Depositor EDS
% Data completeness (in resolution range)	99.9 (27.68-1.73) 100.0 (27.68-1.73)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.172 , 0.208 0.172 , 0.209	Depositor DCC
$R_{free}$ test set	2891 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.1	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5024	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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: GOL, EDO, FG3, EOH

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	0.63	0/2188	0.69	0/2989
1	B	0.62	0/2169	0.71	1/2959 (0.0%)
All	All	0.63	0/4357	0.70	1/5948 (0.0%)

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	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	280	LEU	CA-CB-CG	5.10	127.03	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	288	GLY	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	2138	0	2180	41	0
1	B	2116	0	2201	49	0
2	A	56	0	32	4	0
2	B	56	0	32	4	0
3	A	18	0	24	3	0
3	B	24	0	32	16	0
4	A	16	0	24	0	0
4	B	12	0	18	10	0
5	A	18	0	36	11	0
6	A	280	0	0	8	0
6	B	290	0	0	10	0
All	All	5024	0	4579	93	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (93) 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:B:197:SER:HB3	6:B:644:HOH:O	1.72	0.88
1:B:288:GLY:H	4:B:718:EDO:C2	1.87	0.87
5:A:722:EOH:H23	1:B:119:GLN:HG2	1.61	0.83
1:B:160:LYS:HG2	6:B:304:HOH:O	1.78	0.81
1:B:115:ARG:HH22	3:B:713:GOL:C1	1.92	0.81
1:B:288:GLY:H	4:B:718:EDO:H21	1.46	0.80
2:A:303:FG3:HAA	2:A:303:FG3:HNAQ	1.46	0.80
1:A:69:ASN:HD22	1:A:72:GLN:HE21	1.29	0.78
1:B:115:ARG:HH22	3:B:713:GOL:H11	1.47	0.78
5:A:722:EOH:C2	1:B:119:GLN:HG2	2.14	0.78
1:B:218[B]:THR:HG21	6:B:346:HOH:O	1.85	0.77
2:A:303:FG3:HNAQ	2:A:303:FG3:CA	1.97	0.77
1:A:106:THR:H	5:A:726:EOH:C1	1.98	0.77
1:A:263:ASN:CG	1:A:264:GLY:H	1.89	0.77
1:A:117:THR:OG1	5:A:722:EOH:H21	1.83	0.77
1:A:199:ASN:HD22	3:A:708:GOL:H32	1.50	0.75
1:A:45:GLU:HB3	1:A:195:MET:CE	2.19	0.73
5:A:721:EOH:H22	6:A:438:HOH:O	1.89	0.73
1:A:92:GLN:NE2	6:A:540:HOH:O	2.24	0.70
1:A:45:GLU:HB3	1:A:195:MET:HE1	1.74	0.69
1:B:148:GLN:HE22	3:B:709:GOL:H31	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ILE:HG12	6:A:636:HOH:O	1.92	0.67
2:B:302[A]:FG3:O	6:B:644:HOH:O	2.13	0.67
1:A:263:ASN:CG	1:A:264:GLY:N	2.50	0.64
1:B:69:ASN:CG	1:B:142[B]:VAL:HG21	2.17	0.64
1:A:151:ARG:NH2	1:B:151[A]:ARG:HD2	2.13	0.64
1:A:106:THR:H	5:A:726:EOH:H11	1.62	0.63
1:A:218[B]:THR:HG21	5:A:724:EOH:O	1.98	0.63
2:A:303:FG3:HAI	6:A:608:HOH:O	1.97	0.63
1:B:248:ASP:HB3	6:B:323:HOH:O	1.97	0.63
1:B:224:ALA:O	4:B:718:EDO:H22	1.99	0.62
1:A:75:ALA:HB2	6:A:307:HOH:O	1.98	0.62
1:B:115:ARG:NH2	3:B:713:GOL:H11	2.13	0.61
1:A:169:ARG:HB3	3:B:713:GOL:H31	1.81	0.61
1:B:160:LYS:HE3	6:B:429:HOH:O	1.99	0.61
1:B:11:LEU:HB3	4:B:714:EDO:H22	1.84	0.60
1:A:199:ASN:HD22	3:A:708:GOL:C3	2.13	0.60
1:B:10:GLU:HB3	4:B:714:EDO:H11	1.82	0.60
1:B:288:GLY:N	4:B:718:EDO:H21	2.16	0.59
1:B:276:THR:H	3:B:711:GOL:C1	2.16	0.59
3:B:709:GOL:H12	6:B:333:HOH:O	2.03	0.57
1:A:199:ASN:ND2	3:A:708:GOL:H32	2.19	0.57
1:A:25:ARG:NH1	1:A:151:ARG:HG3	2.20	0.56
1:B:177:LEU:HD22	3:B:709:GOL:H32	1.87	0.55
1:A:148:GLN:HE22	3:B:709:GOL:H31	1.72	0.55
1:A:198[B]:ARG:HD2	6:A:503:HOH:O	2.07	0.54
1:B:69:ASN:OD1	1:B:142[B]:VAL:HG21	2.07	0.54
1:B:115:ARG:NH2	3:B:713:GOL:C1	2.69	0.54
1:B:148:GLN:NE2	3:B:709:GOL:H31	2.22	0.54
1:B:94:ARG:HE	4:B:714:EDO:H21	1.74	0.53
1:B:254:ASP:HB3	1:B:261:PRO:HD3	1.90	0.53
1:A:151:ARG:NH2	1:B:151[A]:ARG:CD	2.71	0.53
1:A:198[A]:ARG:HH21	1:A:278:ARG:H	1.56	0.53
1:B:55:LYS:HE3	6:B:389:HOH:O	2.09	0.53
1:A:114:LEU:HD21	6:A:309:HOH:O	2.09	0.51
1:A:115:ARG:O	5:A:722:EOH:H22	2.10	0.51
1:B:3:ILE:HD13	1:B:26:ALA:HB2	1.92	0.51
1:B:47:HIS:HE2	2:B:302[A]:FG3:HNAQ	1.60	0.50
1:B:143:VAL:HG11	1:B:168[A]:ILE:HD12	1.92	0.50
1:B:186:THR:HG23	2:B:302[B]:FG3:HAJ	1.93	0.49
1:A:151:ARG:HH22	1:B:151[A]:ARG:CD	2.26	0.49
1:B:38:PRO:HB2	3:B:712:GOL:H11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:GLN:HE22	3:B:709:GOL:C3	2.26	0.49
1:B:28[A]:ARG:HH12	1:B:33:ARG:HD3	1.78	0.48
1:B:225:THR:HA	4:B:718:EDO:H22	1.94	0.48
1:B:32:ARG:HG2	1:B:61:VAL:HB	1.96	0.47
1:A:243:PRO:O	5:A:721:EOH:H23	2.16	0.46
1:A:55:LYS:HD3	6:A:455:HOH:O	2.16	0.45
5:A:722:EOH:H21	1:B:119:GLN:HG2	1.98	0.45
1:B:28[A]:ARG:NH1	1:B:33:ARG:HD3	2.32	0.45
1:A:148:GLN:NE2	3:B:709:GOL:C3	2.79	0.45
1:B:94:ARG:HE	4:B:714:EDO:C2	2.29	0.45
1:A:209:ALA:HB3	5:A:721:EOH:H21	1.99	0.45
1:A:88:ASP:O	1:A:92:GLN:HG3	2.17	0.45
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.86	0.44
1:B:147:LEU:O	3:B:709:GOL:H11	2.17	0.44
1:A:225:THR:HA	1:A:289:THR:CB	2.48	0.43
1:B:151[A]:ARG:CZ	6:B:443:HOH:O	2.65	0.43
1:A:288:GLY:N	1:A:289:THR:HA	2.33	0.42
1:B:195[A]:MET:O	2:B:302[A]:FG3:HAK	2.18	0.42
1:A:124:ALA:O	1:A:129:GLY:HA3	2.20	0.42
1:A:151:ARG:HH22	1:B:151[A]:ARG:HD2	1.82	0.41
1:A:214:SER:O	1:A:218[B]:THR:HG22	2.21	0.41
2:A:302:FG3:HAK	2:A:302:FG3:HAA	1.98	0.41
1:B:132:ARG:HB3	1:B:135:HIS:HB2	2.02	0.41
1:B:148:GLN:HE22	3:B:709:GOL:C3	2.30	0.41
1:A:198[A]:ARG:NH2	1:A:278:ARG:H	2.19	0.40
1:B:225:THR:HA	4:B:718:EDO:H11	2.02	0.40
1:B:28[A]:ARG:NH1	1:B:32:ARG:O	2.53	0.40
1:A:225:THR:HG22	1:A:289:THR:CB	2.51	0.40
1:B:28[A]:ARG:HH12	1:B:33:ARG:HA	1.86	0.40
1:A:119:GLN:HG3	6:B:496:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	291/301 (97%)	283 (97%)	8 (3%)	0	100	100
1	B	284/301 (94%)	282 (99%)	2 (1%)	0	100	100
All	All	575/602 (96%)	565 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	216/223 (97%)	212 (98%)	4 (2%)	57	36
1	B	218/223 (98%)	210 (96%)	8 (4%)	34	11
All	All	434/446 (97%)	422 (97%)	12 (3%)	49	19

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	A	198[A]	ARG
1	A	198[B]	ARG
1	A	263	ASN
1	B	1	MET
1	B	20	VAL
1	B	28[A]	ARG
1	B	28[B]	ARG
1	B	32	ARG
1	B	85	THR
1	B	160	LYS
1	B	263	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	148	GLN
1	A	199	ASN
1	A	222	HIS
1	B	148	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

24 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	$\# Z  > 2$
5	EOH	A	721	-	2,2,2	0.42	0	1,1,1	0.36	0
2	FG3	A	303	-	25,30,30	3.30	12 (48%)	31,44,44	2.20	8 (25%)
4	EDO	A	717	-	3,3,3	0.38	0	2,2,2	0.53	0
5	EOH	A	723	-	2,2,2	0.48	0	1,1,1	0.19	0
4	EDO	A	716	-	3,3,3	0.42	0	2,2,2	0.47	0
3	GOL	B	713	-	5,5,5	0.47	0	5,5,5	0.57	0
5	EOH	A	725	-	2,2,2	0.45	0	1,1,1	0.27	0
2	FG3	B	302[B]	-	25,30,30	3.10	11 (44%)	31,44,44	2.40	6 (19%)
3	GOL	B	711	-	5,5,5	0.39	0	5,5,5	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	A	707	-	5,5,5	0.40	0	5,5,5	0.25	0
3	GOL	B	712	-	5,5,5	0.34	0	5,5,5	0.27	0
4	EDO	B	715	-	3,3,3	0.38	0	2,2,2	0.60	0
4	EDO	A	720	-	3,3,3	0.40	0	2,2,2	0.26	0
3	GOL	A	708	-	5,5,5	0.42	0	5,5,5	0.41	0
5	EOH	A	724	-	2,2,2	0.46	0	1,1,1	0.21	0
2	FG3	A	302	-	25,30,30	3.16	11 (44%)	31,44,44	2.20	7 (22%)
3	GOL	A	710	-	5,5,5	0.48	0	5,5,5	0.19	0
4	EDO	A	719	-	3,3,3	0.53	0	2,2,2	0.42	0
3	GOL	B	709	-	5,5,5	0.37	0	5,5,5	0.43	0
5	EOH	A	726	-	2,2,2	0.38	0	1,1,1	0.27	0
4	EDO	B	718	-	3,3,3	0.43	0	2,2,2	0.46	0
5	EOH	A	722	-	2,2,2	0.45	0	1,1,1	0.41	0
2	FG3	B	302[A]	-	25,30,30	3.01	11 (44%)	31,44,44	2.44	9 (29%)
4	EDO	B	714	-	3,3,3	0.47	0	2,2,2	0.25	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
3	GOL	B	711	-	-	0/4/4/4	-
4	EDO	A	716	-	-	1/1/1/1	-
3	GOL	B	709	-	-	2/4/4/4	-
4	EDO	A	719	-	-	1/1/1/1	-
2	FG3	A	303	-	-	4/16/21/21	0/3/3/3
3	GOL	A	707	-	-	3/4/4/4	-
4	EDO	B	718	-	-	1/1/1/1	-
2	FG3	B	302[A]	-	-	8/16/21/21	0/3/3/3
3	GOL	B	713	-	-	4/4/4/4	-
3	GOL	B	712	-	-	4/4/4/4	-
4	EDO	A	717	-	-	1/1/1/1	-
4	EDO	B	714	-	-	1/1/1/1	-
4	EDO	B	715	-	-	0/1/1/1	-
4	EDO	A	720	-	-	0/1/1/1	-
3	GOL	A	708	-	-	2/4/4/4	-
2	FG3	A	302	-	-	5/16/21/21	0/3/3/3
2	FG3	B	302[B]	-	-	3/16/21/21	0/3/3/3
3	GOL	A	710	-	-	4/4/4/4	-



All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	303	FG3	OAE-SBB	9.51	1.54	1.43
2	A	303	FG3	OAF-SBB	9.50	1.54	1.43
2	B	302[A]	FG3	OAE-SBB	9.19	1.54	1.43
2	A	302	FG3	OAE-SBB	8.96	1.53	1.43
2	B	302[B]	FG3	OAF-SBB	8.90	1.53	1.43
2	A	302	FG3	OAF-SBB	8.70	1.53	1.43
2	B	302[B]	FG3	OAE-SBB	7.94	1.52	1.43
2	B	302[A]	FG3	OAF-SBB	7.27	1.51	1.43
2	A	302	FG3	CAT-NAQ	-4.38	1.33	1.39
2	B	302[B]	FG3	CAN-CAX	-3.84	1.33	1.39
2	B	302[A]	FG3	CAT-NAQ	-3.67	1.34	1.39
2	B	302[A]	FG3	CAL-NAP	3.53	1.41	1.34
2	B	302[B]	FG3	CAM-CAY	-3.47	1.34	1.42
2	B	302[B]	FG3	CAB-CAU	-3.46	1.38	1.51
2	A	303	FG3	CAL-NAP	3.33	1.41	1.34
2	A	303	FG3	CAB-CAU	-3.25	1.39	1.51
2	B	302[B]	FG3	CAK-CAZ	-3.21	1.34	1.41
2	B	302[A]	FG3	CAB-CAU	-3.17	1.39	1.51
2	B	302[B]	FG3	CAT-NAQ	-3.14	1.35	1.39
2	A	302	FG3	CAN-CAX	-3.14	1.34	1.39
2	A	303	FG3	CAN-CAX	-3.08	1.34	1.39
2	B	302[B]	FG3	CAL-NAP	3.01	1.40	1.34
2	B	302[A]	FG3	CAM-CAY	-3.00	1.35	1.42
2	A	303	FG3	CAM-CAY	-2.99	1.35	1.42
2	A	302	FG3	CAM-CAV	2.98	1.42	1.37
2	A	302	FG3	CAL-NAP	2.90	1.40	1.34
2	B	302[B]	FG3	CAY-CAZ	-2.90	1.35	1.41
2	B	302[A]	FG3	CAN-CAX	-2.88	1.35	1.39
2	A	303	FG3	CAT-NAQ	-2.81	1.35	1.39
2	A	302	FG3	CAY-CAZ	-2.68	1.35	1.41
2	A	303	FG3	CAK-CAZ	-2.65	1.35	1.41
2	A	302	FG3	CAB-CAU	-2.62	1.41	1.51
2	B	302[A]	FG3	CAY-CAZ	-2.62	1.35	1.41
2	A	303	FG3	CAY-CAZ	-2.60	1.35	1.41
2	B	302[A]	FG3	CAK-CAZ	-2.57	1.35	1.41
2	A	303	FG3	CA-N	2.54	1.53	1.48
2	B	302[B]	FG3	CAX-CAT	-2.50	1.35	1.50
2	B	302[A]	FG3	CAM-CAV	2.44	1.41	1.37
2	A	302	FG3	CAK-CAZ	-2.44	1.36	1.41
2	A	303	FG3	CAM-CAV	2.32	1.41	1.37
2	A	302	FG3	CAM-CAY	-2.30	1.36	1.42
2	A	303	FG3	CAX-CAT	-2.27	1.36	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	302	FG3	CAX-CAT	-2.26	1.36	1.50
2	B	302[A]	FG3	CAX-CAT	-2.22	1.36	1.50
2	B	302[B]	FG3	CAM-CAV	2.03	1.40	1.37

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302[A]	FG3	OAF-SBB-OAE	-8.27	109.38	119.55
2	B	302[B]	FG3	OAF-SBB-OAE	-8.02	109.69	119.55
2	A	303	FG3	OAF-SBB-OAE	-7.00	110.95	119.55
2	A	302	FG3	C-CA-N	5.75	122.14	114.00
2	A	302	FG3	OAF-SBB-OAE	-5.43	112.87	119.55
2	B	302[B]	FG3	CAU-CAL-NAP	-5.36	118.50	124.81
2	B	302[B]	FG3	CAL-NAP-CAW	5.11	121.34	115.91
2	B	302[A]	FG3	CAU-CAL-NAP	-5.03	118.89	124.81
2	A	302	FG3	CAU-CAL-NAP	-4.87	119.08	124.81
2	A	302	FG3	CAL-NAP-CAW	4.58	120.78	115.91
2	A	303	FG3	CAI-CAW-NAP	-4.53	120.31	125.28
2	B	302[A]	FG3	CAL-NAP-CAW	4.50	120.70	115.91
2	B	302[B]	FG3	CAI-CAW-NAP	-4.03	120.86	125.28
2	B	302[A]	FG3	CAI-CAW-NAP	-3.99	120.90	125.28
2	A	303	FG3	SBB-CAW-NAP	3.96	123.14	115.18
2	A	303	FG3	CAU-CAL-NAP	-3.68	120.48	124.81
2	B	302[A]	FG3	CAT-NAQ-SBB	-3.59	118.72	123.36
2	A	302	FG3	CAI-CAW-NAP	-3.58	121.35	125.28
2	A	303	FG3	CAL-NAP-CAW	3.52	119.65	115.91
2	B	302[A]	FG3	C-CA-N	2.79	117.96	114.00
2	B	302[A]	FG3	CAJ-CAV-CAM	-2.69	117.19	120.81
2	B	302[B]	FG3	OAD-CAT-NAQ	2.59	124.27	121.08
2	A	302	FG3	CAT-NAQ-SBB	-2.51	120.12	123.36
2	B	302[A]	FG3	CAA-OAR-CAV	2.49	122.92	117.51
2	A	303	FG3	OAD-CAT-NAQ	2.44	124.08	121.08
2	A	302	FG3	CAJ-CAV-CAM	-2.38	117.61	120.81
2	B	302[B]	FG3	C-CA-N	-2.23	110.84	114.00
2	B	302[A]	FG3	SBB-CAW-NAP	2.15	119.50	115.18
2	A	303	FG3	CAN-CAY-CAZ	2.03	108.04	106.27
2	A	303	FG3	CAI-CAH-CAU	-2.01	118.69	121.38

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	302[A]	FG3	OAD-CAT-CAX-CAN
2	B	302[B]	FG3	OAD-CAT-CAX-CAN
3	B	712	GOL	O1-C1-C2-C3
3	B	713	GOL	C1-C2-C3-O3
2	B	302[B]	FG3	CAJ-CAV-OAR-CAA
2	B	302[B]	FG3	CAM-CAV-OAR-CAA
2	A	302	FG3	CAT-NAQ-SBB-OAF
2	A	302	FG3	CAM-CAV-OAR-CAA
3	B	709	GOL	O1-C1-C2-O2
3	B	713	GOL	O1-C1-C2-O2
2	A	302	FG3	CAJ-CAV-OAR-CAA
2	B	302[A]	FG3	CAI-CAW-SBB-NAQ
3	A	707	GOL	O1-C1-C2-C3
3	A	708	GOL	O1-C1-C2-C3
3	A	710	GOL	C1-C2-C3-O3
3	B	709	GOL	O1-C1-C2-C3
3	B	712	GOL	C1-C2-C3-O3
3	B	713	GOL	O1-C1-C2-C3
2	A	302	FG3	CAT-NAQ-SBB-CAW
3	A	707	GOL	O1-C1-C2-O2
3	A	710	GOL	O2-C2-C3-O3
3	B	712	GOL	O1-C1-C2-O2
3	B	712	GOL	O2-C2-C3-O3
3	B	713	GOL	O2-C2-C3-O3
4	A	717	EDO	O1-C1-C2-O2
4	B	718	EDO	O1-C1-C2-O2
2	A	303	FG3	CAI-CAW-SBB-NAQ
2	A	303	FG3	NAP-CAW-SBB-OAE
2	B	302[A]	FG3	NAP-CAW-SBB-OAE
2	B	302[A]	FG3	CAI-CAW-SBB-OAE
2	A	302	FG3	CAT-NAQ-SBB-OAE
3	A	710	GOL	O1-C1-C2-O2
2	B	302[A]	FG3	C-CA-N-CAX
2	A	303	FG3	CAI-CAW-SBB-OAE
4	A	716	EDO	O1-C1-C2-O2
2	B	302[A]	FG3	NAP-CAW-SBB-OAF
2	B	302[A]	FG3	CAI-CAW-SBB-OAF
4	B	714	EDO	O1-C1-C2-O2
3	A	710	GOL	O1-C1-C2-C3
2	B	302[A]	FG3	C-CA-N-CAZ
2	A	303	FG3	OAD-CAT-CAX-CAN
3	A	707	GOL	O2-C2-C3-O3
4	A	719	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	708	GOL	O1-C1-C2-O2

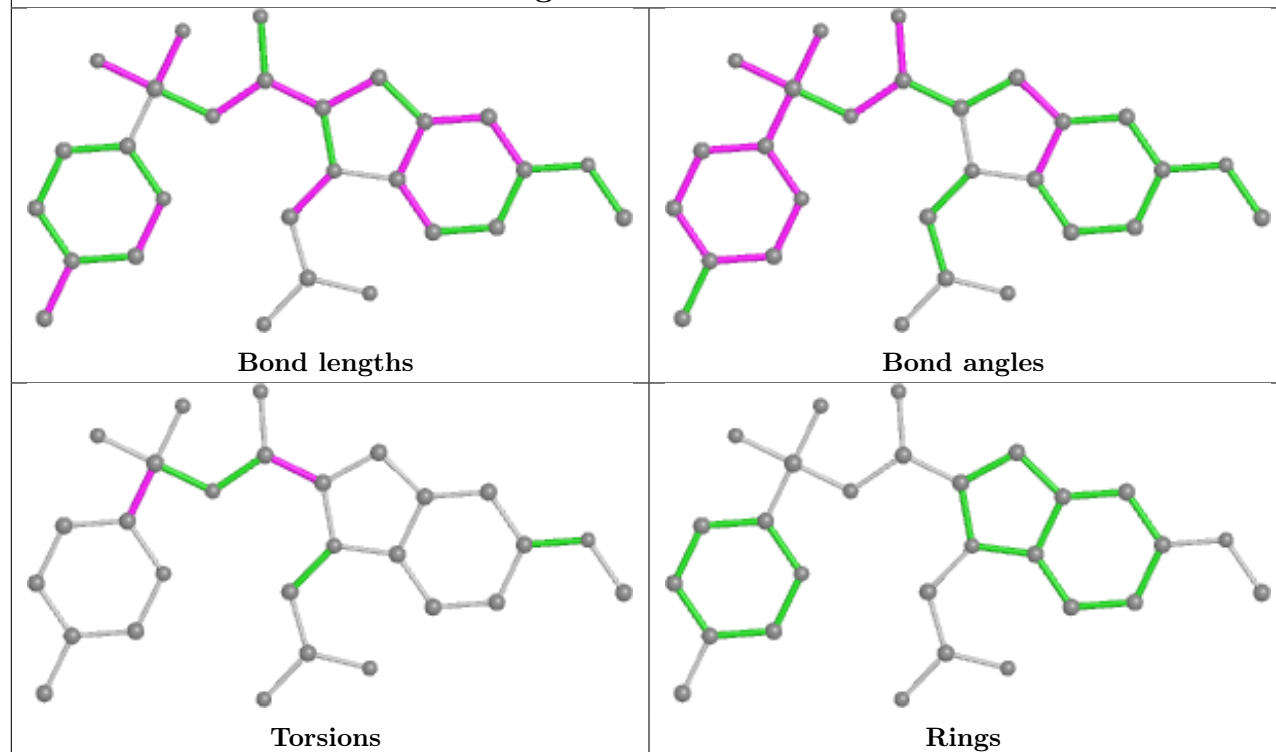
There are no ring outliers.

15 monomers are involved in 48 short contacts:

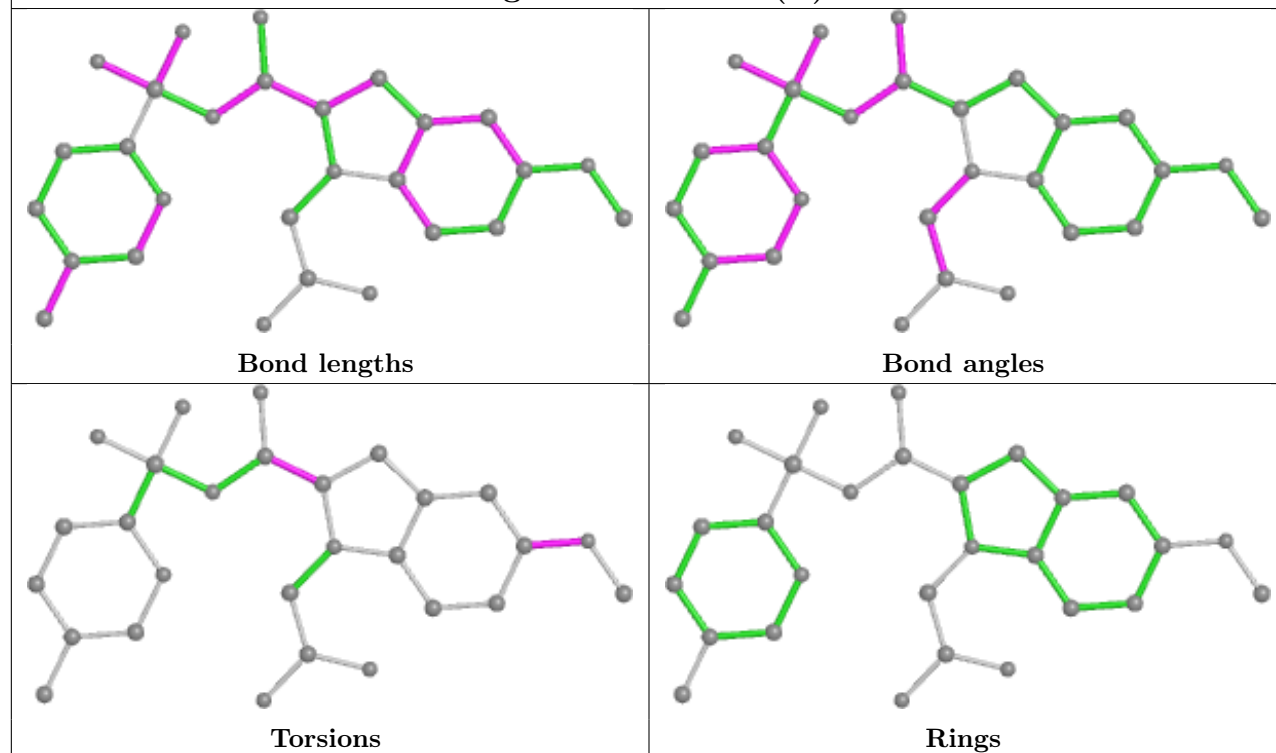
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	721	EOH	3	0
2	A	303	FG3	3	0
3	B	713	GOL	5	0
2	B	302[B]	FG3	1	0
3	B	711	GOL	1	0
3	B	712	GOL	1	0
3	A	708	GOL	3	0
5	A	724	EOH	1	0
2	A	302	FG3	1	0
3	B	709	GOL	9	0
5	A	726	EOH	2	0
4	B	718	EDO	6	0
5	A	722	EOH	5	0
2	B	302[A]	FG3	3	0
4	B	714	EDO	4	0

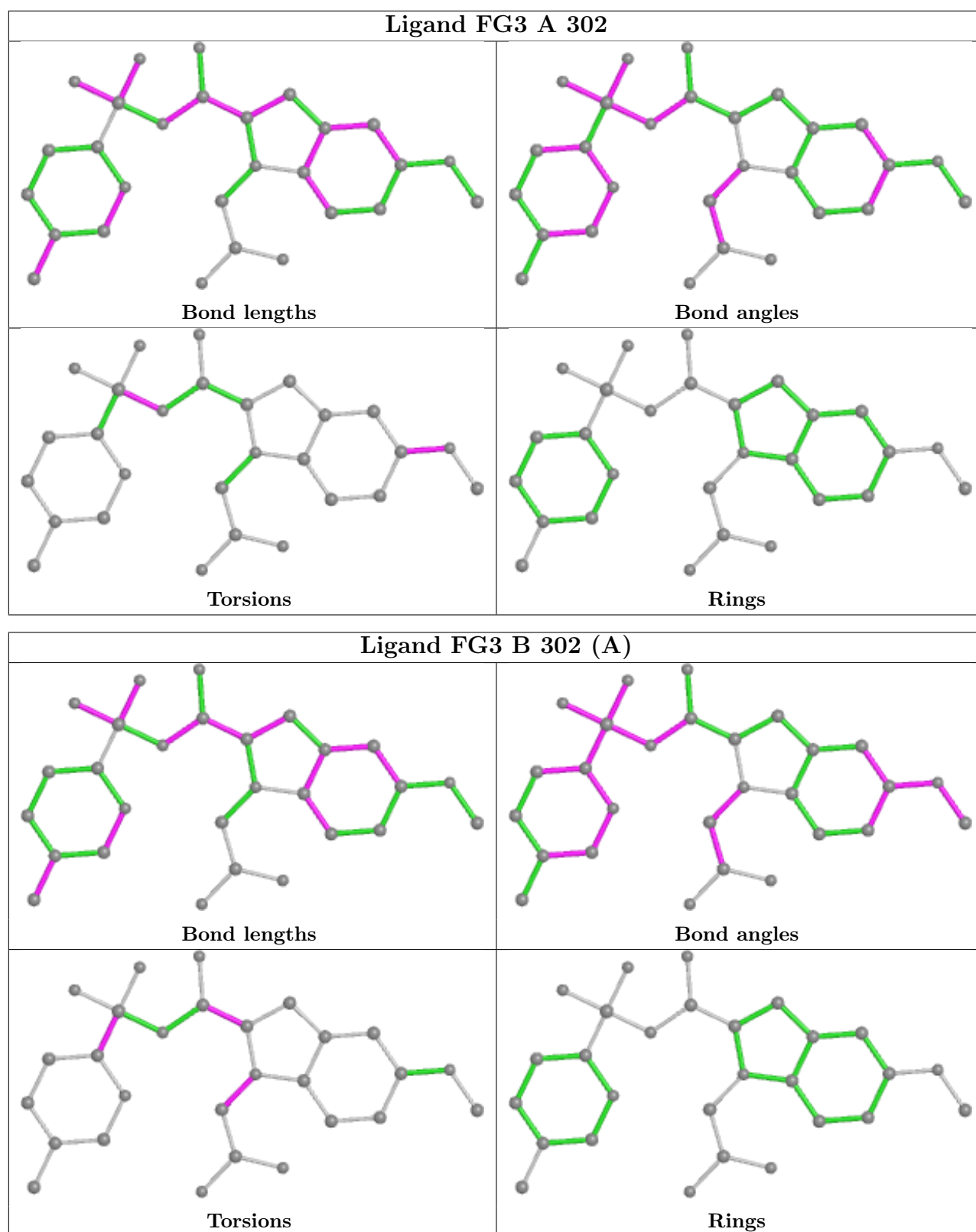
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

## Ligand FG3 A 303



## Ligand FG3 B 302 (B)





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	288/301 (95%)	0.01	10 (3%)	44 49	10, 18, 34, 51	4 (1%)
1	B	278/301 (92%)	0.19	20 (7%)	15 19	10, 17, 36, 66	1 (0%)
All	All	566/602 (94%)	0.10	30 (5%)	26 31	10, 18, 35, 66	5 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	83	PRO	10.8
1	A	290	PHE	8.7
1	B	84	ARG	7.9
1	A	3	ILE	7.8
1	B	85	THR	7.5
1	B	71	MET	7.1
1	B	262	LEU	6.8
1	A	289	THR	5.7
1	A	76	GLY	5.2
1	A	75	ALA	4.9
1	B	288	GLY	4.9
1	B	263	ASN	4.8
1	B	72	GLN	4.8
1	B	1	MET	4.8
1	B	86	PRO	4.2
1	A	4	PRO	4.0
1	B	201	TYR	3.3
1	B	2	ALA	3.2
1	B	87	ASP	3.1
1	A	260	MET	3.0
1	A	243	PRO	3.0
1	B	69	ASN	3.0
1	B	287	ILE	2.6
1	B	70	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	200	ARG	2.5
1	B	88	ASP	2.4
1	A	74	GLY	2.4
1	A	77	GLY	2.1
1	B	261	PRO	2.1
1	B	131	PRO	2.1

## 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	GOL	B	711	6/6	0.65	0.31	72,74,74,74	0
4	EDO	B	714	4/4	0.67	0.23	57,58,58,59	0
5	EOH	A	723	3/3	0.68	0.34	28,28,29,30	0
5	EOH	A	722	3/3	0.77	0.18	25,25,28,28	0
5	EOH	A	724	3/3	0.79	0.22	31,31,31,31	0
3	GOL	A	708	6/6	0.80	0.22	50,51,52,52	0
3	GOL	B	712	6/6	0.80	0.20	42,47,47,49	0
3	GOL	A	710	6/6	0.84	0.20	39,42,42,43	0
3	GOL	A	707	6/6	0.85	0.28	54,55,55,56	0
2	FG3	A	303	28/28	0.85	0.18	32,33,41,42	0
5	EOH	A	721	3/3	0.85	0.10	46,46,46,46	0
3	GOL	B	709	6/6	0.89	0.14	36,37,38,41	0
4	EDO	B	718	4/4	0.90	0.23	41,43,43,43	0
5	EOH	A	726	3/3	0.90	0.23	24,24,25,28	0
3	GOL	B	713	6/6	0.91	0.15	38,42,43,44	0
5	EOH	A	725	3/3	0.92	0.09	32,32,32,33	0
4	EDO	A	719	4/4	0.92	0.09	27,29,29,30	0

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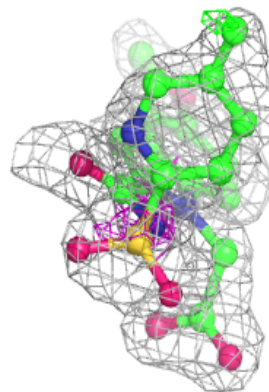
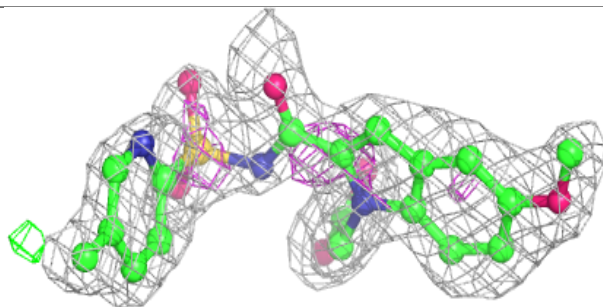
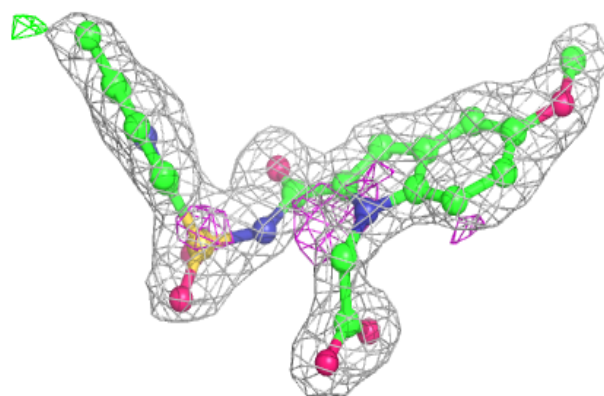
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	A	717	4/4	0.94	0.09	32,35,35,35	0
4	EDO	A	716	4/4	0.94	0.11	24,24,25,26	0
2	FG3	A	302	28/28	0.95	0.09	17,19,24,25	0
2	FG3	B	302[A]	28/28	0.95	0.15	11,14,24,25	28
2	FG3	B	302[B]	28/28	0.95	0.15	28,30,32,32	28
4	EDO	B	715	4/4	0.96	0.10	19,23,23,26	0
4	EDO	A	720	4/4	0.96	0.15	28,30,31,33	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.

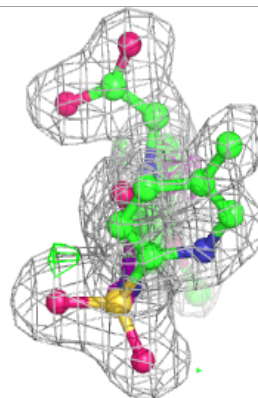
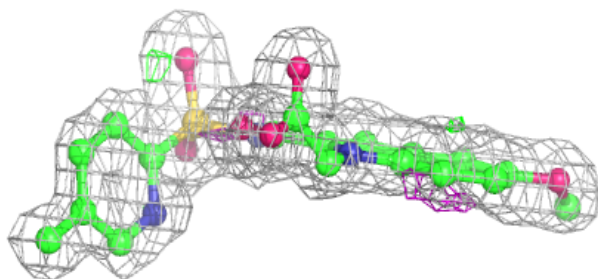
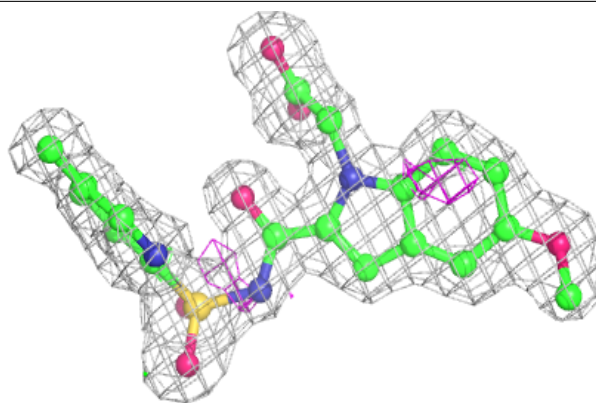
**Electron density around FG3 A 303:**

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)

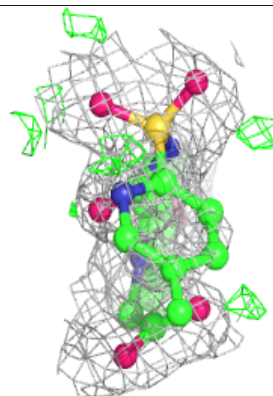
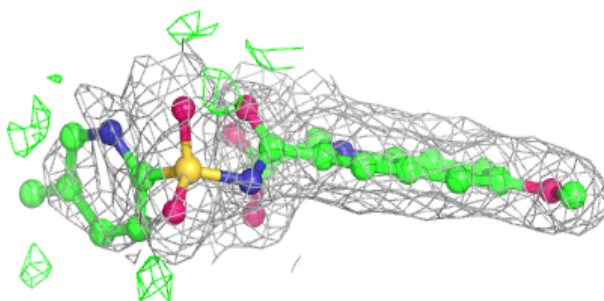
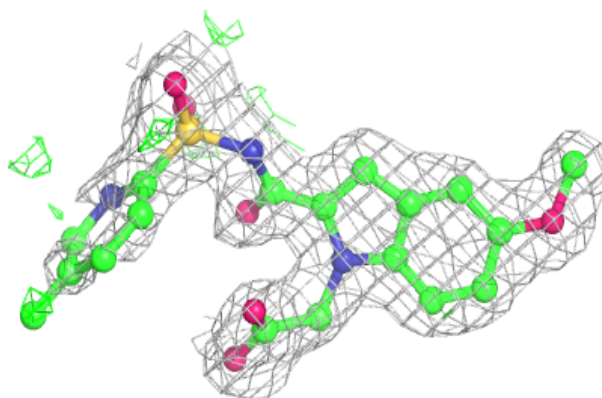


**Electron density around FG3 A 302:**

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

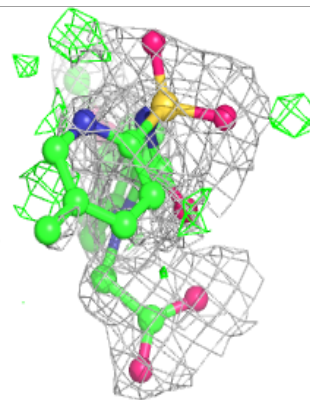
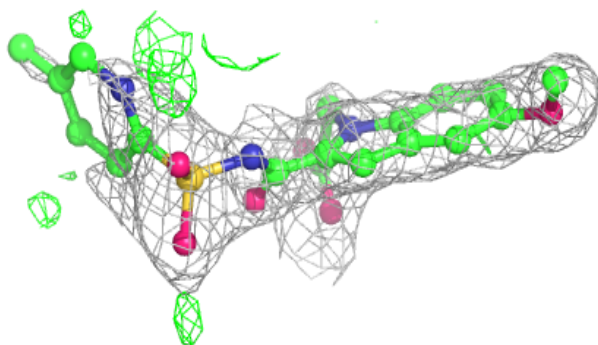
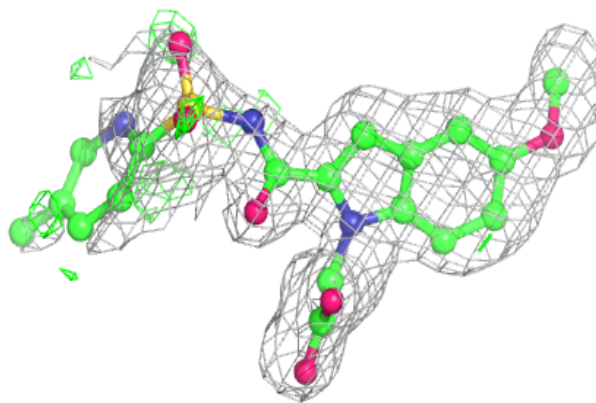
**Electron density around FG3 B 302 (A):**

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



**Electron density around FG3 B 302 (B):**

$2mF_o - DF_c$  (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.