



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:42 PM UTC

PDB ID : 6TG2 / pdb_00006tg2
Title : Structure of the PBP/SBP MotA in complex with mannopinic acid from *A.tumefaciens* R10
Authors : Morera, S.; Marty, L.
Deposited on : 2019-11-14
Resolution : 2.21 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

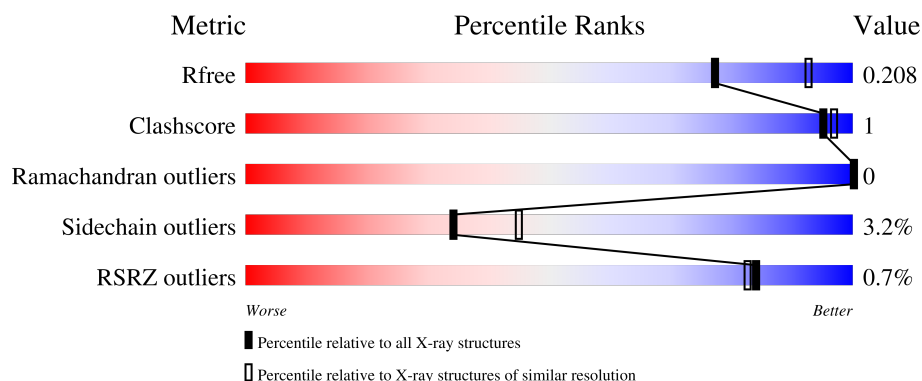
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	351	
1	B	351	
1	C	351	
1	D	351	

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	N72	A	401	X	-	-	-
2	N72	B	401	X	-	-	-
2	N72	C	401	X	-	-	-
2	N72	D	401	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10389 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 MotA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2509	1594	424	482	9			
1	B	325	Total	C	N	O	S	0	0	0
			2498	1588	420	481	9			
1	C	326	Total	C	N	O	S	0	0	0
			2511	1595	426	482	8			
1	D	323	Total	C	N	O	S	0	0	0
			2482	1579	416	478	9			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	MET	-	initiating methionine	UNP Q44384
A	11	GLY	-	expression tag	UNP Q44384
A	12	SER	-	expression tag	UNP Q44384
A	13	SER	-	expression tag	UNP Q44384
A	14	HIS	-	expression tag	UNP Q44384
A	15	HIS	-	expression tag	UNP Q44384
A	16	HIS	-	expression tag	UNP Q44384
A	17	HIS	-	expression tag	UNP Q44384
A	18	HIS	-	expression tag	UNP Q44384
A	19	HIS	-	expression tag	UNP Q44384
A	20	SER	-	expression tag	UNP Q44384
A	21	SER	-	expression tag	UNP Q44384
A	22	GLY	-	expression tag	UNP Q44384
A	23	LEU	-	expression tag	UNP Q44384
A	24	VAL	-	expression tag	UNP Q44384
A	25	PRO	-	expression tag	UNP Q44384
A	26	ARG	-	expression tag	UNP Q44384
A	27	GLY	-	expression tag	UNP Q44384
A	28	SER	-	expression tag	UNP Q44384
A	29	HIS	-	expression tag	UNP Q44384
A	30	MET	-	expression tag	UNP Q44384

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Chain	Residue	Modelled	Actual	Comment	Reference
A	355	HIS	-	expression tag	UNP Q44384
A	356	HIS	-	expression tag	UNP Q44384
A	357	HIS	-	expression tag	UNP Q44384
A	358	HIS	-	expression tag	UNP Q44384
A	359	HIS	-	expression tag	UNP Q44384
A	360	HIS	-	expression tag	UNP Q44384
B	10	MET	-	initiating methionine	UNP Q44384
B	11	GLY	-	expression tag	UNP Q44384
B	12	SER	-	expression tag	UNP Q44384
B	13	SER	-	expression tag	UNP Q44384
B	14	HIS	-	expression tag	UNP Q44384
B	15	HIS	-	expression tag	UNP Q44384
B	16	HIS	-	expression tag	UNP Q44384
B	17	HIS	-	expression tag	UNP Q44384
B	18	HIS	-	expression tag	UNP Q44384
B	19	HIS	-	expression tag	UNP Q44384
B	20	SER	-	expression tag	UNP Q44384
B	21	SER	-	expression tag	UNP Q44384
B	22	GLY	-	expression tag	UNP Q44384
B	23	LEU	-	expression tag	UNP Q44384
B	24	VAL	-	expression tag	UNP Q44384
B	25	PRO	-	expression tag	UNP Q44384
B	26	ARG	-	expression tag	UNP Q44384
B	27	GLY	-	expression tag	UNP Q44384
B	28	SER	-	expression tag	UNP Q44384
B	29	HIS	-	expression tag	UNP Q44384
B	30	MET	-	expression tag	UNP Q44384
B	355	HIS	-	expression tag	UNP Q44384
B	356	HIS	-	expression tag	UNP Q44384
B	357	HIS	-	expression tag	UNP Q44384
B	358	HIS	-	expression tag	UNP Q44384
B	359	HIS	-	expression tag	UNP Q44384
B	360	HIS	-	expression tag	UNP Q44384
C	10	MET	-	initiating methionine	UNP Q44384
C	11	GLY	-	expression tag	UNP Q44384
C	12	SER	-	expression tag	UNP Q44384
C	13	SER	-	expression tag	UNP Q44384
C	14	HIS	-	expression tag	UNP Q44384
C	15	HIS	-	expression tag	UNP Q44384
C	16	HIS	-	expression tag	UNP Q44384
C	17	HIS	-	expression tag	UNP Q44384
C	18	HIS	-	expression tag	UNP Q44384

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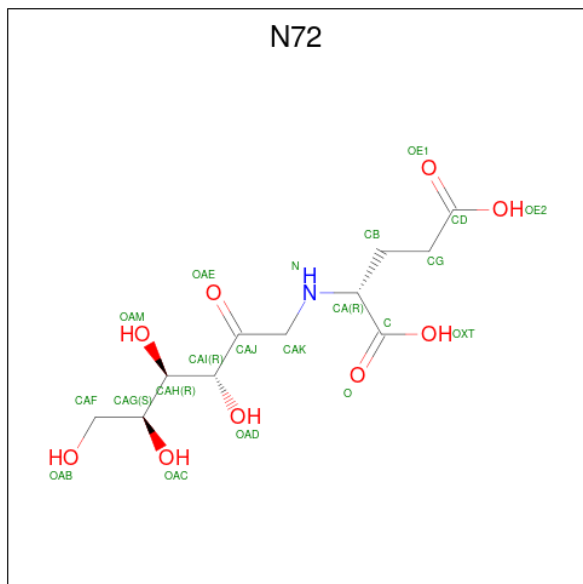
Chain	Residue	Modelled	Actual	Comment	Reference
C	19	HIS	-	expression tag	UNP Q44384
C	20	SER	-	expression tag	UNP Q44384
C	21	SER	-	expression tag	UNP Q44384
C	22	GLY	-	expression tag	UNP Q44384
C	23	LEU	-	expression tag	UNP Q44384
C	24	VAL	-	expression tag	UNP Q44384
C	25	PRO	-	expression tag	UNP Q44384
C	26	ARG	-	expression tag	UNP Q44384
C	27	GLY	-	expression tag	UNP Q44384
C	28	SER	-	expression tag	UNP Q44384
C	29	HIS	-	expression tag	UNP Q44384
C	30	MET	-	expression tag	UNP Q44384
C	355	HIS	-	expression tag	UNP Q44384
C	356	HIS	-	expression tag	UNP Q44384
C	357	HIS	-	expression tag	UNP Q44384
C	358	HIS	-	expression tag	UNP Q44384
C	359	HIS	-	expression tag	UNP Q44384
C	360	HIS	-	expression tag	UNP Q44384
D	10	MET	-	initiating methionine	UNP Q44384
D	11	GLY	-	expression tag	UNP Q44384
D	12	SER	-	expression tag	UNP Q44384
D	13	SER	-	expression tag	UNP Q44384
D	14	HIS	-	expression tag	UNP Q44384
D	15	HIS	-	expression tag	UNP Q44384
D	16	HIS	-	expression tag	UNP Q44384
D	17	HIS	-	expression tag	UNP Q44384
D	18	HIS	-	expression tag	UNP Q44384
D	19	HIS	-	expression tag	UNP Q44384
D	20	SER	-	expression tag	UNP Q44384
D	21	SER	-	expression tag	UNP Q44384
D	22	GLY	-	expression tag	UNP Q44384
D	23	LEU	-	expression tag	UNP Q44384
D	24	VAL	-	expression tag	UNP Q44384
D	25	PRO	-	expression tag	UNP Q44384
D	26	ARG	-	expression tag	UNP Q44384
D	27	GLY	-	expression tag	UNP Q44384
D	28	SER	-	expression tag	UNP Q44384
D	29	HIS	-	expression tag	UNP Q44384
D	30	MET	-	expression tag	UNP Q44384
D	355	HIS	-	expression tag	UNP Q44384
D	356	HIS	-	expression tag	UNP Q44384
D	357	HIS	-	expression tag	UNP Q44384

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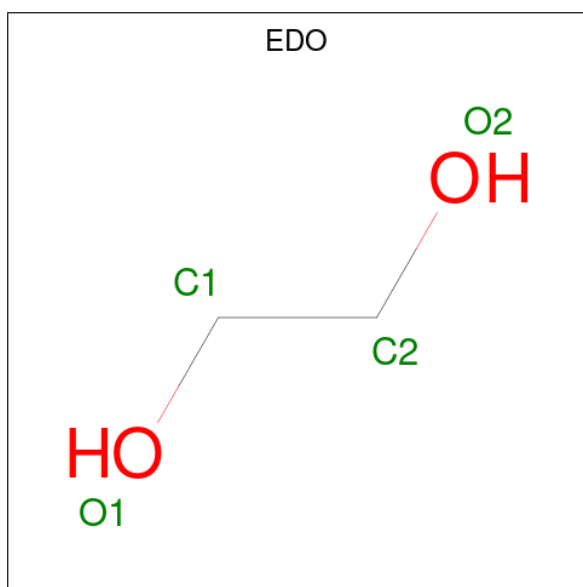
Chain	Residue	Modelled	Actual	Comment	Reference
D	358	HIS	-	expression tag	UNP Q44384
D	359	HIS	-	expression tag	UNP Q44384
D	360	HIS	-	expression tag	UNP Q44384

- Molecule 2 is (2 {R})-2-[[[(3 {R},4 {R},5 {S})-3,4,5,6-tetrakis(oxidanyl)-2-oxidanylidene-h exyl]amino]pentanedioic acid (CCD ID: N72) (formula: C₁₁H₁₉NO₉) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	11	1	9		
2	B	1	Total	C	N	O	0	0
			21	11	1	9		
2	C	1	Total	C	N	O	0	0
			21	11	1	9		
2	D	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

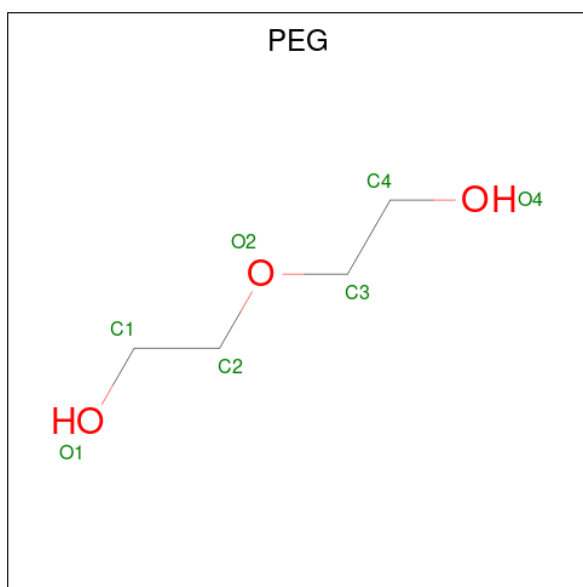


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Ca 3 3	0	0
4	B	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			7	4	3		

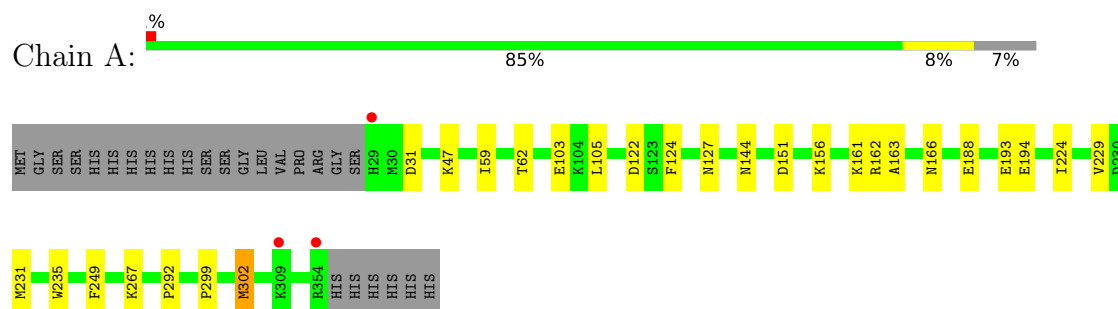
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	77	Total	O	0	0
			77	77		
6	B	67	Total	O	0	0
			67	67		
6	C	56	Total	O	0	0
			56	56		
6	D	69	Total	O	0	0
			69	69		

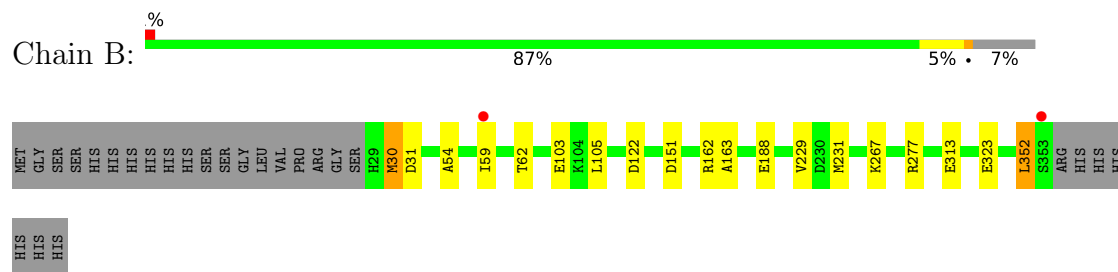
3 Residue-property plots [i](#)

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.

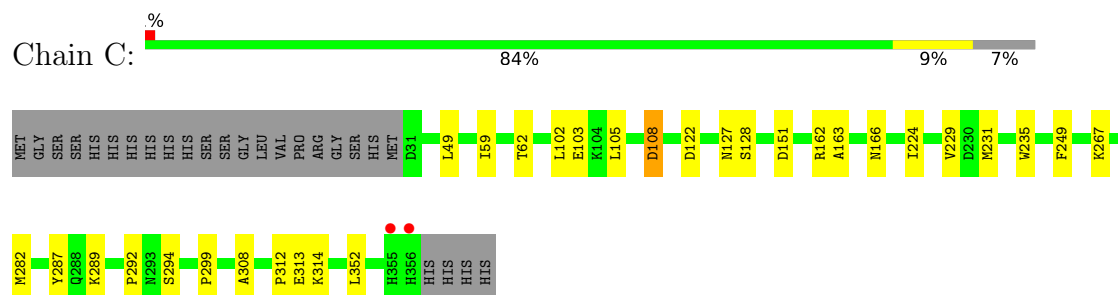
• Molecule 1: MotA



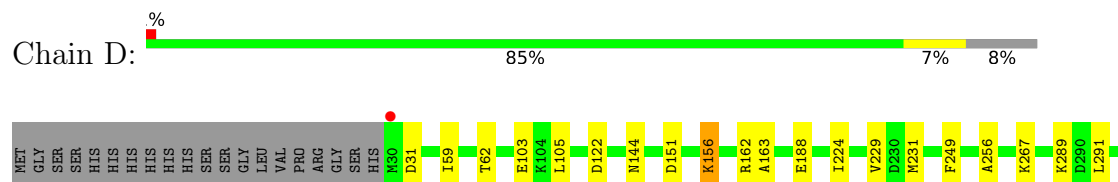
• Molecule 1: MotA

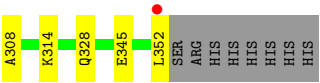


• Molecule 1: MotA



• Molecule 1: MotA





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.92Å 132.13Å 69.46Å 90.00° 91.23° 90.00°	Depositor
Resolution (Å)	31.19 – 2.21 31.19 – 2.21	Depositor EDS
% Data completeness (in resolution range)	97.8 (31.19-2.21) 98.3 (31.19-2.21)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.185 , 0.218 (Not available) , 0.208	Depositor DCC
R_{free} test set	3015 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.011 for l,k,-h 0.042 for h,-k,-l 0.026 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10389	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PEG, N72, CA

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	0.86	0/2572	1.25	10/3497 (0.3%)
1	B	0.85	0/2561	1.28	10/3483 (0.3%)
1	C	0.84	0/2575	1.26	13/3502 (0.4%)
1	D	0.86	1/2544 (0.0%)	1.23	5/3460 (0.1%)
All	All	0.85	1/10252 (0.0%)	1.26	38/13942 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	291	LEU	CA-C	5.09	1.58	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	352	LEU	CA-C-N	6.42	133.25	121.70
1	B	352	LEU	C-N-CA	6.42	133.25	121.70
1	B	30	MET	CA-C-N	6.34	129.84	120.90
1	B	30	MET	C-N-CA	6.34	129.84	120.90
1	B	122	ASP	CA-CB-CG	6.28	118.88	112.60
1	C	312	PRO	CA-C-N	6.28	129.01	120.54
1	C	312	PRO	C-N-CA	6.28	129.01	120.54
1	A	31	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	122	ASP	CA-CB-CG	5.90	118.50	112.60
1	C	151	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	151	ASP	CA-CB-CG	5.80	118.40	112.60
1	D	122	ASP	CA-CB-CG	5.79	118.39	112.60
1	D	151	ASP	CA-CB-CG	5.76	118.36	112.60
1	C	122	ASP	CA-CB-CG	5.75	118.35	112.60
1	B	31	ASP	CA-CB-CG	5.71	118.31	112.60
1	B	151	ASP	CA-CB-CG	5.70	118.30	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	127	ASN	CA-CB-CG	5.33	117.94	112.60
1	C	108	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	124	PHE	CA-CB-CG	5.30	119.10	113.80
1	C	235	TRP	CA-C-N	5.28	125.95	120.03
1	C	235	TRP	C-N-CA	5.28	125.95	120.03
1	C	287	TYR	CA-C-N	5.24	127.55	120.38
1	C	287	TYR	C-N-CA	5.24	127.55	120.38
1	A	235	TRP	CA-C-N	5.23	125.89	120.03
1	A	235	TRP	C-N-CA	5.23	125.89	120.03
1	C	128	SER	N-CA-C	5.23	116.79	108.79
1	A	193	GLU	CA-C-N	5.21	127.22	120.44
1	A	193	GLU	C-N-CA	5.21	127.22	120.44
1	D	188	GLU	N-CA-C	-5.20	105.53	111.14
1	D	31	ASP	CA-CB-CG	5.18	117.78	112.60
1	C	352	LEU	CA-C-N	5.15	128.54	120.82
1	C	352	LEU	C-N-CA	5.15	128.54	120.82
1	A	127	ASN	CA-CB-CG	5.10	117.70	112.60
1	D	144	ASN	CA-CB-CG	5.07	117.67	112.60
1	B	188	GLU	N-CA-C	-5.06	105.66	111.07
1	A	144	ASN	CA-CB-CG	5.04	117.64	112.60
1	B	54	ALA	CA-C-N	5.03	126.97	120.44
1	B	54	ALA	C-N-CA	5.03	126.97	120.44

There are no chirality outliers.

There are no planarity outliers.

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	2509	0	2428	8	0
1	B	2498	0	2415	3	0
1	C	2511	0	2426	7	0
1	D	2482	0	2403	7	0
2	A	21	0	0	0	0
2	B	21	0	0	0	0
2	C	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	21	0	0	0	0
3	A	12	0	18	0	0
3	B	4	0	6	0	0
3	C	8	0	12	0	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	C	7	0	10	0	0
6	A	77	0	0	0	0
6	B	67	0	0	0	0
6	C	56	0	0	0	0
6	D	69	0	0	0	0
All	All	10389	0	9718	24	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (24) 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:D:162:ARG:HG3	1:D:231:MET:HG3	1.82	0.62
1:B:162:ARG:HG3	1:B:231:MET:HG3	1.82	0.61
1:A:292:PRO:HG3	1:A:299:PRO:HD3	1.85	0.59
1:C:163:ALA:HB2	1:C:229:VAL:HG11	1.86	0.57
1:B:103:GLU:HG2	1:B:267:LYS:HA	1.87	0.56
1:C:292:PRO:HG3	1:C:299:PRO:HD3	1.88	0.56
1:A:103:GLU:HG2	1:A:267:LYS:HA	1.88	0.55
1:D:103:GLU:HG2	1:D:267:LYS:HA	1.88	0.55
1:B:163:ALA:HB2	1:B:229:VAL:HG11	1.89	0.55
1:C:103:GLU:HG2	1:C:267:LYS:HA	1.90	0.53
1:D:289:LYS:HB2	1:D:308:ALA:HB2	1.91	0.51
1:C:49:LEU:HB3	1:C:282:MET:HB2	1.92	0.50
1:D:163:ALA:HB2	1:D:229:VAL:HG11	1.92	0.50
1:A:163:ALA:HB2	1:A:229:VAL:HG11	1.97	0.46
1:A:162:ARG:HG3	1:A:231:MET:HG3	1.98	0.45
1:C:289:LYS:HB2	1:C:308:ALA:HB2	1.98	0.45
1:D:256:ALA:HB3	1:D:328:GLN:HG2	1.98	0.44
1:A:161:LYS:HB2	1:A:161:LYS:NZ	2.33	0.43
1:D:224:ILE:HG23	1:D:249:PHE:CG	2.53	0.43
1:A:188:GLU:HG2	1:D:156:LYS:HG2	2.01	0.42
1:C:162:ARG:HG3	1:C:231:MET:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:ILE:HG23	1:C:249:PHE:CG	2.55	0.41
1:A:302:MET:HA	1:A:302:MET:HE2	2.02	0.41
1:A:224:ILE:HG23	1:A:249:PHE:CG	2.56	0.41

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	324/351 (92%)	319 (98%)	5 (2%)	0	100	100
1	B	323/351 (92%)	318 (98%)	5 (2%)	0	100	100
1	C	324/351 (92%)	317 (98%)	7 (2%)	0	100	100
1	D	321/351 (92%)	313 (98%)	8 (2%)	0	100	100
All	All	1292/1404 (92%)	1267 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	252/274 (92%)	244 (97%)	8 (3%)	34	45
1	B	251/274 (92%)	243 (97%)	8 (3%)	34	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	252/274 (92%)	243 (96%)	9 (4%)	31	40
1	D	249/274 (91%)	242 (97%)	7 (3%)	38	50
All	All	1004/1096 (92%)	972 (97%)	32 (3%)	34	45

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

Mol	Chain	Res	Type
1	A	47	LYS
1	A	59	ILE
1	A	62	THR
1	A	105	LEU
1	A	156	LYS
1	A	166	ASN
1	A	194	GLU
1	A	302	MET
1	B	30	MET
1	B	59	ILE
1	B	62	THR
1	B	105	LEU
1	B	277	ARG
1	B	313	GLU
1	B	323	GLU
1	B	352	LEU
1	C	59	ILE
1	C	62	THR
1	C	102	LEU
1	C	105	LEU
1	C	108	ASP
1	C	166	ASN
1	C	294	SER
1	C	313	GLU
1	C	314	LYS
1	D	59	ILE
1	D	62	THR
1	D	105	LEU
1	D	156	LYS
1	D	314	LYS
1	D	345	GLU
1	D	352	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	129	ASN
1	A	167	GLN
1	A	240	GLN
1	A	257	GLN
1	B	67	GLN
1	B	87	GLN
1	B	111	ASN
1	B	127	ASN
1	B	166	ASN
1	B	167	GLN
1	B	240	GLN
1	B	244	ASN
1	B	257	GLN
1	B	334	ASN
1	B	339	HIS
1	C	111	ASN
1	C	127	ASN
1	C	240	GLN
1	C	257	GLN
1	D	67	GLN
1	D	111	ASN
1	D	127	ASN
1	D	144	ASN
1	D	166	ASN
1	D	240	GLN
1	D	244	ASN
1	D	257	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 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
3	EDO	C	403	-	3,3,3	0.77	0	2,2,2	0.22	0
3	EDO	B	402	-	3,3,3	0.71	0	2,2,2	0.04	0
3	EDO	A	402	-	3,3,3	0.76	0	2,2,2	0.25	0
3	EDO	C	402	-	3,3,3	0.57	0	2,2,2	0.19	0
5	PEG	C	404	-	6,6,6	0.92	0	5,5,5	0.34	0
2	N72	A	401	-	20,20,20	1.52	3 (15%)	20,26,26	1.86	5 (25%)
2	N72	B	401	-	20,20,20	1.50	4 (20%)	20,26,26	1.44	3 (15%)
2	N72	D	401	-	20,20,20	1.36	2 (10%)	20,26,26	1.63	6 (30%)
3	EDO	A	404	-	3,3,3	0.54	0	2,2,2	0.30	0
2	N72	C	401	-	20,20,20	1.47	4 (20%)	20,26,26	1.48	5 (25%)
3	EDO	A	403	-	3,3,3	0.52	0	2,2,2	0.37	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	EDO	C	403	-	-	0/1/1/1	-
3	EDO	B	402	-	-	1/1/1/1	-
3	EDO	A	402	-	-	0/1/1/1	-
3	EDO	C	402	-	-	0/1/1/1	-
5	PEG	C	404	-	-	2/4/4/4	-
2	N72	A	401	-	3/3/7/8	7/27/28/28	-
2	N72	B	401	-	3/3/7/8	7/27/28/28	-
2	N72	D	401	-	3/3/7/8	7/27/28/28	-
3	EDO	A	404	-	-	0/1/1/1	-
2	N72	C	401	-	3/3/7/8	7/27/28/28	-
3	EDO	A	403	-	-	1/1/1/1	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	N72	CAK-CAJ	3.92	1.57	1.51
2	A	401	N72	CAK-CAJ	3.81	1.56	1.51
2	B	401	N72	CAK-CAJ	3.73	1.56	1.51
2	D	401	N72	CAK-CAJ	3.00	1.55	1.51
2	D	401	N72	CG-CD	2.93	1.57	1.50
2	C	401	N72	CAK-N	-2.66	1.43	1.46
2	B	401	N72	CG-CD	2.63	1.56	1.50
2	A	401	N72	CG-CD	2.55	1.56	1.50
2	C	401	N72	CG-CD	2.37	1.56	1.50
2	A	401	N72	CAK-N	-2.28	1.43	1.46
2	B	401	N72	O-C	2.25	1.28	1.22
2	C	401	N72	O-C	2.14	1.28	1.22
2	B	401	N72	CAK-N	-2.07	1.44	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	N72	CAK-CAJ-CAI	4.35	123.56	116.43
2	D	401	N72	CAK-N-CA	-4.05	105.63	113.93
2	B	401	N72	CAK-CAJ-CAI	3.38	121.97	116.43
2	C	401	N72	CAK-CAJ-CAI	3.09	121.49	116.43
2	A	401	N72	OAE-CAJ-CAK	-2.90	117.35	121.23
2	A	401	N72	OXT-C-CA	2.66	122.50	113.51
2	B	401	N72	CAK-N-CA	-2.60	108.59	113.93
2	D	401	N72	CAK-CAJ-CAI	2.52	120.56	116.43
2	C	401	N72	OXT-C-O	-2.48	118.46	124.08
2	A	401	N72	CAK-N-CA	-2.47	108.87	113.93
2	A	401	N72	OXT-C-O	-2.47	118.48	124.08
2	D	401	N72	OXT-C-CA	2.43	121.74	113.51
2	D	401	N72	OXT-C-O	-2.38	118.68	124.08
2	D	401	N72	OAE-CAJ-CAK	-2.33	118.11	121.23
2	C	401	N72	CAG-CAH-CAI	2.29	115.80	112.05
2	C	401	N72	OXT-C-CA	2.19	120.91	113.51
2	D	401	N72	OAM-CAH-CAG	2.11	113.72	108.93
2	C	401	N72	OAE-CAJ-CAK	-2.04	118.51	121.23
2	B	401	N72	OXT-C-CA	2.01	120.30	113.51

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	401	N72	CA

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Mol	Chain	Res	Type	Atom
2	A	401	N72	CAG
2	A	401	N72	CAI
2	B	401	N72	CA
2	B	401	N72	CAG
2	B	401	N72	CAI
2	C	401	N72	CA
2	C	401	N72	CAG
2	C	401	N72	CAI
2	D	401	N72	CA
2	D	401	N72	CAG
2	D	401	N72	CAI

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	N72	C-CA-N-CAK
2	A	401	N72	CB-CA-N-CAK
2	B	401	N72	C-CA-N-CAK
2	B	401	N72	CB-CA-N-CAK
2	C	401	N72	C-CA-N-CAK
2	D	401	N72	OAE-CAJ-CAK-N
2	B	401	N72	OAE-CAJ-CAK-N
2	C	401	N72	OAE-CAJ-CAK-N
3	A	403	EDO	O1-C1-C2-O2
2	A	401	N72	OAE-CAJ-CAK-N
5	C	404	PEG	O2-C3-C4-O4
3	B	402	EDO	O1-C1-C2-O2
2	D	401	N72	C-CA-CB-CG
5	C	404	PEG	C1-C2-O2-C3
2	C	401	N72	CB-CA-N-CAK
2	D	401	N72	CB-CA-N-CAK
2	D	401	N72	C-CA-N-CAK
2	C	401	N72	O-C-CA-CB
2	C	401	N72	OXT-C-CA-CB
2	A	401	N72	OXT-C-CA-CB
2	C	401	N72	OE1-CD-CG-CB
2	A	401	N72	OE2-CD-CG-CB
2	D	401	N72	OE1-CD-CG-CB
2	C	401	N72	OE2-CD-CG-CB
2	D	401	N72	OE2-CD-CG-CB
2	A	401	N72	OE1-CD-CG-CB
2	B	401	N72	OE1-CD-CG-CB

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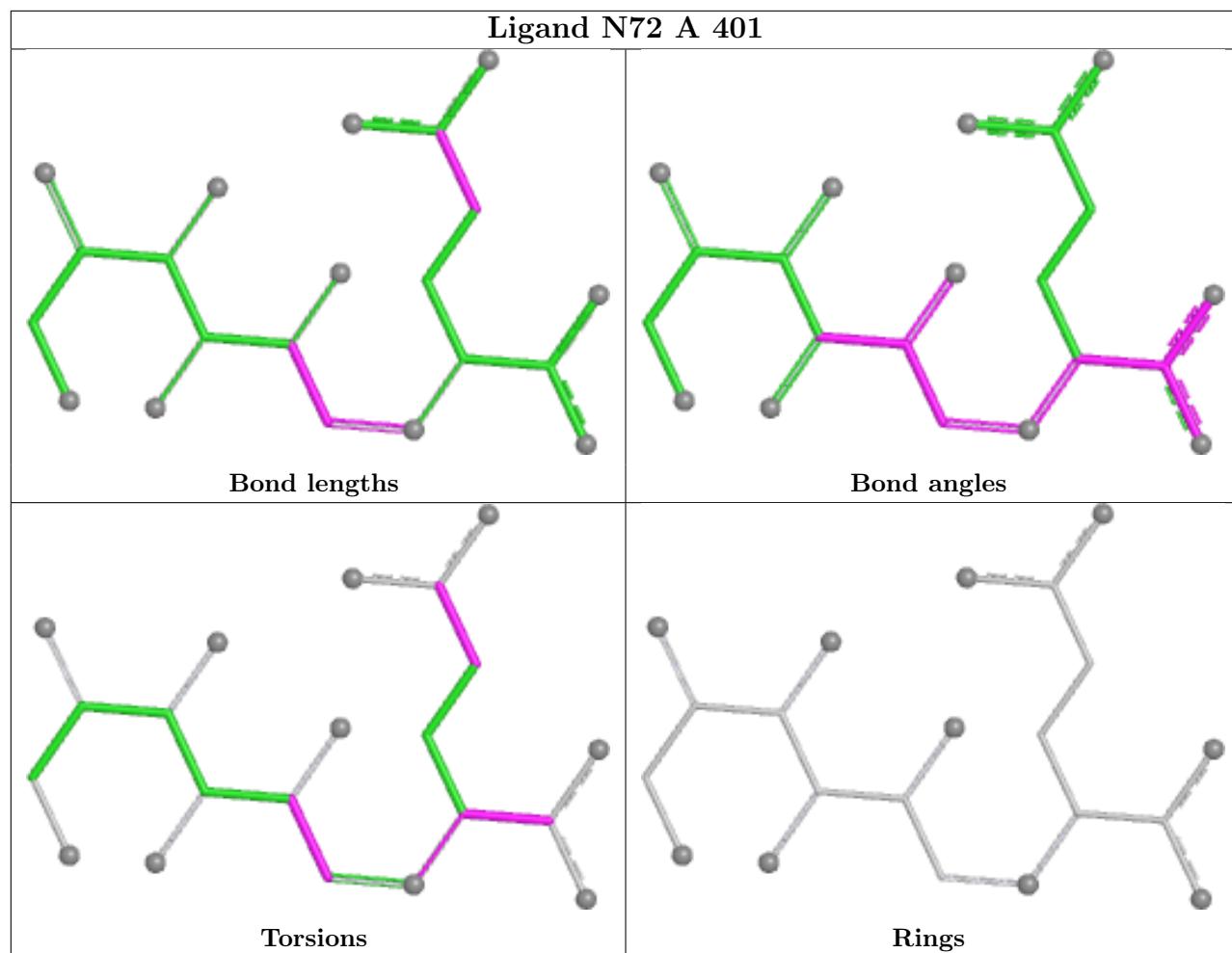
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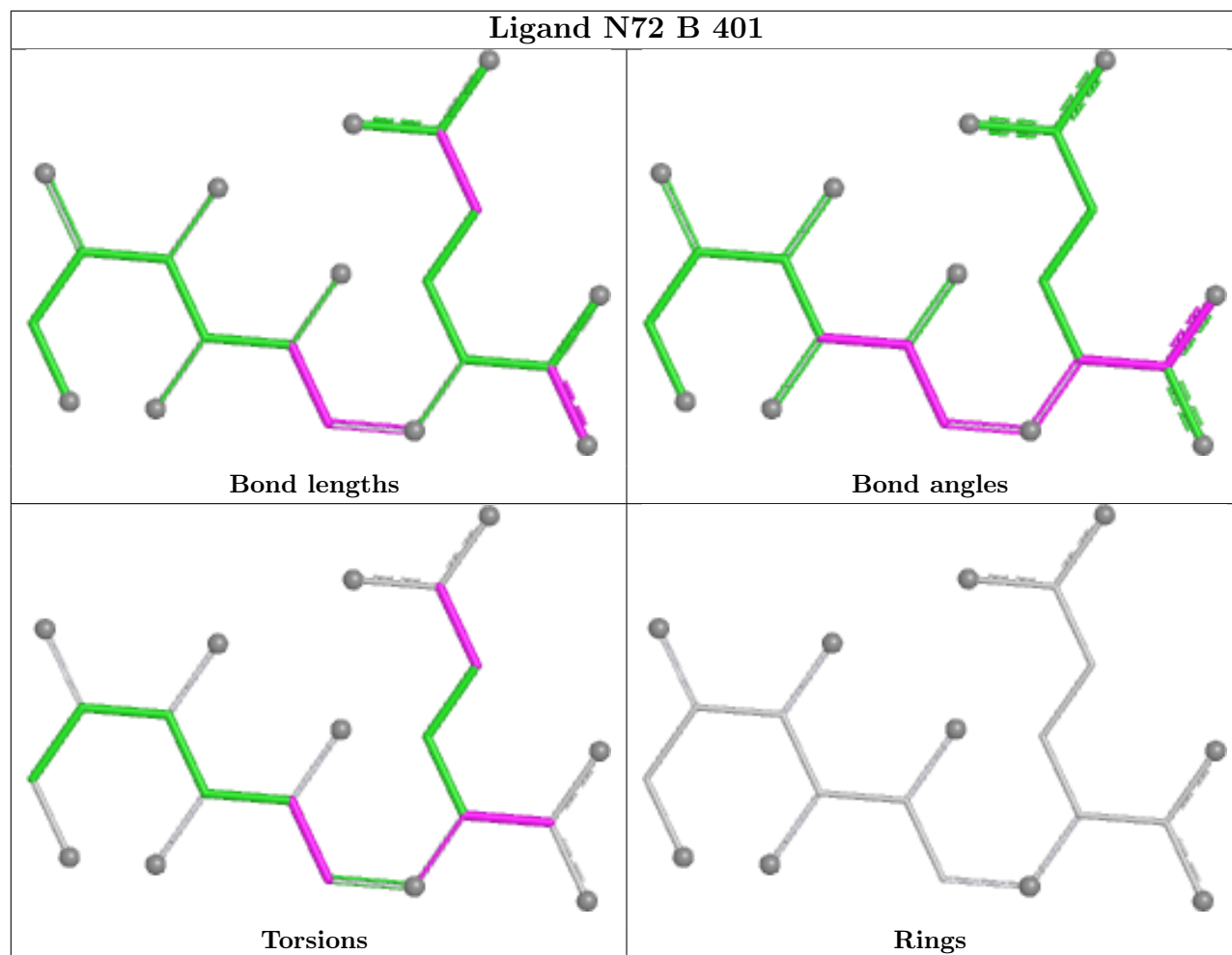
Mol	Chain	Res	Type	Atoms
2	B	401	N72	OE2-CD-CG-CB
2	A	401	N72	O-C-CA-CB
2	D	401	N72	N-CA-CB-CG
2	B	401	N72	OXT-C-CA-CB
2	B	401	N72	O-C-CA-CB

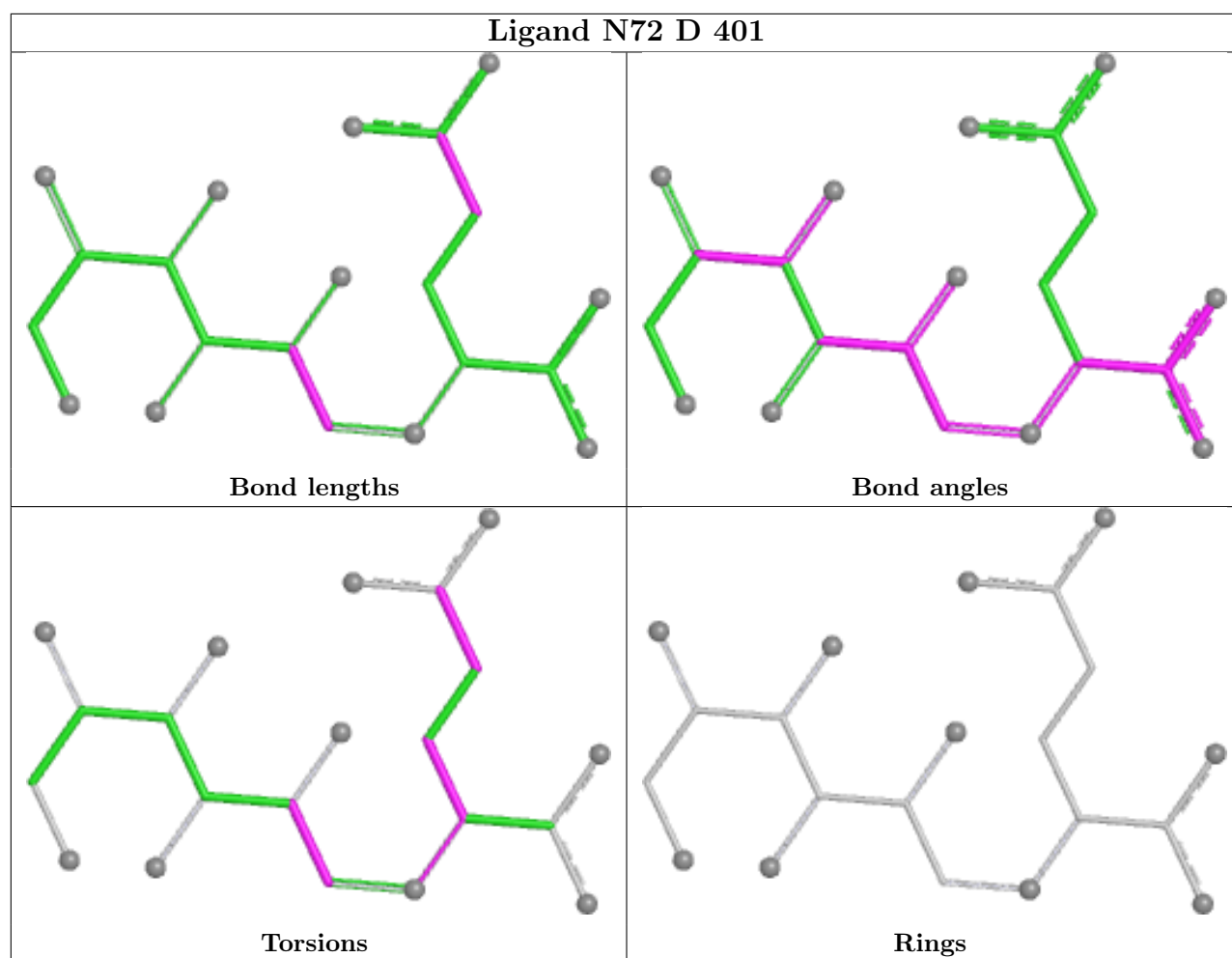
There are no ring outliers.

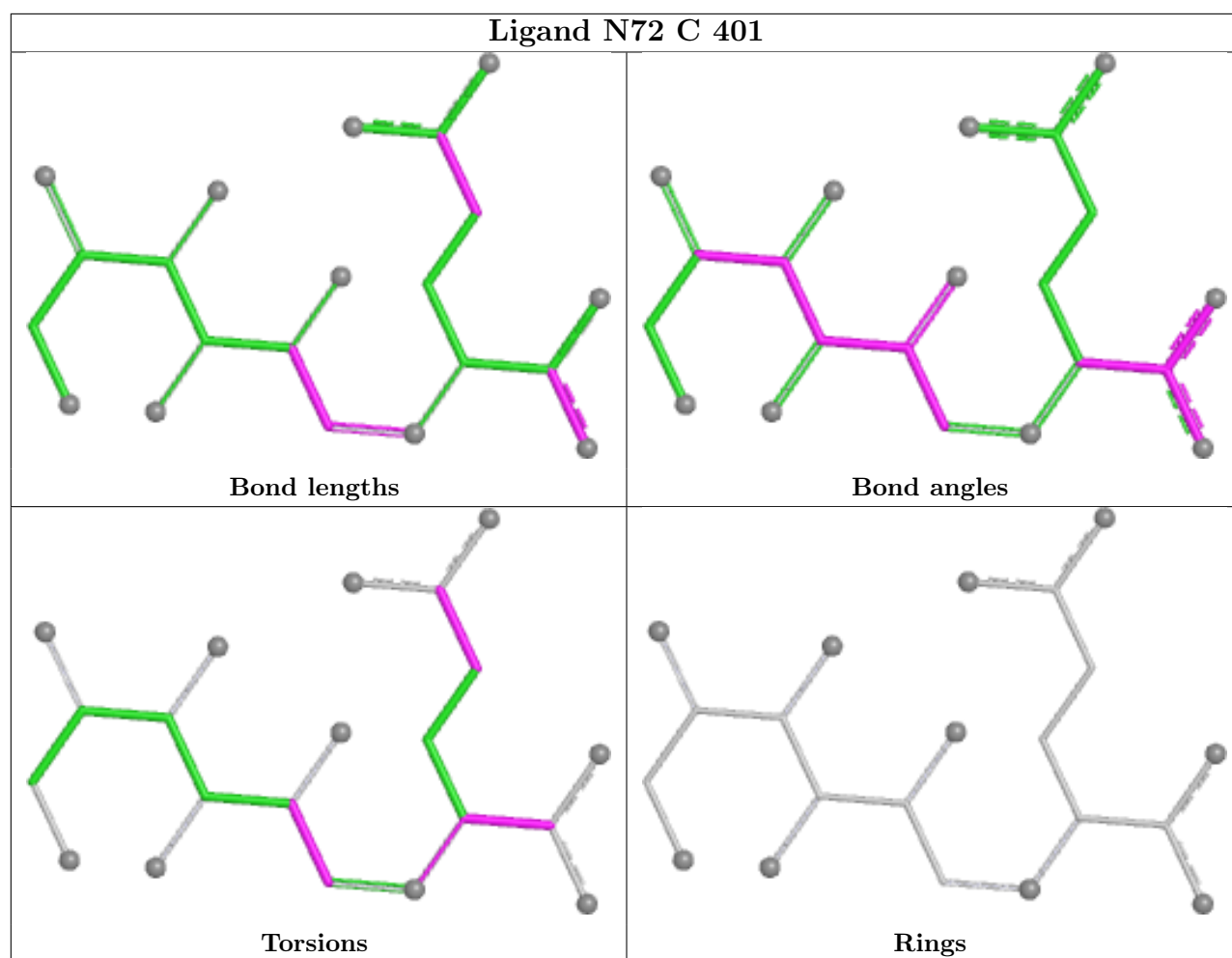
No monomer is involved in short contacts.

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	326/351 (92%)	-0.06	3 (0%) 81 79	24, 38, 65, 108	0
1	B	325/351 (92%)	-0.04	2 (0%) 85 84	25, 40, 67, 82	0
1	C	326/351 (92%)	-0.03	2 (0%) 85 84	25, 42, 68, 113	0
1	D	323/351 (92%)	-0.08	2 (0%) 85 84	24, 39, 69, 83	0
All	All	1300/1404 (92%)	-0.05	9 (0%) 84 83	24, 40, 67, 113	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	30	MET	2.7
1	B	59	ILE	2.6
1	A	29	HIS	2.4
1	C	356	HIS	2.4
1	A	354	ARG	2.4
1	B	353	SER	2.2
1	A	309	LYS	2.1
1	D	352	LEU	2.1
1	C	355	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

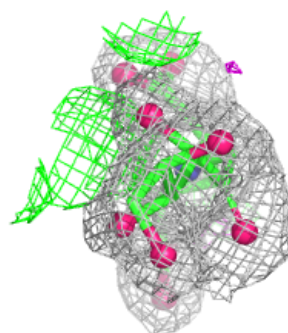
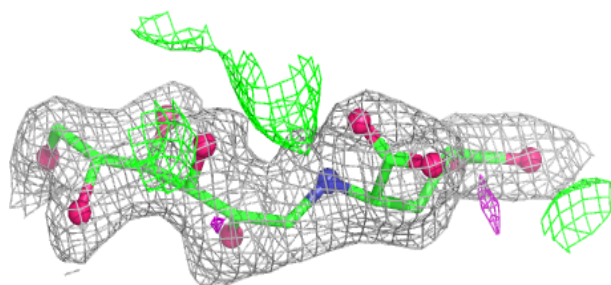
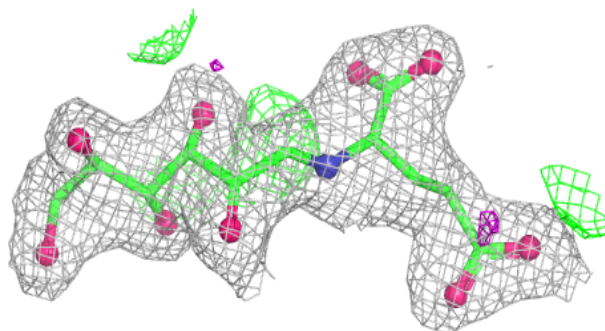
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	A	403	4/4	0.55	0.21	75,76,77,77	0
3	EDO	A	404	4/4	0.67	0.12	75,76,76,76	0
3	EDO	C	402	4/4	0.75	0.12	58,59,60,62	0
5	PEG	C	404	7/7	0.78	0.17	66,66,68,69	0
3	EDO	B	402	4/4	0.79	0.13	51,53,54,55	0
3	EDO	C	403	4/4	0.81	0.14	44,47,49,51	0
4	CA	A	406	1/1	0.86	0.12	87,87,87,87	0
3	EDO	A	402	4/4	0.88	0.11	45,47,48,48	0
4	CA	D	402	1/1	0.89	0.09	83,83,83,83	0
2	N72	D	401	21/21	0.92	0.08	27,31,35,37	0
2	N72	C	401	21/21	0.93	0.07	27,32,42,45	0
2	N72	B	401	21/21	0.94	0.07	18,31,36,38	0
2	N72	A	401	21/21	0.94	0.06	24,34,37,39	0
4	CA	A	407	1/1	0.95	0.13	62,62,62,62	0
4	CA	B	403	1/1	0.97	0.13	55,55,55,55	0
4	CA	A	405	1/1	0.98	0.05	48,48,48,48	0

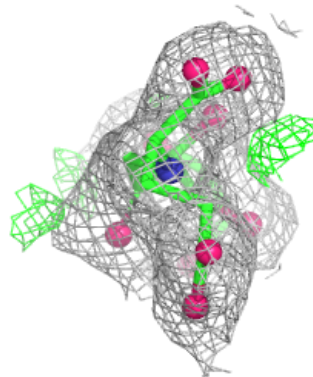
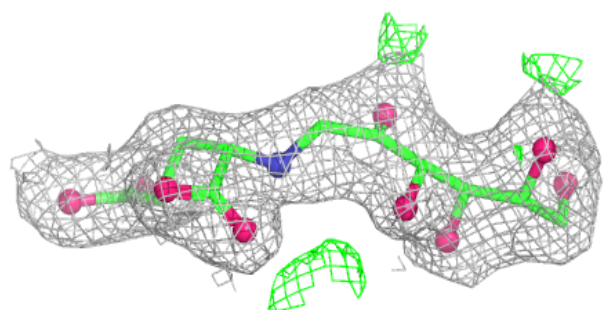
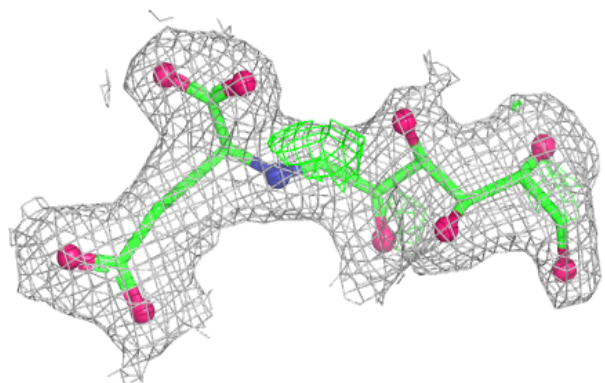
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around N72 D 401:

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

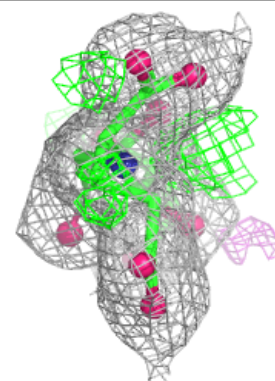
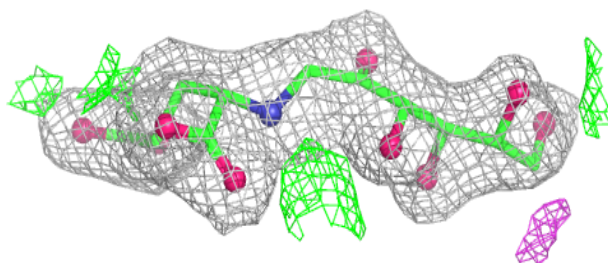
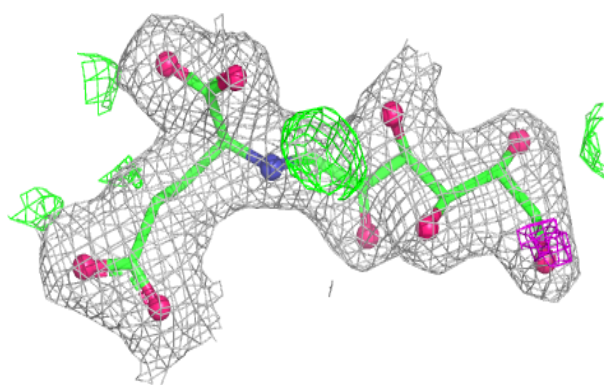
**Electron density around N72 C 401:**

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

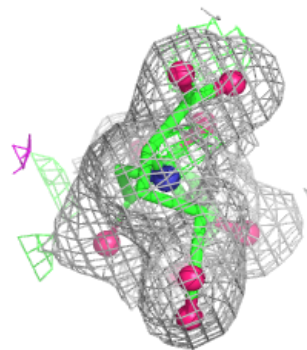
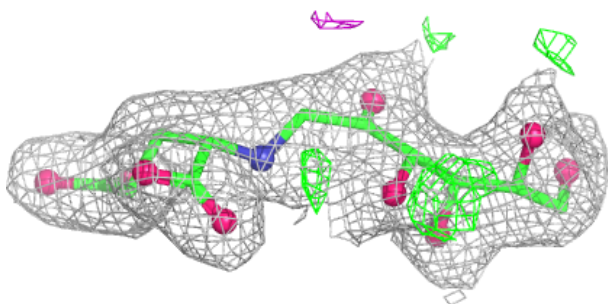
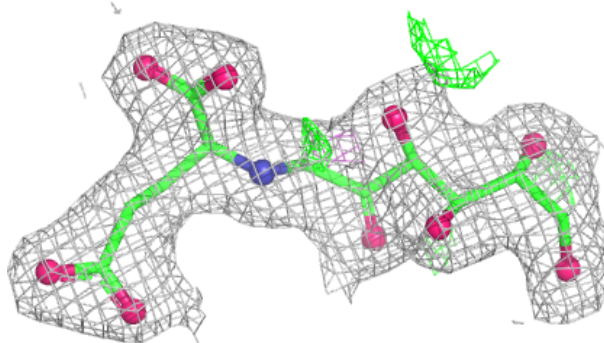


Electron density around N72 B 401:

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

**Electron density around N72 A 401:**

$2mF_o-DF_c$ (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.