



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:03 PM UTC

PDB ID : 9E2B / pdb_00009e2b
Title : Structure of a solute binding protein from Desulfonauticus sp. bound to L-tryptophan
Authors : Rahman, M.; Frkic, R.L.; Smith, O.B.; Jackson, C.J.
Deposited on : 2024-10-22
Resolution : 1.80 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

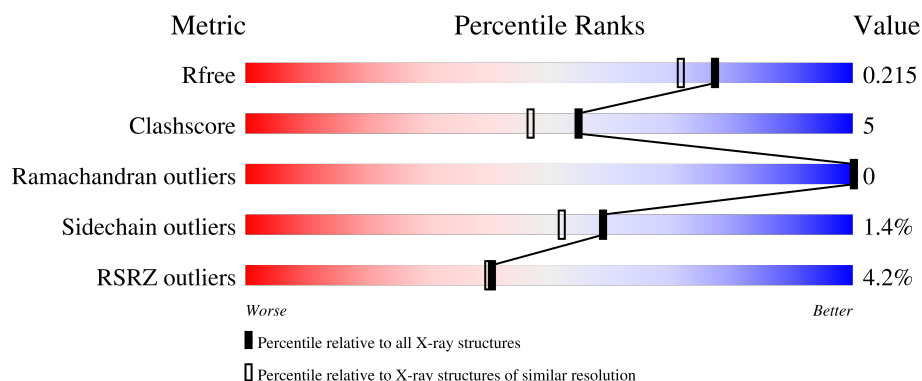
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	270	2% 87% 6% 7%
1	B	270	% 82% 11% 7%
1	C	270	3% 88% 7% .
1	D	270	4% 84% 8% . 6%
1	E	270	% 82% 11% 7%

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Mol	Chain	Length	Quality of chain
1	F	270	

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	EDO	A	308	-	-	X	-
4	PEG	B	303	-	-	X	-
4	PEG	D	302	-	-	X	-
6	PG4	E	302	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13301 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 ABC-type transporter, periplasmic subunit family 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	1	0
			2028	1318	347	358	5			
1	B	252	Total	C	N	O	S	0	0	0
			2018	1312	343	358	5			
1	C	258	Total	C	N	O	S	0	1	0
			2066	1345	350	366	5			
1	D	253	Total	C	N	O	S	0	2	0
			2045	1327	352	361	5			
1	E	251	Total	C	N	O	S	0	1	0
			2023	1315	343	360	5			
1	F	251	Total	C	N	O	S	0	0	0
			2008	1306	341	356	5			

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLY	-	expression tag	UNP A0A101DJ27
A	5	SER	-	expression tag	UNP A0A101DJ27
A	6	SER	-	expression tag	UNP A0A101DJ27
A	7	HIS	-	expression tag	UNP A0A101DJ27
A	8	HIS	-	expression tag	UNP A0A101DJ27
A	9	HIS	-	expression tag	UNP A0A101DJ27
A	10	HIS	-	expression tag	UNP A0A101DJ27
A	11	HIS	-	expression tag	UNP A0A101DJ27
A	12	HIS	-	expression tag	UNP A0A101DJ27
A	13	SER	-	expression tag	UNP A0A101DJ27
A	14	SER	-	expression tag	UNP A0A101DJ27
A	15	GLY	-	expression tag	UNP A0A101DJ27
A	16	GLU	-	expression tag	UNP A0A101DJ27
A	17	ASN	-	expression tag	UNP A0A101DJ27
A	18	LEU	-	expression tag	UNP A0A101DJ27
A	19	TYR	-	expression tag	UNP A0A101DJ27
A	20	PHE	-	expression tag	UNP A0A101DJ27

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Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLN	-	expression tag	UNP A0A101DJ27
A	22	GLY	-	expression tag	UNP A0A101DJ27
B	4	GLY	-	expression tag	UNP A0A101DJ27
B	5	SER	-	expression tag	UNP A0A101DJ27
B	6	SER	-	expression tag	UNP A0A101DJ27
B	7	HIS	-	expression tag	UNP A0A101DJ27
B	8	HIS	-	expression tag	UNP A0A101DJ27
B	9	HIS	-	expression tag	UNP A0A101DJ27
B	10	HIS	-	expression tag	UNP A0A101DJ27
B	11	HIS	-	expression tag	UNP A0A101DJ27
B	12	HIS	-	expression tag	UNP A0A101DJ27
B	13	SER	-	expression tag	UNP A0A101DJ27
B	14	SER	-	expression tag	UNP A0A101DJ27
B	15	GLY	-	expression tag	UNP A0A101DJ27
B	16	GLU	-	expression tag	UNP A0A101DJ27
B	17	ASN	-	expression tag	UNP A0A101DJ27
B	18	LEU	-	expression tag	UNP A0A101DJ27
B	19	TYR	-	expression tag	UNP A0A101DJ27
B	20	PHE	-	expression tag	UNP A0A101DJ27
B	21	GLN	-	expression tag	UNP A0A101DJ27
B	22	GLY	-	expression tag	UNP A0A101DJ27
C	4	GLY	-	expression tag	UNP A0A101DJ27
C	5	SER	-	expression tag	UNP A0A101DJ27
C	6	SER	-	expression tag	UNP A0A101DJ27
C	7	HIS	-	expression tag	UNP A0A101DJ27
C	8	HIS	-	expression tag	UNP A0A101DJ27
C	9	HIS	-	expression tag	UNP A0A101DJ27
C	10	HIS	-	expression tag	UNP A0A101DJ27
C	11	HIS	-	expression tag	UNP A0A101DJ27
C	12	HIS	-	expression tag	UNP A0A101DJ27
C	13	SER	-	expression tag	UNP A0A101DJ27
C	14	SER	-	expression tag	UNP A0A101DJ27
C	15	GLY	-	expression tag	UNP A0A101DJ27
C	16	GLU	-	expression tag	UNP A0A101DJ27
C	17	ASN	-	expression tag	UNP A0A101DJ27
C	18	LEU	-	expression tag	UNP A0A101DJ27
C	19	TYR	-	expression tag	UNP A0A101DJ27
C	20	PHE	-	expression tag	UNP A0A101DJ27
C	21	GLN	-	expression tag	UNP A0A101DJ27
C	22	GLY	-	expression tag	UNP A0A101DJ27
D	4	GLY	-	expression tag	UNP A0A101DJ27
D	5	SER	-	expression tag	UNP A0A101DJ27

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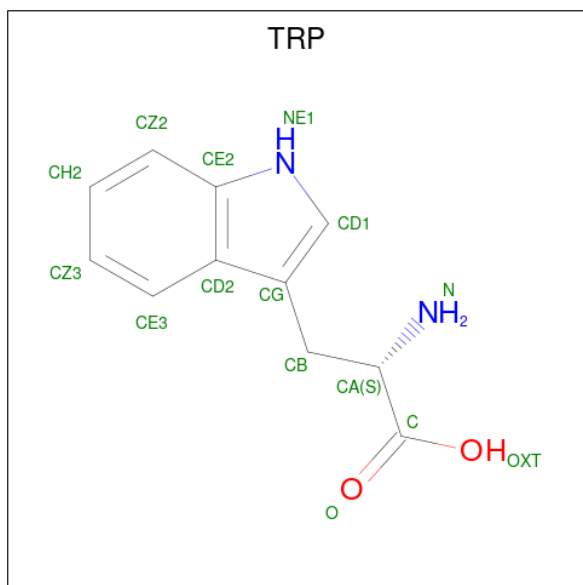
Chain	Residue	Modelled	Actual	Comment	Reference
D	6	SER	-	expression tag	UNP A0A101DJ27
D	7	HIS	-	expression tag	UNP A0A101DJ27
D	8	HIS	-	expression tag	UNP A0A101DJ27
D	9	HIS	-	expression tag	UNP A0A101DJ27
D	10	HIS	-	expression tag	UNP A0A101DJ27
D	11	HIS	-	expression tag	UNP A0A101DJ27
D	12	HIS	-	expression tag	UNP A0A101DJ27
D	13	SER	-	expression tag	UNP A0A101DJ27
D	14	SER	-	expression tag	UNP A0A101DJ27
D	15	GLY	-	expression tag	UNP A0A101DJ27
D	16	GLU	-	expression tag	UNP A0A101DJ27
D	17	ASN	-	expression tag	UNP A0A101DJ27
D	18	LEU	-	expression tag	UNP A0A101DJ27
D	19	TYR	-	expression tag	UNP A0A101DJ27
D	20	PHE	-	expression tag	UNP A0A101DJ27
D	21	GLN	-	expression tag	UNP A0A101DJ27
D	22	GLY	-	expression tag	UNP A0A101DJ27
E	4	GLY	-	expression tag	UNP A0A101DJ27
E	5	SER	-	expression tag	UNP A0A101DJ27
E	6	SER	-	expression tag	UNP A0A101DJ27
E	7	HIS	-	expression tag	UNP A0A101DJ27
E	8	HIS	-	expression tag	UNP A0A101DJ27
E	9	HIS	-	expression tag	UNP A0A101DJ27
E	10	HIS	-	expression tag	UNP A0A101DJ27
E	11	HIS	-	expression tag	UNP A0A101DJ27
E	12	HIS	-	expression tag	UNP A0A101DJ27
E	13	SER	-	expression tag	UNP A0A101DJ27
E	14	SER	-	expression tag	UNP A0A101DJ27
E	15	GLY	-	expression tag	UNP A0A101DJ27
E	16	GLU	-	expression tag	UNP A0A101DJ27
E	17	ASN	-	expression tag	UNP A0A101DJ27
E	18	LEU	-	expression tag	UNP A0A101DJ27
E	19	TYR	-	expression tag	UNP A0A101DJ27
E	20	PHE	-	expression tag	UNP A0A101DJ27
E	21	GLN	-	expression tag	UNP A0A101DJ27
E	22	GLY	-	expression tag	UNP A0A101DJ27
F	4	GLY	-	expression tag	UNP A0A101DJ27
F	5	SER	-	expression tag	UNP A0A101DJ27
F	6	SER	-	expression tag	UNP A0A101DJ27
F	7	HIS	-	expression tag	UNP A0A101DJ27
F	8	HIS	-	expression tag	UNP A0A101DJ27
F	9	HIS	-	expression tag	UNP A0A101DJ27

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Chain	Residue	Modelled	Actual	Comment	Reference
F	10	HIS	-	expression tag	UNP A0A101DJ27
F	11	HIS	-	expression tag	UNP A0A101DJ27
F	12	HIS	-	expression tag	UNP A0A101DJ27
F	13	SER	-	expression tag	UNP A0A101DJ27
F	14	SER	-	expression tag	UNP A0A101DJ27
F	15	GLY	-	expression tag	UNP A0A101DJ27
F	16	GLU	-	expression tag	UNP A0A101DJ27
F	17	ASN	-	expression tag	UNP A0A101DJ27
F	18	LEU	-	expression tag	UNP A0A101DJ27
F	19	TYR	-	expression tag	UNP A0A101DJ27
F	20	PHE	-	expression tag	UNP A0A101DJ27
F	21	GLN	-	expression tag	UNP A0A101DJ27
F	22	GLY	-	expression tag	UNP A0A101DJ27

- Molecule 2 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



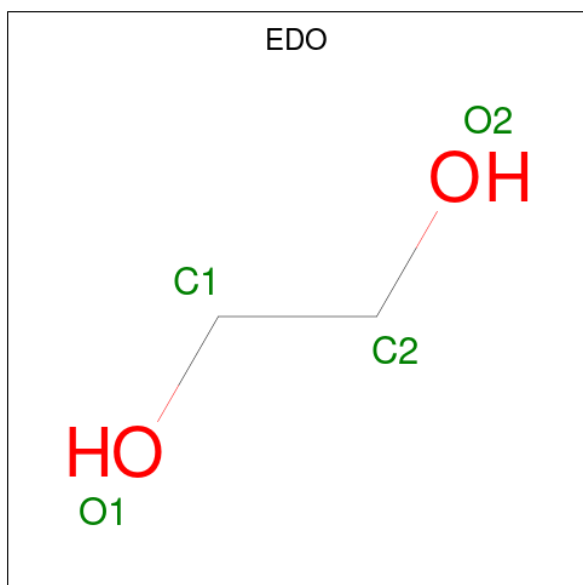
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	2	2		
2	B	1	Total	C	N	O	0	0
			15	11	2	2		
2	C	1	Total	C	N	O	0	0
			15	11	2	2		
2	D	1	Total	C	N	O	0	0
			15	11	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	N	O	0	0
			15	11	2	2		
2	F	1	Total	C	N	O	0	0
			15	11	2	2		

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



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

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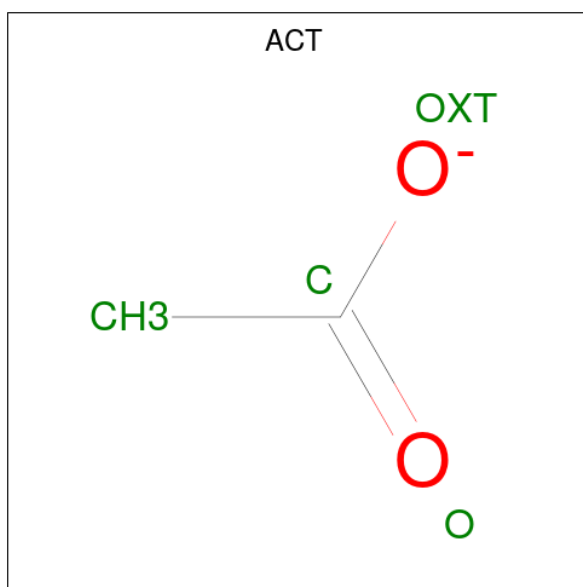
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



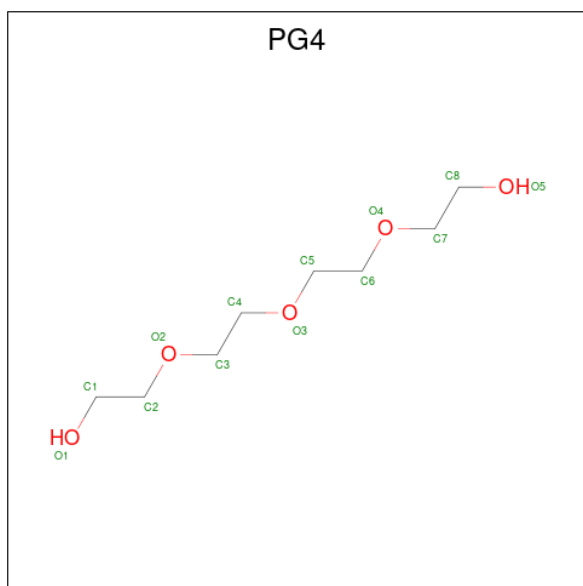
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			13	8	5		

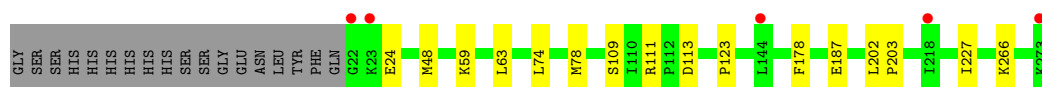
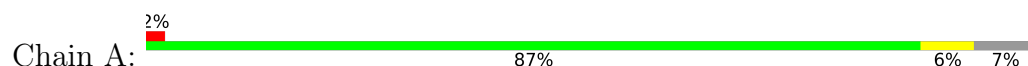
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	191	Total	O	0	0
			191	191		
7	B	184	Total	O	0	0
			184	184		
7	C	117	Total	O	0	0
			117	117		
7	D	133	Total	O	0	0
			133	133		
7	E	134	Total	O	0	0
			134	134		
7	F	130	Total	O	0	0
			130	130		

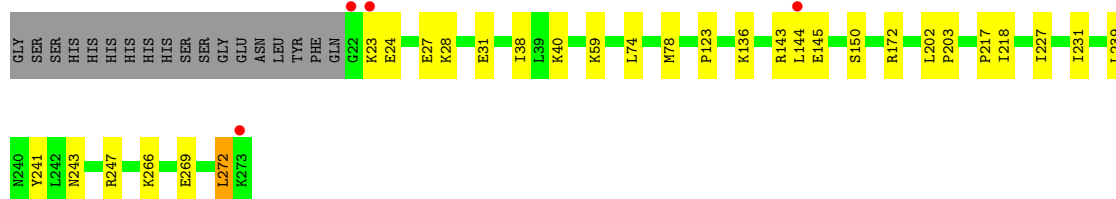
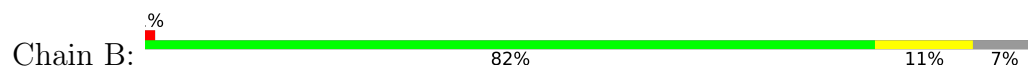
3 Residue-property plots [i](#)

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.

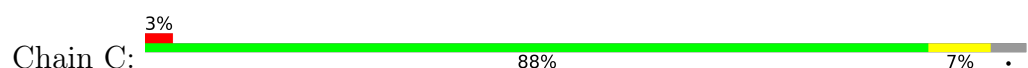
- Molecule 1: ABC-type transporter, periplasmic subunit family 3



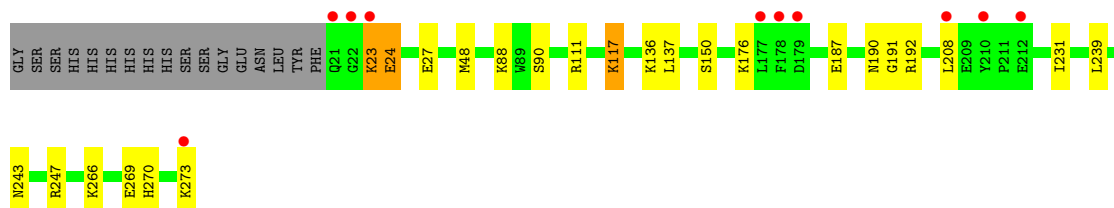
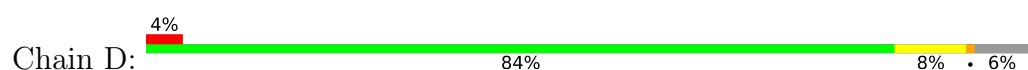
- Molecule 1: ABC-type transporter, periplasmic subunit family 3



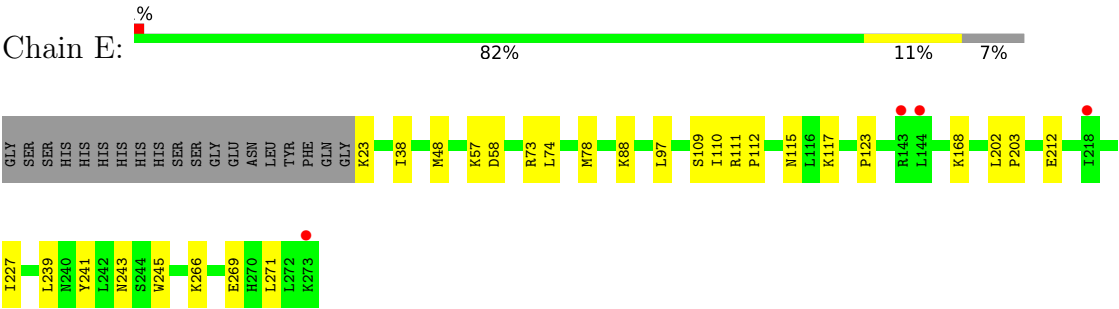
- Molecule 1: ABC-type transporter, periplasmic subunit family 3



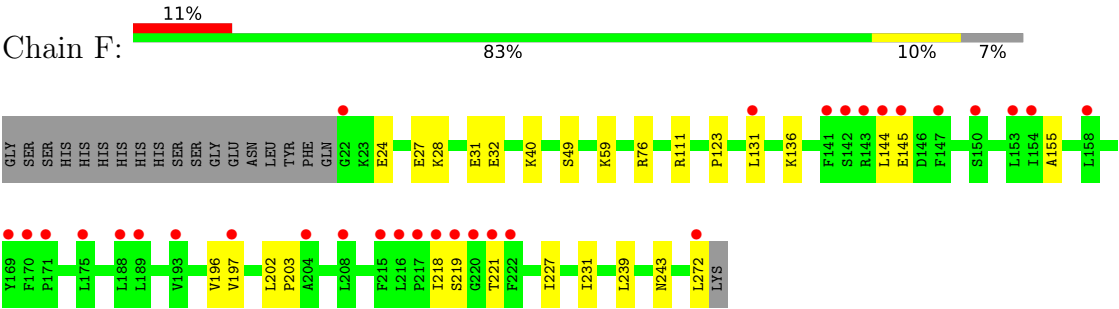
- Molecule 1: ABC-type transporter, periplasmic subunit family 3



- Molecule 1: ABC-type transporter, periplasmic subunit family 3



• Molecule 1: ABC-type transporter, periplasmic subunit family 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.51Å 74.59Å 92.35Å 98.21° 91.24° 119.84°	Depositor
Resolution (Å)	39.14 – 1.80 39.14 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (39.14-1.80) 97.7 (39.14-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.185 , 0.216 0.184 , 0.215	Depositor DCC
R_{free} test set	7977 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13301	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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, ACT, PEG, PG4

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	0.33	0/2076	0.51	0/2803
1	B	0.36	0/2066	0.57	2/2788 (0.1%)
1	C	0.36	0/2115	0.56	0/2856
1	D	0.33	0/2093	0.55	0/2824
1	E	0.41	0/2071	0.59	0/2795
1	F	0.27	0/2056	0.44	0/2777
All	All	0.35	0/12477	0.54	2/16843 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	272	LEU	N-CA-C	6.08	113.76	108.78
1	B	272	LEU	CB-CA-C	-5.28	109.47	117.07

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	2028	0	2074	22	0
1	B	2018	0	2061	22	0
1	C	2066	0	2099	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2045	0	2088	20	0
1	E	2023	0	2063	19	0
1	F	2008	0	2048	20	0
2	A	15	0	9	1	0
2	B	15	0	9	0	0
2	C	15	0	9	0	0
2	D	15	0	9	0	0
2	E	15	0	9	1	0
2	F	15	0	9	0	0
3	A	28	0	42	15	0
3	B	4	0	6	0	0
3	C	12	0	18	1	0
3	D	16	0	24	2	0
3	E	16	0	24	1	0
3	F	16	0	24	2	0
4	B	7	0	10	5	0
4	C	7	0	10	3	0
4	D	7	0	10	5	0
5	C	4	0	3	0	0
5	D	4	0	3	0	0
6	E	13	0	18	7	0
7	A	191	0	0	0	0
7	B	184	0	0	3	0
7	C	117	0	0	0	0
7	D	133	0	0	3	0
7	E	134	0	0	1	0
7	F	130	0	0	4	0
All	All	13301	0	12679	121	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 5.

All (121) 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:111[B]:ARG:HE	3:A:308:EDO:H21	1.05	1.16
1:A:111[A]:ARG:HE	3:A:308:EDO:H21	1.05	1.15
1:A:111[A]:ARG:NE	3:A:308:EDO:H21	1.70	1.05
1:A:111[A]:ARG:HE	3:A:308:EDO:C2	1.71	1.01
1:A:111[B]:ARG:NE	3:A:308:EDO:H21	1.75	1.00
1:A:111[B]:ARG:HE	3:A:308:EDO:C2	1.75	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:302:PEG:H32	1:F:239:LEU:HD13	1.59	0.83
1:B:239:LEU:HD13	4:D:302:PEG:H32	1.63	0.80
1:D:243:ASN:HD22	4:D:302:PEG:H21	1.53	0.73
1:F:144:LEU:HD11	1:F:218:ILE:HG21	1.75	0.68
1:E:239:LEU:HD13	6:E:302:PG4:H82	1.75	0.68
1:B:247:ARG:HH22	4:B:303:PEG:H11	1.59	0.67
6:E:302:PG4:H62	1:F:243:ASN:HD22	1.60	0.67
1:B:247:ARG:HH12	4:B:303:PEG:H22	1.62	0.64
1:A:111[A]:ARG:CG	3:A:308:EDO:H21	2.29	0.63
1:A:111[B]:ARG:CD	3:A:308:EDO:H21	2.29	0.61
1:A:74:LEU:O	1:A:78:MET:HG3	2.01	0.60
1:B:247:ARG:HH22	4:B:303:PEG:C1	2.16	0.59
1:F:28:LYS:HE2	1:F:32:GLU:OE2	2.03	0.58
1:A:111[B]:ARG:CG	3:A:308:EDO:H21	2.34	0.58
1:F:231:ILE:HD11	1:F:239:LEU:HG	1.86	0.57
1:B:24:GLU:HG3	1:B:28:LYS:HD2	1.87	0.57
6:E:302:PG4:C6	1:F:243:ASN:HD22	2.18	0.56
1:C:143:ARG:NH2	1:C:146:ASP:OD1	2.37	0.56
1:A:24:GLU:H	1:A:24:GLU:CD	2.14	0.55
1:B:144:LEU:HD23	1:B:218:ILE:HD13	1.88	0.55
1:B:59:LYS:HB3	1:B:272:LEU:O	2.06	0.55
1:D:247:ARG:HE	3:D:304:EDO:H22	1.73	0.54
1:B:145:GLU:HG2	7:B:512:HOH:O	2.07	0.54
4:C:302:PEG:H11	7:F:473:HOH:O	2.08	0.53
1:C:243:ASN:HD22	4:C:302:PEG:H21	1.74	0.53
1:C:270:HIS:HA	1:C:273:LYS:HE3	1.91	0.53
1:C:231:ILE:HD11	1:C:239:LEU:HG	1.91	0.53
1:E:109:SER:HG	2:E:301:TRP:N	2.07	0.52
1:F:27:GLU:O	1:F:31:GLU:HG3	2.09	0.52
1:C:20:PHE:O	1:C:23:LYS:HG2	2.09	0.51
1:D:231:ILE:HD11	1:D:239:LEU:HG	1.92	0.51
1:A:63:LEU:HD12	3:A:303:EDO:H12	1.91	0.51
1:A:109:SER:HG	2:A:301:TRP:N	2.09	0.51
1:B:231:ILE:HD11	1:B:239:LEU:HG	1.92	0.51
1:D:88:LYS:NZ	7:D:404:HOH:O	2.42	0.51
1:D:190:ASN:HB2	1:D:192:ARG:HD2	1.92	0.51
1:E:97:LEU:HD11	1:E:117:LYS:HD2	1.93	0.50
1:E:73:ARG:HG2	1:E:245:TRP:HZ2	1.76	0.50
1:E:266:LYS:HE2	1:E:269:GLU:HG3	1.93	0.50
1:B:27:GLU:O	1:B:31:GLU:HG3	2.11	0.50
1:A:111[A]:ARG:HG3	3:A:308:EDO:H21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:LYS:HE2	7:B:424:HOH:O	2.10	0.50
1:A:202:LEU:HB3	1:A:203:PRO:HD3	1.93	0.49
1:B:38:ILE:HG21	1:B:78:MET:HE1	1.94	0.49
1:D:187:GLU:HA	1:D:192:ARG:HD3	1.94	0.49
1:F:40:LYS:HG3	7:F:412:HOH:O	2.12	0.49
1:F:155:ALA:HB3	1:F:196:VAL:HG22	1.95	0.49
1:F:59:LYS:HB3	1:F:272:LEU:O	2.13	0.49
1:F:111:ARG:NH2	7:F:404:HOH:O	2.46	0.49
1:F:221:THR:OG1	3:F:302:EDO:H11	2.12	0.49
1:C:32:GLU:HG2	1:E:23:LYS:HD2	1.95	0.49
1:E:202:LEU:HB3	1:E:203:PRO:HD3	1.94	0.49
1:D:208:LEU:HG	7:D:431:HOH:O	2.14	0.48
1:B:202:LEU:HB3	1:B:203:PRO:HD3	1.95	0.48
1:E:243:ASN:HD22	6:E:302:PG4:H21	1.79	0.48
7:B:494:HOH:O	4:D:302:PEG:H11	2.14	0.48
1:D:247:ARG:HE	3:D:304:EDO:C2	2.27	0.48
1:D:270:HIS:ND1	1:D:273:LYS:HD3	2.29	0.48
1:B:74:LEU:O	1:B:78:MET:HG3	2.14	0.47
1:D:24:GLU:H	1:D:24:GLU:HG3	1.35	0.47
1:C:88:LYS:HA	1:C:88:LYS:HD2	1.68	0.47
1:E:38:ILE:HG21	1:E:78:MET:HE1	1.97	0.47
1:D:176:LYS:HE3	1:D:187:GLU:OE1	2.15	0.46
1:E:58:ASP:HB2	1:E:271:LEU:O	2.16	0.46
1:F:218:ILE:HD12	1:F:219:SER:H	1.79	0.46
1:A:111[A]:ARG:NE	3:A:308:EDO:C2	2.48	0.46
1:D:117:LYS:HA	1:D:117:LYS:HD2	1.80	0.46
1:E:168:LYS:NZ	7:E:402:HOH:O	2.48	0.46
1:C:38:ILE:HG21	1:C:78:MET:HE1	1.97	0.46
1:B:243:ASN:HD22	4:B:303:PEG:H31	1.81	0.46
1:F:24:GLU:H	1:F:24:GLU:CD	2.23	0.46
1:D:137:LEU:HD11	1:D:191:GLY:O	2.16	0.46
1:A:178:PHE:CZ	1:A:187:GLU:HG3	2.51	0.45
6:E:302:PG4:H32	6:E:302:PG4:H51	1.66	0.45
1:C:254:TRP:HE1	3:C:304:EDO:H21	1.80	0.45
1:D:23:LYS:HE3	1:D:23:LYS:HB3	1.68	0.45
1:A:113:ASP:OD1	3:A:308:EDO:H22	2.16	0.44
1:D:88:LYS:HE3	1:D:90:SER:OG	2.17	0.44
1:B:150:SER:HA	1:B:172:ARG:O	2.18	0.44
1:F:131:LEU:HD12	1:F:197:VAL:HG22	1.98	0.44
1:C:146:ASP:O	1:C:149:LYS:HD2	2.18	0.43
1:F:123:PRO:HA	1:F:227:ILE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:LYS:NZ	1:B:269:GLU:OE2	2.26	0.43
1:D:111[B]:ARG:HG2	7:D:498:HOH:O	2.18	0.43
1:B:123:PRO:HA	1:B:227:ILE:O	2.18	0.43
1:A:111[A]:ARG:NH2	3:A:308:EDO:O2	2.47	0.43
1:E:266:LYS:O	1:E:269:GLU:HB2	2.18	0.43
1:A:111[B]:ARG:HG3	3:A:308:EDO:H12	2.00	0.42
1:E:78:MET:HG2	1:E:241:TYR:CE1	2.54	0.42
1:E:111:ARG:HA	1:E:112:PRO:HD3	1.90	0.42
1:F:76:ARG:HD2	7:F:409:HOH:O	2.20	0.42
1:C:78:MET:HE2	1:C:78:MET:HB3	1.80	0.42
1:B:78:MET:HG2	1:B:241:TYR:CE1	2.54	0.42
1:F:49:SER:HA	3:F:305:EDO:H11	2.02	0.42
1:F:136:LYS:HD3	1:F:136:LYS:HA	1.76	0.42
1:B:40:LYS:HB2	1:B:40:LYS:HE2	1.84	0.42
1:D:247:ARG:HH12	4:D:302:PEG:H12	1.85	0.42
1:B:143:ARG:HE	1:B:145:GLU:HG3	1.85	0.42
1:E:74:LEU:O	1:E:78:MET:HG3	2.20	0.41
1:F:202:LEU:HB3	1:F:203:PRO:HD3	2.01	0.41
1:A:123:PRO:HA	1:A:227:ILE:O	2.21	0.41
1:D:243:ASN:ND2	4:D:302:PEG:H21	2.27	0.41
1:E:123:PRO:HA	1:E:227:ILE:O	2.20	0.41
1:C:182:ALA:O	1:C:186:GLN:HG3	2.20	0.41
1:B:217:PRO:C	1:B:218:ILE:HG13	2.45	0.41
1:C:150:SER:HA	1:C:172:ARG:O	2.20	0.41
4:B:303:PEG:H31	4:B:303:PEG:H12	1.83	0.41
1:D:23:LYS:HD2	1:D:27:GLU:OE1	2.21	0.41
1:C:23:LYS:HG3	1:C:28:LYS:HD3	2.02	0.41
1:D:266:LYS:O	1:D:269:GLU:HB2	2.21	0.41
1:E:110:ILE:C	1:E:111:ARG:HG2	2.46	0.40
6:E:302:PG4:H31	6:E:302:PG4:H11	1.74	0.40
1:E:73:ARG:HD2	3:E:306:EDO:H21	2.02	0.40
1:E:243:ASN:HB2	6:E:302:PG4:H21	2.03	0.40
1:A:266:LYS:HB3	1:A:266:LYS:HE2	1.86	0.40

There are no symmetry-related clashes.

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	251/270 (93%)	248 (99%)	3 (1%)	0	100	100
1	B	250/270 (93%)	247 (99%)	3 (1%)	0	100	100
1	C	257/270 (95%)	255 (99%)	2 (1%)	0	100	100
1	D	253/270 (94%)	250 (99%)	3 (1%)	0	100	100
1	E	250/270 (93%)	247 (99%)	3 (1%)	0	100	100
1	F	249/270 (92%)	245 (98%)	4 (2%)	0	100	100
All	All	1510/1620 (93%)	1492 (99%)	18 (1%)	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	213/228 (93%)	211 (99%)	2 (1%)	70	67
1	B	212/228 (93%)	210 (99%)	2 (1%)	70	67
1	C	215/228 (94%)	213 (99%)	2 (1%)	70	67
1	D	214/228 (94%)	208 (97%)	6 (3%)	38	26
1	E	213/228 (93%)	207 (97%)	6 (3%)	38	26
1	F	211/228 (92%)	210 (100%)	1 (0%)	81	80
All	All	1278/1368 (93%)	1259 (98%)	19 (2%)	59	49

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	MET
1	A	59	LYS
1	B	23	LYS
1	B	136	LYS
1	C	48	MET
1	C	88	LYS
1	D	23	LYS
1	D	24	GLU
1	D	48	MET
1	D	117	LYS
1	D	136	LYS
1	D	150	SER
1	E	48	MET
1	E	57	LYS
1	E	88	LYS
1	E	115	ASN
1	E	212[A]	GLU
1	E	212[B]	GLU
1	F	145	GLU

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

Mol	Chain	Res	Type
1	B	186	GLN
1	D	174	GLN
1	D	213	GLN
1	D	260	HIS
1	E	139	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

35 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	$\# Z > 2$
3	EDO	F	304	-	3,3,3	0.42	0	2,2,2	0.48	0
3	EDO	E	304	-	3,3,3	0.38	0	2,2,2	0.48	0
3	EDO	D	307	-	3,3,3	0.43	0	2,2,2	0.51	0
3	EDO	F	302	-	3,3,3	0.44	0	2,2,2	0.25	0
3	EDO	D	305	-	3,3,3	0.40	0	2,2,2	0.49	0
3	EDO	F	305	-	3,3,3	0.39	0	2,2,2	0.49	0
6	PG4	E	302	-	12,12,12	0.14	0	11,11,11	0.13	0
3	EDO	E	306	-	3,3,3	0.08	0	2,2,2	0.19	0
3	EDO	F	303	-	3,3,3	0.42	0	2,2,2	0.40	0
3	EDO	E	303	-	3,3,3	0.41	0	2,2,2	0.55	0
2	TRP	A	301	-	15,16,16	0.99	1 (6%)	18,22,22	0.66	1 (5%)
3	EDO	A	307	-	3,3,3	0.39	0	2,2,2	0.51	0
3	EDO	A	308	-	3,3,3	0.15	0	2,2,2	0.24	0
3	EDO	A	304	-	3,3,3	0.47	0	2,2,2	0.38	0
4	PEG	D	302	-	6,6,6	0.12	0	5,5,5	0.19	0
3	EDO	A	305	-	3,3,3	0.45	0	2,2,2	0.27	0
5	ACT	C	305	-	3,3,3	1.45	1 (33%)	3,3,3	1.34	0
3	EDO	C	304	-	3,3,3	0.41	0	2,2,2	0.44	0
3	EDO	A	302	-	3,3,3	0.47	0	2,2,2	0.30	0
2	TRP	B	301	-	15,16,16	0.72	0	18,22,22	0.82	1 (5%)
3	EDO	B	302	-	3,3,3	0.48	0	2,2,2	0.38	0
4	PEG	C	302	-	6,6,6	0.14	0	5,5,5	0.31	0
4	PEG	B	303	-	6,6,6	0.10	0	5,5,5	0.33	0
3	EDO	A	306	-	3,3,3	0.40	0	2,2,2	0.50	0
3	EDO	D	304	-	3,3,3	0.46	0	2,2,2	0.36	0
3	EDO	C	306	-	3,3,3	0.28	0	2,2,2	0.58	0
3	EDO	A	303	-	3,3,3	0.44	0	2,2,2	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	C	303	-	3,3,3	0.43	0	2,2,2	0.47	0
5	ACT	D	306	-	3,3,3	1.01	0	3,3,3	1.40	0
2	TRP	E	301	-	15,16,16	0.75	0	18,22,22	0.75	1 (5%)
3	EDO	D	303	-	3,3,3	0.47	0	2,2,2	0.27	0
3	EDO	E	305	-	3,3,3	0.44	0	2,2,2	0.35	0
2	TRP	F	301	-	15,16,16	0.74	1 (6%)	18,22,22	0.79	1 (5%)
2	TRP	C	301	-	15,16,16	0.79	1 (6%)	18,22,22	0.74	1 (5%)
2	TRP	D	301	-	15,16,16	0.82	1 (6%)	18,22,22	0.71	1 (5%)

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	F	304	-	-	1/1/1/1	-
3	EDO	E	304	-	-	0/1/1/1	-
3	EDO	D	307	-	-	1/1/1/1	-
3	EDO	F	302	-	-	1/1/1/1	-
3	EDO	D	305	-	-	0/1/1/1	-
3	EDO	F	305	-	-	0/1/1/1	-
6	PG4	E	302	-	-	7/10/10/10	-
3	EDO	E	306	-	-	1/1/1/1	-
3	EDO	F	303	-	-	0/1/1/1	-
3	EDO	E	303	-	-	1/1/1/1	-
2	TRP	A	301	-	-	0/8/8/8	0/2/2/2
3	EDO	A	307	-	-	1/1/1/1	-
3	EDO	A	308	-	-	1/1/1/1	-
3	EDO	A	304	-	-	0/1/1/1	-
4	PEG	D	302	-	-	3/4/4/4	-
3	EDO	A	305	-	-	1/1/1/1	-
3	EDO	C	304	-	-	0/1/1/1	-
3	EDO	A	302	-	-	1/1/1/1	-
2	TRP	B	301	-	-	0/8/8/8	0/2/2/2
3	EDO	B	302	-	-	0/1/1/1	-
4	PEG	C	302	-	-	3/4/4/4	-
4	PEG	B	303	-	-	2/4/4/4	-
3	EDO	A	306	-	-	0/1/1/1	-
3	EDO	D	304	-	-	1/1/1/1	-
3	EDO	C	306	-	-	1/1/1/1	-
3	EDO	A	303	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	303	-	-	0/1/1/1	-
2	TRP	E	301	-	-	0/8/8/8	0/2/2/2
3	EDO	D	303	-	-	0/1/1/1	-
3	EDO	E	305	-	-	0/1/1/1	-
2	TRP	F	301	-	-	1/8/8/8	0/2/2/2
2	TRP	C	301	-	-	1/8/8/8	0/2/2/2
2	TRP	D	301	-	-	0/8/8/8	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	TRP	OXT-C	-2.44	1.22	1.30
2	A	301	TRP	OXT-C	-2.41	1.23	1.30
2	F	301	TRP	OXT-C	-2.23	1.23	1.30
5	C	305	ACT	CH3-C	2.21	1.57	1.49
2	C	301	TRP	OXT-C	-2.14	1.23	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	TRP	OXT-C-O	-2.89	117.52	124.08
2	B	301	TRP	OXT-C-O	-2.72	117.92	124.08
2	E	301	TRP	OXT-C-O	-2.65	118.06	124.08
2	D	301	TRP	OXT-C-O	-2.48	118.45	124.08
2	C	301	TRP	OXT-C-O	-2.47	118.47	124.08
2	A	301	TRP	OXT-C-O	-2.14	119.23	124.08

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	302	PG4	C1-C2-O2-C3
6	E	302	PG4	O3-C5-C6-O4
4	C	302	PEG	O2-C3-C4-O4
6	E	302	PG4	O1-C1-C2-O2
4	B	303	PEG	C1-C2-O2-C3
6	E	302	PG4	C3-C4-O3-C5
3	A	305	EDO	O1-C1-C2-O2
3	A	308	EDO	O1-C1-C2-O2
4	B	303	PEG	O1-C1-C2-O2
4	C	302	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	D	302	PEG	O2-C3-C4-O4
3	A	302	EDO	O1-C1-C2-O2
3	D	304	EDO	O1-C1-C2-O2
3	E	306	EDO	O1-C1-C2-O2
3	F	302	EDO	O1-C1-C2-O2
4	D	302	PEG	C1-C2-O2-C3
4	C	302	PEG	C1-C2-O2-C3
6	E	302	PG4	O4-C7-C8-O5
6	E	302	PG4	C5-C6-O4-C7
4	D	302	PEG	O1-C1-C2-O2
3	E	303	EDO	O1-C1-C2-O2
3	A	303	EDO	O1-C1-C2-O2
3	A	307	EDO	O1-C1-C2-O2
3	C	306	EDO	O1-C1-C2-O2
3	D	307	EDO	O1-C1-C2-O2
2	C	301	TRP	OXT-C-CA-N
3	F	304	EDO	O1-C1-C2-O2
2	F	301	TRP	OXT-C-CA-N
6	E	302	PG4	C6-C5-O3-C4

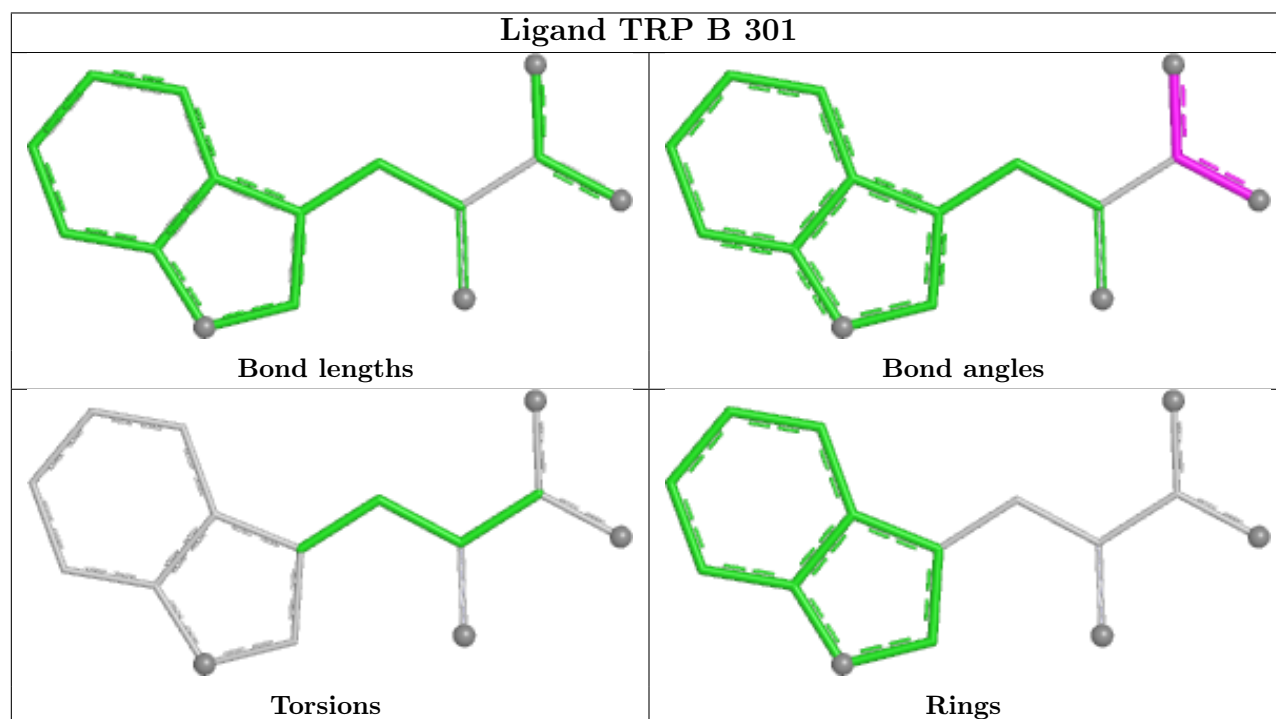
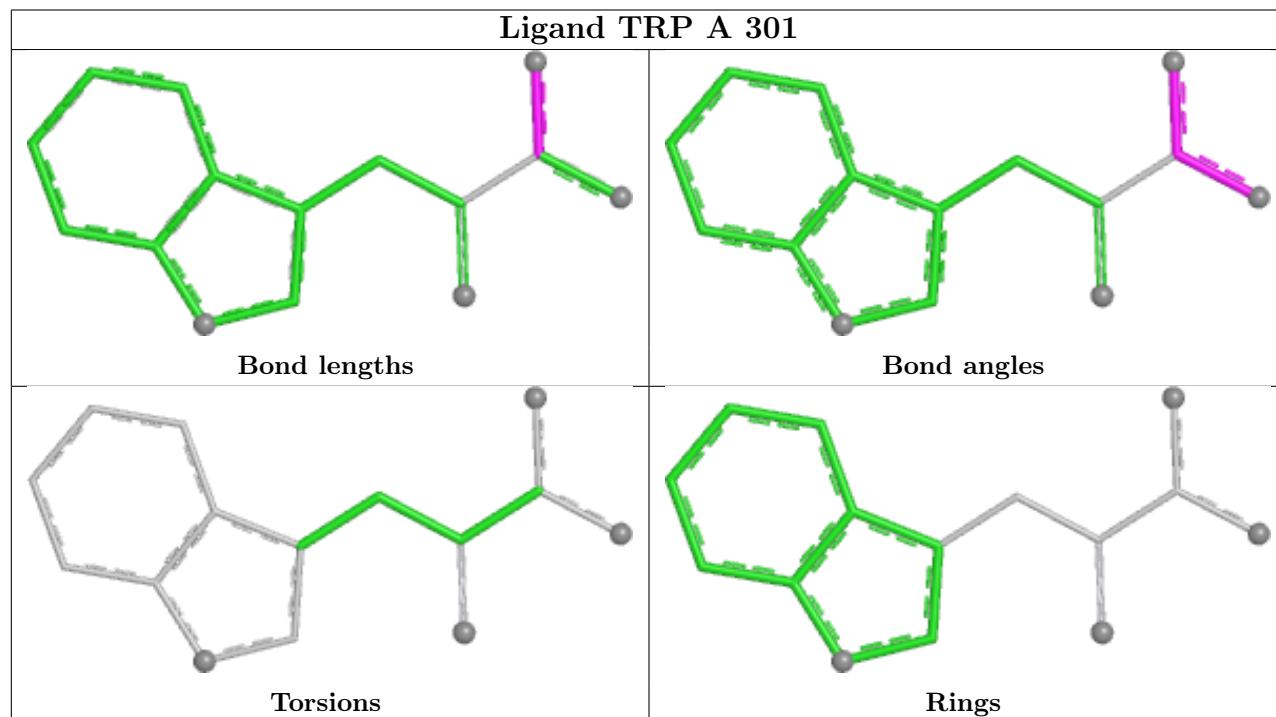
There are no ring outliers.

13 monomers are involved in 43 short contacts:

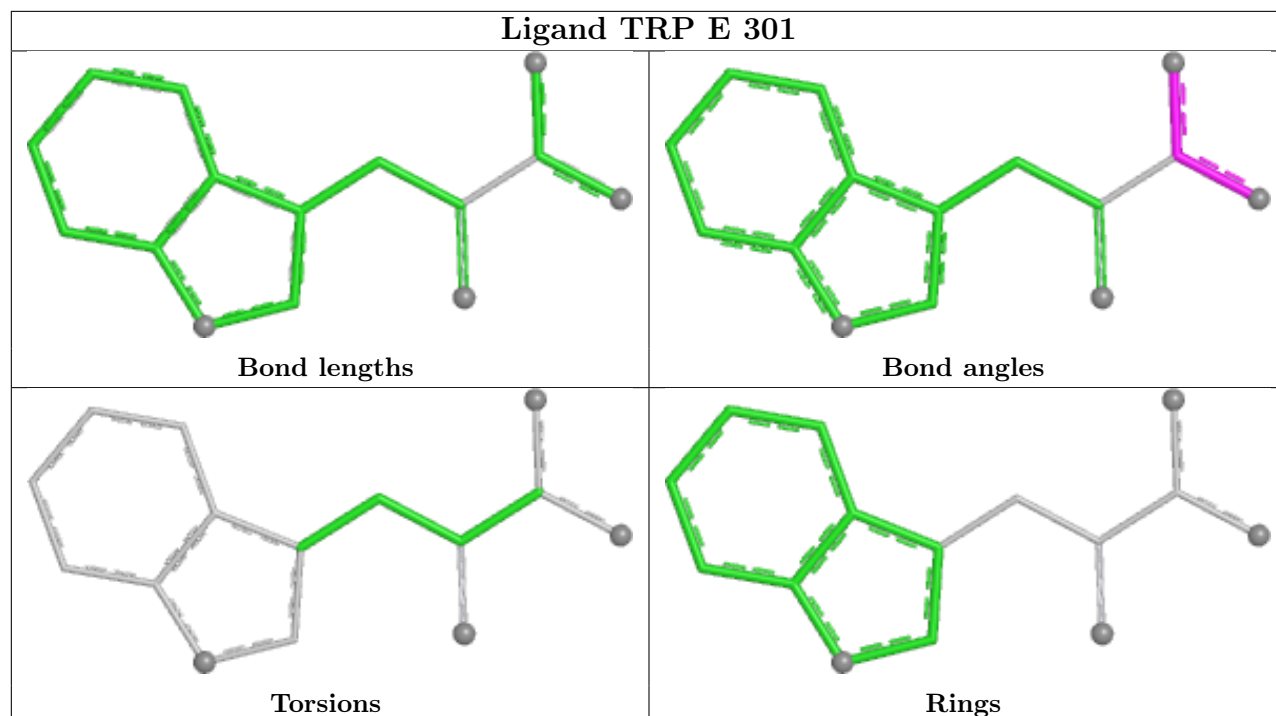
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	302	EDO	1	0
3	F	305	EDO	1	0
6	E	302	PG4	7	0
3	E	306	EDO	1	0
2	A	301	TRP	1	0
3	A	308	EDO	14	0
4	D	302	PEG	5	0
3	C	304	EDO	1	0
4	C	302	PEG	3	0
4	B	303	PEG	5	0
3	D	304	EDO	2	0
3	A	303	EDO	1	0
2	E	301	TRP	1	0

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

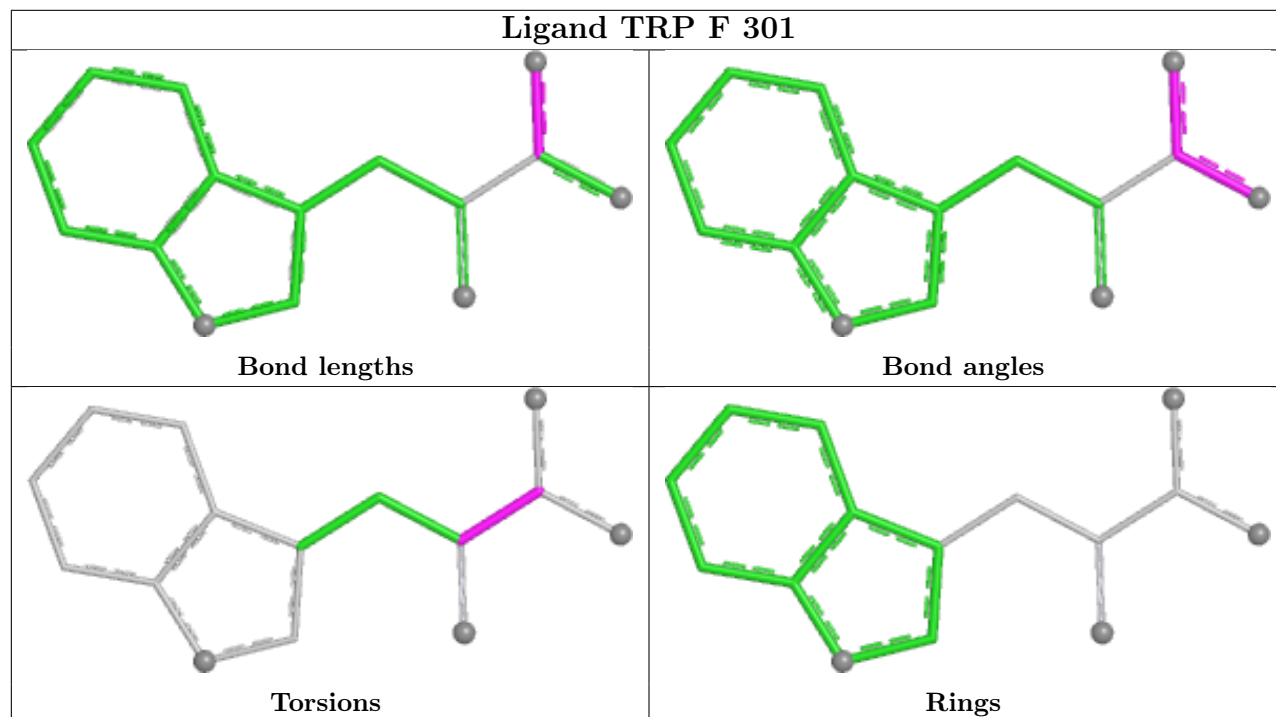
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

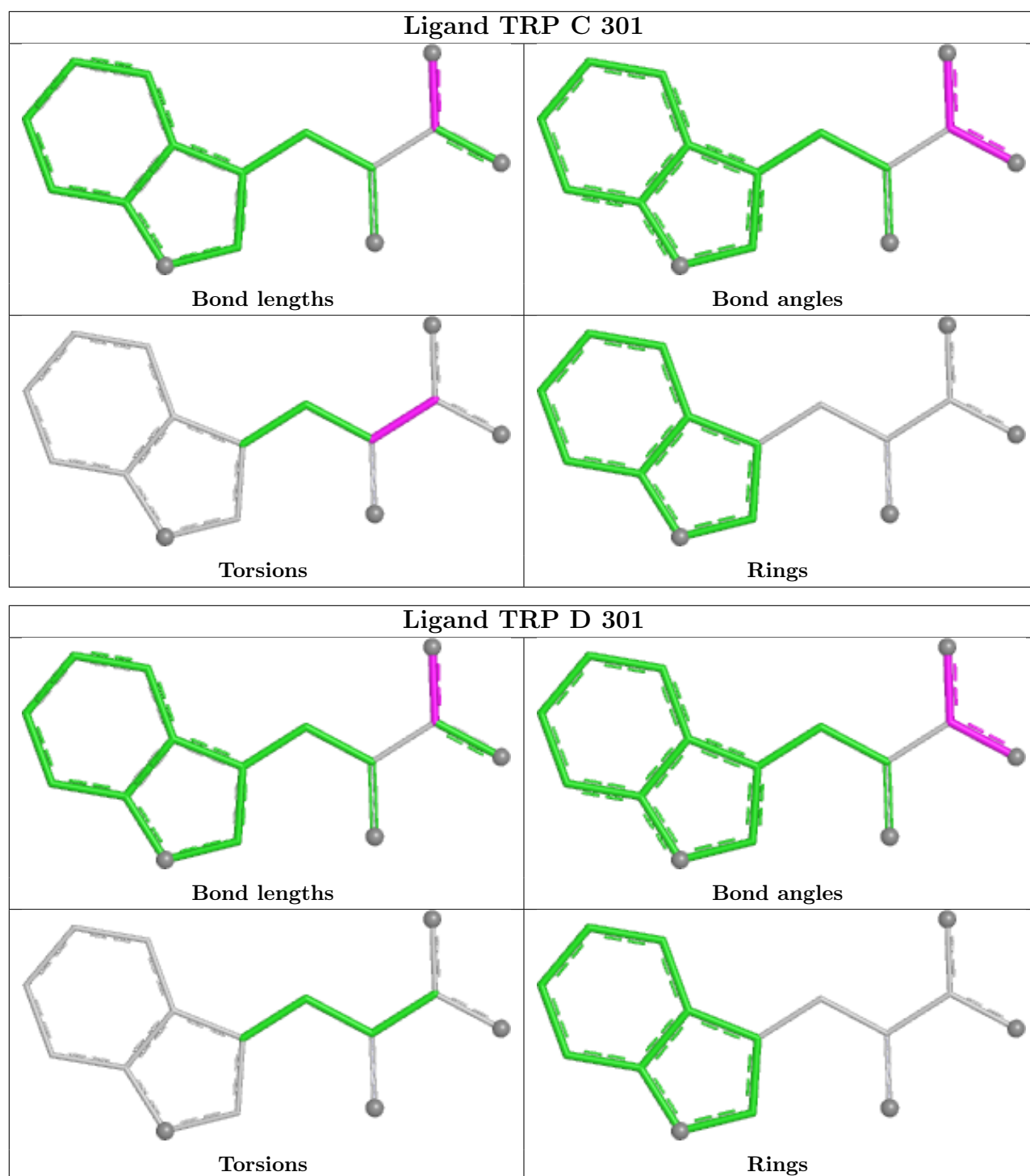


Ligand TRP E 301



Ligand TRP F 301





5.7 Other polymers [i](#)

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, 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	252/270 (93%)	-0.31	5 (1%)	65 65	12, 25, 42, 66	1 (0%)
1	B	252/270 (93%)	-0.22	4 (1%)	70 71	18, 27, 46, 83	0
1	C	258/270 (95%)	0.11	9 (3%)	47 47	16, 32, 54, 79	1 (0%)
1	D	253/270 (93%)	0.10	10 (3%)	42 41	12, 29, 63, 76	2 (0%)
1	E	251/270 (92%)	-0.01	4 (1%)	70 71	19, 32, 53, 83	1 (0%)
1	F	251/270 (92%)	0.64	31 (12%)	8 6	25, 37, 62, 79	0
All	All	1517/1620 (93%)	0.05	63 (4%)	40 40	12, 30, 57, 83	5 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	19	TYR	5.6
1	C	18	LEU	5.2
1	C	17	ASN	4.9
1	A	22	GLY	4.9
1	C	20	PHE	3.9
1	D	210	TYR	3.9
1	F	144	LEU	3.9
1	F	222	PHE	3.5
1	B	22	GLY	3.5
1	D	21	GLN	3.4
1	F	153	LEU	3.4
1	F	188	LEU	3.4
1	F	215	PHE	3.4
1	F	141	PHE	3.3
1	E	273	LYS	3.3
1	E	218	ILE	3.2
1	C	22	GLY	3.2
1	D	208	LEU	3.2
1	F	131	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	22	GLY	3.2
1	A	144	LEU	3.1
1	D	178	PHE	3.1
1	C	16	GLU	3.0
1	E	144	LEU	3.0
1	F	154	ILE	3.0
1	F	216	LEU	2.9
1	F	143	ARG	2.9
1	F	220	GLY	2.9
1	D	22	GLY	2.9
1	F	204	ALA	2.8
1	A	273	LYS	2.8
1	F	221	THR	2.7
1	F	142	SER	2.7
1	B	273	LYS	2.7
1	D	273	LYS	2.7
1	C	24	GLU	2.6
1	F	145	GLU	2.6
1	F	219	SER	2.6
1	F	218	ILE	2.6
1	B	144	LEU	2.5
1	F	208	LEU	2.5
1	F	272	LEU	2.5
1	F	193	VAL	2.5
1	D	23	LYS	2.5
1	C	21	GLN	2.4
1	F	147	PHE	2.4
1	F	170	PHE	2.4
1	D	179	ASP	2.3
1	D	177	LEU	2.3
1	F	175	LEU	2.3
1	A	23	LYS	2.3
1	F	150	SER	2.3
1	C	273	LYS	2.3
1	F	189	LEU	2.2
1	D	212	GLU	2.1
1	B	23	LYS	2.1
1	E	143	ARG	2.1
1	A	218	ILE	2.1
1	F	169	TYR	2.1
1	F	197	VAL	2.1
1	F	217	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	158	LEU	2.0
1	F	171	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	F	304	4/4	0.70	0.17	52,54,59,60	0
3	EDO	D	303	4/4	0.71	0.17	47,50,53,59	0
3	EDO	E	306	4/4	0.72	0.20	49,50,53,60	0
3	EDO	D	307	4/4	0.74	0.19	42,46,46,49	0
3	EDO	E	305	4/4	0.78	0.15	43,48,52,55	0
3	EDO	C	304	4/4	0.79	0.18	45,48,49,52	0
3	EDO	A	308	4/4	0.79	0.22	37,40,42,46	0
3	EDO	D	305	4/4	0.81	0.26	38,39,49,54	0
3	EDO	A	302	4/4	0.83	0.14	41,46,49,50	0
3	EDO	A	306	4/4	0.83	0.15	38,39,47,50	0
6	PG4	E	302	13/13	0.84	0.18	23,29,37,39	13
3	EDO	E	304	4/4	0.85	0.19	32,45,47,48	0
3	EDO	E	303	4/4	0.87	0.15	35,39,42,43	0
3	EDO	F	302	4/4	0.87	0.14	50,52,54,54	0
3	EDO	C	306	4/4	0.87	0.12	34,36,37,47	0
4	PEG	B	303	7/7	0.87	0.18	18,27,35,45	7
3	EDO	A	303	4/4	0.87	0.14	36,38,44,50	0
3	EDO	F	303	4/4	0.88	0.12	48,50,58,59	0
3	EDO	D	304	4/4	0.88	0.21	35,36,42,46	0
3	EDO	C	303	4/4	0.89	0.15	36,37,44,48	0
4	PEG	C	302	7/7	0.89	0.12	25,31,37,38	0

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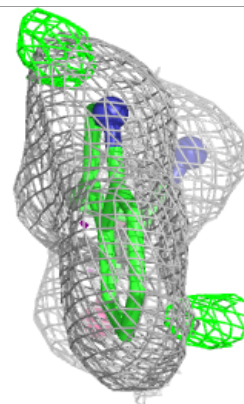
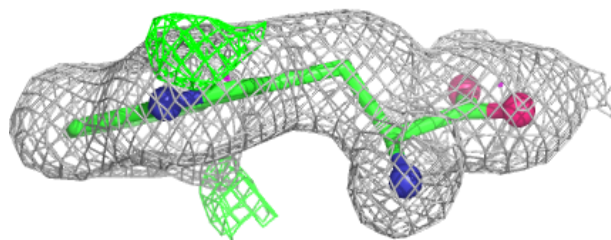
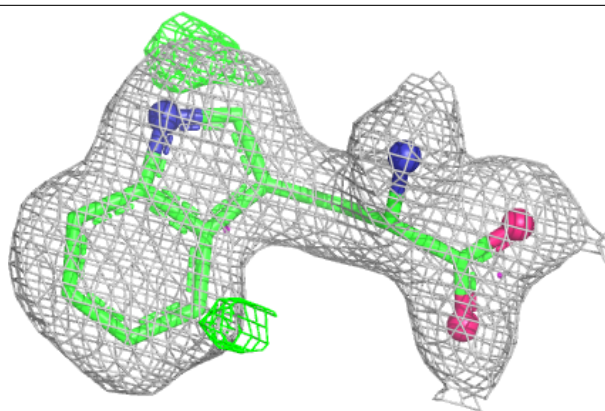
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PEG	D	302	7/7	0.89	0.12	25,27,38,39	0
3	EDO	A	304	4/4	0.89	0.18	33,38,42,46	0
3	EDO	A	305	4/4	0.90	0.13	26,27,34,35	0
3	EDO	B	302	4/4	0.90	0.15	34,36,39,46	0
2	TRP	E	301	15/15	0.92	0.08	23,29,32,32	0
5	ACT	D	306	4/4	0.93	0.08	24,30,33,42	0
3	EDO	F	305	4/4	0.94	0.09	32,36,42,50	0
3	EDO	A	307	4/4	0.94	0.13	26,29,37,44	0
2	TRP	A	301	15/15	0.95	0.07	17,21,24,25	0
2	TRP	F	301	15/15	0.95	0.08	26,33,39,41	0
2	TRP	B	301	15/15	0.95	0.07	18,23,28,29	0
5	ACT	C	305	4/4	0.95	0.14	33,34,35,37	0
2	TRP	C	301	15/15	0.95	0.08	20,25,37,38	0
2	TRP	D	301	15/15	0.95	0.08	18,23,39,39	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.

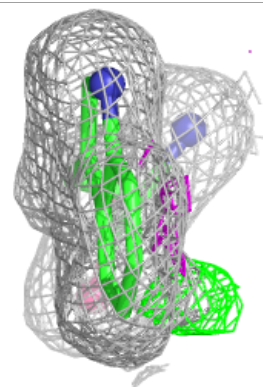
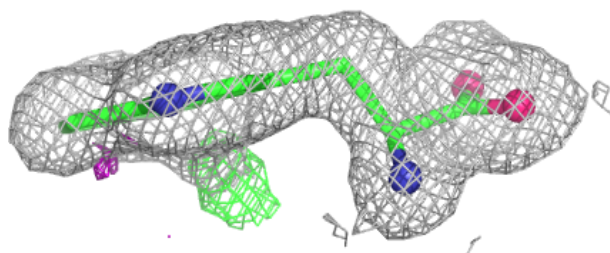
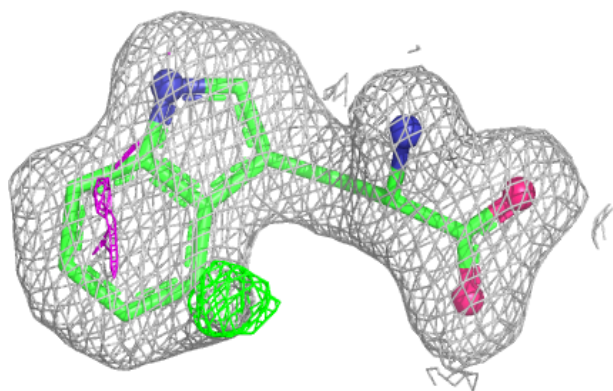
Electron density around TRP E 301:

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

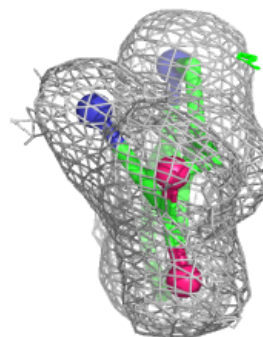
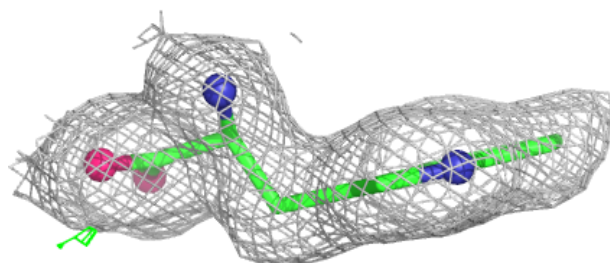
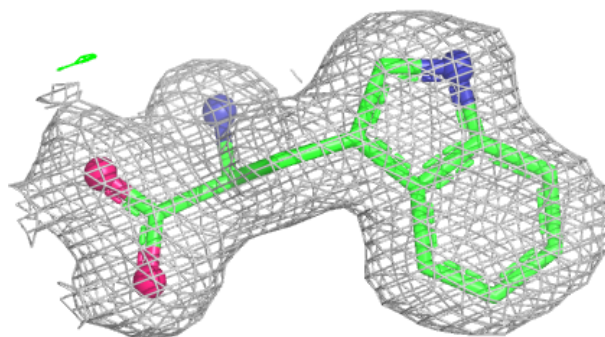


Electron density around TRP A 301:

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

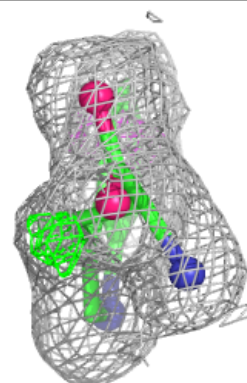
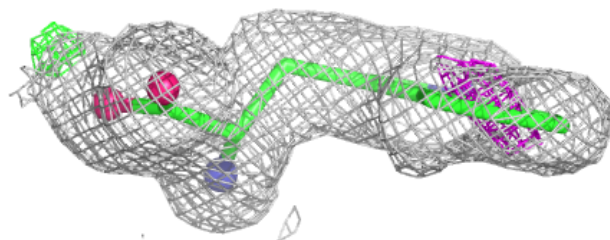
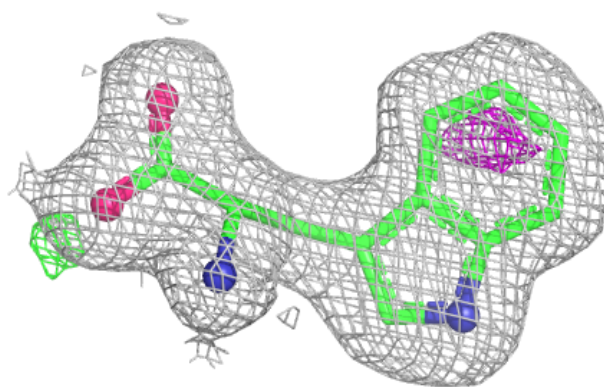
**Electron density around TRP F 301:**

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

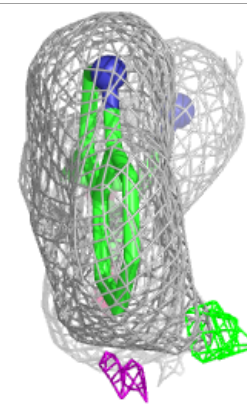
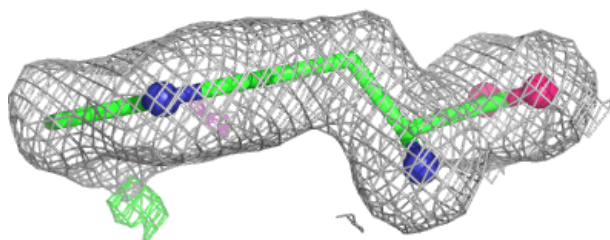
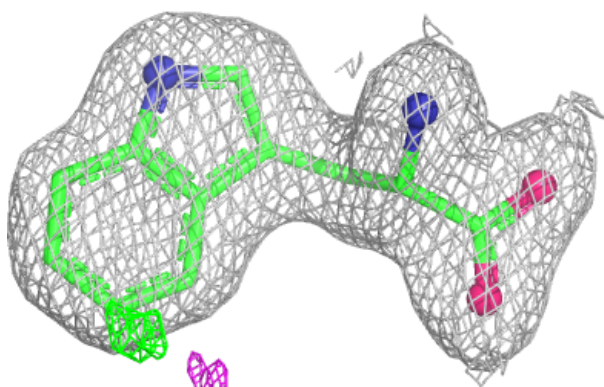


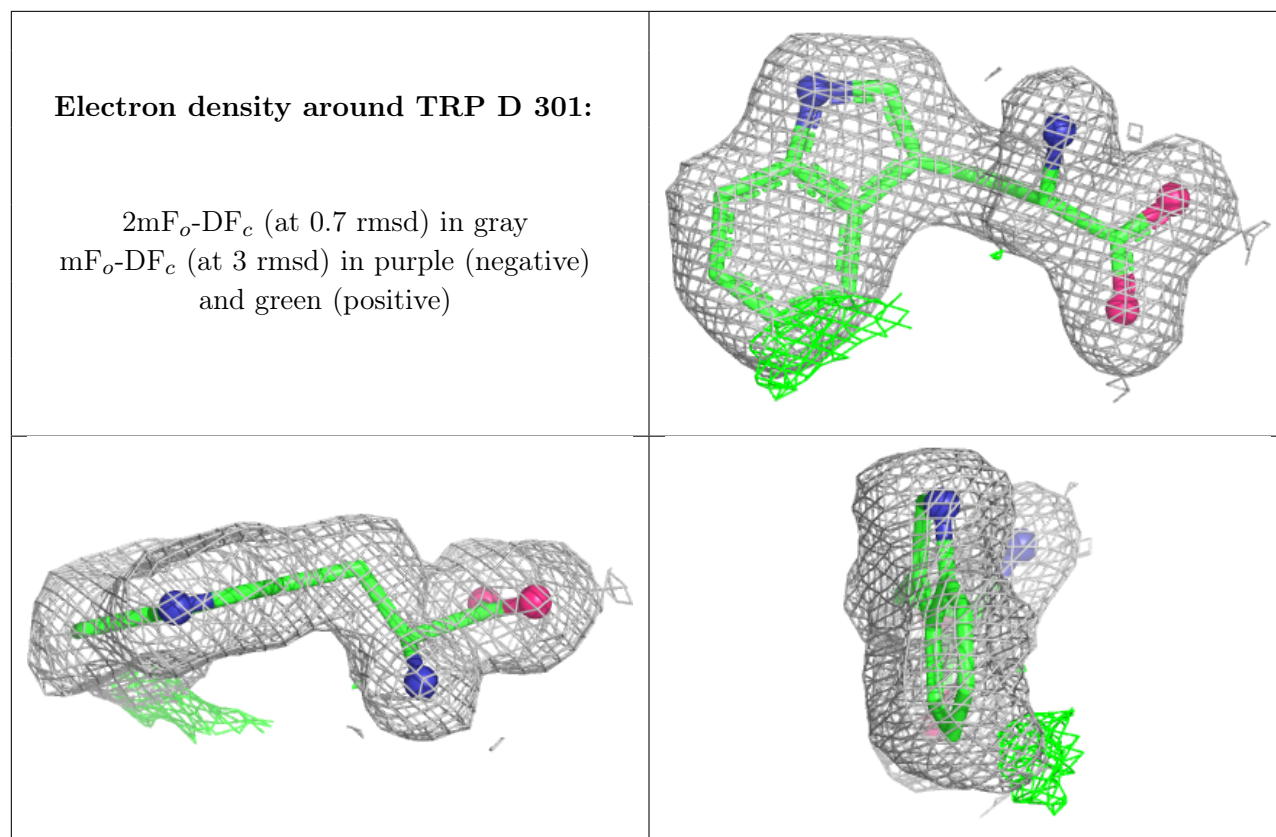
Electron density around TRP B 301:

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

**Electron density around TRP C 301:**

$2mF_o-DF_c$ (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.