



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 02:47 AM UTC

PDB ID : 6G5L / pdb_00006g5l
Title : Crystal structure of human carbonic anhydrase isozyme XII with 4-chloro-2-(cyclohexylamino)-N-(2-hydroxyethyl)-5-sulfamoyl-benzamide
Authors : Smirnov, A.; Manakova, E.; Grazulis, S.
Deposited on : 2018-03-29
Resolution : 1.21 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

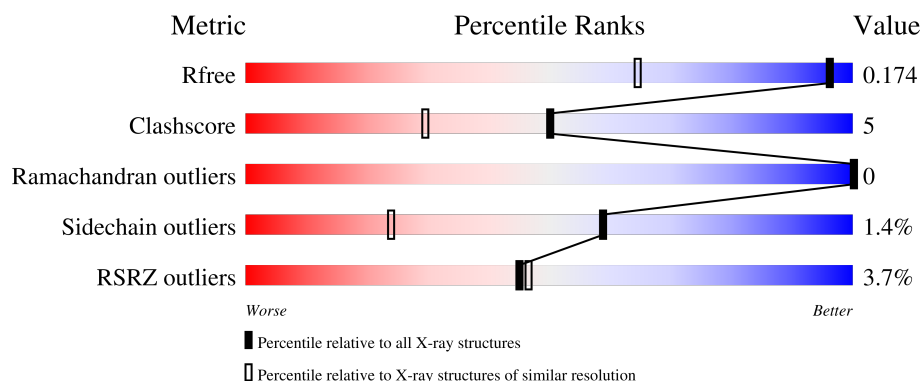
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.21 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	2002 (1.24-1.20)
Clashscore	190562	2061 (1.24-1.20)
Ramachandran outliers	187476	2009 (1.24-1.20)
Sidechain outliers	187428	2008 (1.24-1.20)
RSRZ outliers	180081	2000 (1.24-1.20)

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	263	2% 85% 13% ..
1	B	263	3% 86% 12% ..
1	C	263	9% 71% 26% ..
1	D	263	2% 86% 13% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	B	306	-	X	-	-
4	EDO	D	303	-	-	X	-
4	EDO	D	308	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9747 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 Carbonic anhydrase 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	7	0
			2150	1365	365	412	8			
1	B	261	Total	C	N	O	S	0	6	0
			2126	1351	362	406	7			
1	C	261	Total	C	N	O	S	0	4	0
			2108	1345	356	400	7			
1	D	261	Total	C	N	O	S	0	5	0
			2117	1346	357	407	7			

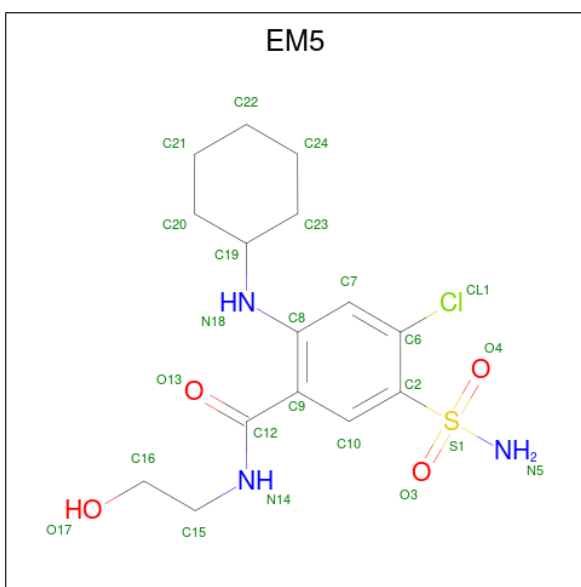
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O43570
B	1	MET	-	initiating methionine	UNP O43570
C	1	MET	-	initiating methionine	UNP O43570
D	1	MET	-	initiating methionine	UNP O43570

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

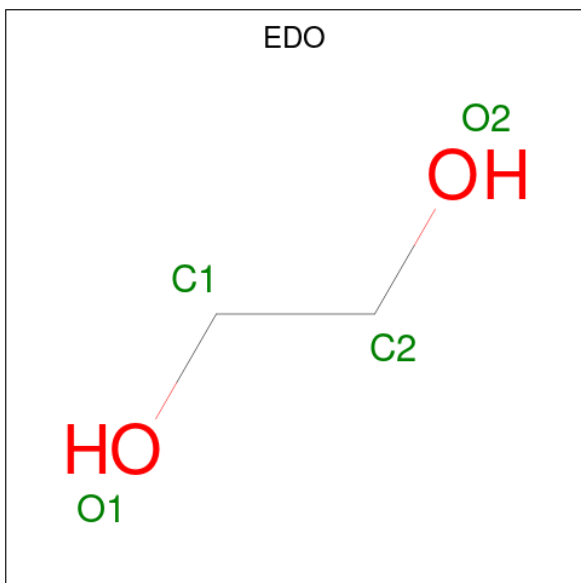
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 4-chloranyl-2-(cyclohexylamino)- {N}-(2-hydroxyethyl)-5-sulfamoyl-benzamide (CCD ID: EM5) (formula: C₁₅H₂₂ClN₃O₄S).



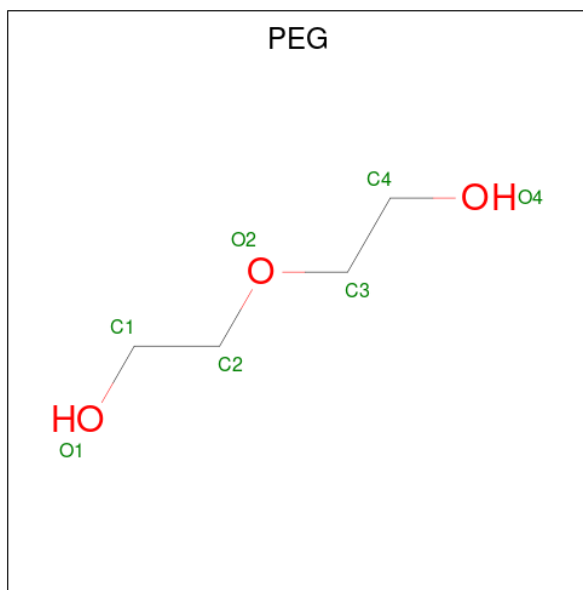
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 48	C 30	Cl 2	N 6	O 8	S 2	0	1
3	B	1	Total 48	C 30	Cl 2	N 6	O 8	S 2	0	1
3	C	1	Total 24	C 15	Cl 1	N 3	O 4	S 1	0	0
3	D	1	Total 24	C 15	Cl 1	N 3	O 4	S 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

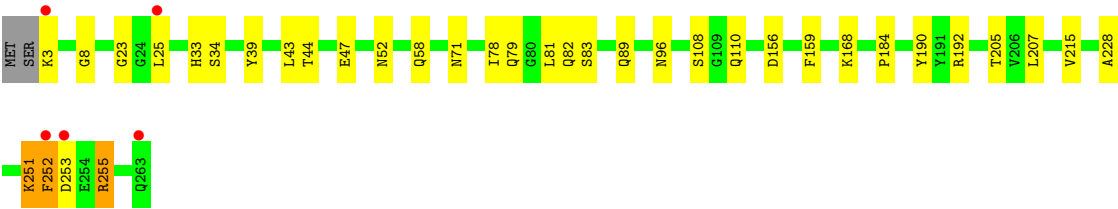
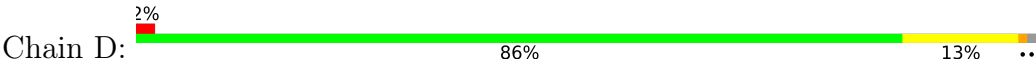
- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	284	Total	O	0	0
			284	284		
6	B	278	Total	O	0	0
			278	278		
6	C	212	Total	O	0	0
			212	212		
6	D	262	Total	O	0	0
			262	262		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.13Å 74.23Å 91.53Å 90.00° 108.64° 90.00°	Depositor
Resolution (Å)	73.08 – 1.21 73.08 – 1.21	Depositor EDS
% Data completeness (in resolution range)	95.7 (73.08-1.21) 95.7 (73.08-1.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.81 (at 1.21Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.136 , 0.173 0.136 , 0.174	Depositor DCC
R_{free} test set	28370 reflections (9.55%)	wwPDB-VP
Wilson B-factor (Å ²)	12.6	Xtrriage
Anisotropy	0.224	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	9747	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7036e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, EDO, PEG, EM5

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.65	15/2213 (0.7%)	1.35	13/3012 (0.4%)
1	B	1.69	28/2190 (1.3%)	1.37	12/2983 (0.4%)
1	C	1.89	50/2172 (2.3%)	1.59	18/2959 (0.6%)
1	D	1.67	21/2180 (1.0%)	1.36	7/2969 (0.2%)
All	All	1.73	114/8755 (1.3%)	1.42	50/11923 (0.4%)

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	B	0	1
1	C	0	1
All	All	0	2

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	ASP	CA-C	-10.10	1.40	1.52
1	C	96	ASN	N-CA	9.53	1.55	1.45
1	C	69	LYS	N-CA	8.27	1.56	1.46
1	D	81	LEU	CA-C	8.08	1.63	1.53
1	A	184	PRO	CA-C	-7.90	1.44	1.53
1	B	136	SER	C-O	-7.80	1.14	1.23
1	C	209	THR	N-CA	-7.66	1.37	1.46
1	C	54	SER	N-CA	7.48	1.55	1.45
1	C	152	ASN	C-O	7.47	1.32	1.24
1	C	166	LYS	CA-C	-7.42	1.42	1.52
1	C	93	HIS	CG-CD2	7.28	1.43	1.35
1	B	252	PHE	CA-C	7.17	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	LEU	CA-C	-7.12	1.43	1.52
1	C	49	GLN	N-CA	6.86	1.54	1.46
1	C	228	ALA	N-CA	-6.82	1.37	1.46
1	B	101	HIS	C-O	6.82	1.32	1.23
1	C	261	PHE	CA-C	-6.79	1.44	1.52
1	C	213	ASN	C-O	-6.62	1.16	1.24
1	C	166	LYS	CA-CB	6.58	1.64	1.53
1	A	33	HIS	CA-C	-6.50	1.44	1.52
1	C	162	LEU	CA-C	-6.47	1.43	1.52
1	C	153	PRO	CA-CB	6.47	1.62	1.53
1	D	81	LEU	N-CA	6.45	1.53	1.45
1	C	75	ASP	CA-C	6.41	1.61	1.52
1	C	143	ALA	CA-C	-6.40	1.45	1.52
1	A	81	LEU	C-O	6.35	1.32	1.23
1	A	189	GLU	CA-C	6.35	1.60	1.52
1	B	174	VAL	CA-C	6.31	1.58	1.52
1	B	135	LYS	N-CA	6.25	1.53	1.45
1	A	184	PRO	C-O	6.24	1.33	1.23
1	D	83	SER	N-CA	6.20	1.53	1.46
1	A	78	ILE	CA-CB	6.17	1.62	1.54
1	C	118	ILE	C-O	6.13	1.31	1.24
1	B	35	ASP	CA-C	-6.11	1.44	1.52
1	B	223	LEU	CA-CB	6.10	1.62	1.53
1	C	223	LEU	CA-C	-6.08	1.45	1.52
1	B	161	HIS	CB-CG	-6.07	1.41	1.50
1	B	184	PRO	CA-C	-6.06	1.43	1.52
1	D	44	THR	CA-CB	6.05	1.62	1.53
1	C	90	LEU	N-CA	-6.02	1.38	1.45
1	D	71	ASN	CA-C	-6.00	1.45	1.52
1	C	9	PRO	CA-CB	6.00	1.62	1.53
1	B	255	ARG	CA-CB	5.99	1.62	1.53
1	B	255	ARG	CA-C	5.97	1.61	1.53
1	D	39	TYR	N-CA	-5.95	1.38	1.46
1	C	235	ASP	N-CA	5.92	1.54	1.46
1	A	255	ARG	N-CA	5.91	1.53	1.45
1	D	96	ASN	N-CA	5.87	1.51	1.46
1	B	164	HIS	C-O	5.87	1.31	1.24
1	C	141	VAL	N-CA	-5.86	1.39	1.46
1	C	78	ILE	CA-CB	5.79	1.61	1.54
1	C	222	LEU	C-N	5.77	1.41	1.33
1	D	52	ASN	N-CA	-5.74	1.39	1.46
1	C	90	LEU	CB-CG	5.72	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	157	LYS	CA-C	-5.70	1.45	1.52
1	A	7	PHE	C-O	-5.68	1.17	1.23
1	C	229	LEU	CA-C	-5.68	1.46	1.52
1	D	81	LEU	C-O	-5.68	1.17	1.23
1	D	190	TYR	CA-C	-5.68	1.45	1.52
1	D	184	PRO	CA-C	-5.65	1.46	1.53
1	C	116	LEU	CA-C	5.63	1.59	1.52
1	B	79	GLN	N-CA	5.63	1.52	1.46
1	B	126	TYR	CA-C	-5.62	1.45	1.52
1	B	5	THR	CA-CB	5.56	1.61	1.53
1	C	226	GLU	N-CA	5.55	1.53	1.46
1	C	113	ALA	C-N	5.53	1.40	1.33
1	D	8	GLY	C-O	5.53	1.31	1.24
1	D	23	GLY	C-O	5.49	1.29	1.24
1	A	160	SER	N-CA	5.48	1.53	1.46
1	C	141	VAL	C-O	5.47	1.29	1.24
1	C	204	PRO	N-CA	5.47	1.51	1.47
1	B	162	LEU	N-CA	5.47	1.52	1.46
1	C	38	GLN	CD-NE2	-5.46	1.21	1.33
1	C	146	ILE	N-CA	5.42	1.52	1.46
1	A	126	TYR	CA-CB	5.38	1.60	1.54
1	B	228	ALA	CA-CB	-5.38	1.45	1.53
1	C	178	ASN	N-CA	-5.36	1.39	1.46
1	A	184	PRO	CA-CB	5.35	1.62	1.53
1	C	224	ALA	N-CA	5.34	1.52	1.46
1	D	33	HIS	N-CA	5.33	1.52	1.45
1	D	255	ARG	CA-C	5.29	1.59	1.52
1	B	109	GLY	C-O	5.29	1.31	1.24
1	C	57	LYS	C-O	5.27	1.30	1.23
1	A	49	GLN	N-CA	5.26	1.52	1.46
1	B	58	GLN	N-CA	5.25	1.52	1.45
1	C	144	VAL	CA-C	5.25	1.59	1.52
1	C	168	LYS	C-O	5.24	1.30	1.23
1	D	82	GLN	N-CA	5.23	1.53	1.46
1	C	260	SER	C-O	5.23	1.30	1.24
1	D	215	VAL	CA-C	-5.22	1.48	1.52
1	B	166[A]	LYS	C-O	5.21	1.30	1.24
1	B	166[B]	LYS	C-O	5.21	1.30	1.24
1	D	168	LYS	N-CA	-5.18	1.39	1.46
1	B	9	PRO	C-O	-5.17	1.17	1.24
1	D	184	PRO	CA-CB	5.16	1.62	1.53
1	C	172	ALA	C-O	-5.16	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	43	LEU	CA-C	-5.13	1.45	1.52
1	A	57	LYS	N-CA	5.12	1.51	1.45
1	B	262	SER	CA-C	-5.11	1.46	1.52
1	C	118	ILE	CA-CB	-5.10	1.47	1.53
1	C	35	ASP	CA-C	-5.10	1.45	1.52
1	C	64	ASN	N-CA	-5.09	1.40	1.46
1	C	75	ASP	CA-CB	-5.05	1.44	1.53
1	C	169	GLY	N-CA	5.05	1.52	1.44
1	C	231	CYS	CA-C	5.05	1.59	1.52
1	C	257	VAL	CA-CB	-5.05	1.48	1.54
1	C	30	ILE	C-O	5.05	1.29	1.23
1	B	136	SER	N-CA	5.03	1.52	1.46
1	B	96	ASN	C-O	-5.03	1.19	1.24
1	C	67	SER	C-O	5.03	1.29	1.23
1	B	33	HIS	N-CA	5.03	1.52	1.45
1	B	8	GLY	C-O	5.02	1.30	1.24
1	B	184	PRO	C-N	5.02	1.40	1.33
1	D	251	LYS	N-CA	5.00	1.52	1.46

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	252	PHE	CA-CB-CG	-6.87	106.93	113.80
1	B	164	HIS	CA-C-O	6.85	126.96	119.15
1	C	230	TYR	N-CA-C	-6.82	99.08	109.85
1	D	159	PHE	N-CA-C	6.74	119.46	111.71
1	C	229	LEU	N-CA-C	6.52	120.24	110.14
1	D	82	GLN	N-CA-C	-6.51	105.20	113.01
1	C	8	GLY	CA-C-N	-6.46	111.76	119.84
1	C	8	GLY	C-N-CA	-6.46	111.76	119.84
1	C	7	PHE	N-CA-C	6.38	116.42	108.19
1	B	163	GLN	CA-C-N	6.37	133.28	122.26
1	B	163	GLN	C-N-CA	6.37	133.28	122.26
1	B	98	ASN	N-CA-C	-6.37	105.51	113.28
1	A	159	PHE	N-CA-C	6.21	118.85	111.71
1	C	239	PRO	CB-CA-C	-6.18	102.89	110.98
1	D	253	ASP	CA-C-O	-5.84	114.76	121.54
1	A	111	HIS	CB-CG-CD2	-5.83	123.63	131.20
1	B	262	SER	CA-C-N	5.82	132.17	121.70
1	B	262	SER	C-N-CA	5.82	132.17	121.70
1	A	8	GLY	CA-C-N	-5.76	114.07	121.04
1	A	8	GLY	C-N-CA	-5.76	114.07	121.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	PHE	N-CA-CB	5.68	119.81	110.39
1	C	91	HIS	CA-CB-CG	-5.67	108.13	113.80
1	C	34	SER	CA-CB-OG	-5.57	99.97	111.10
1	C	205	THR	CA-CB-OG1	-5.50	101.35	109.60
1	A	219	GLN	CB-CG-CD	5.47	121.91	112.60
1	C	117	HIS	ND1-CG-CD2	5.44	111.54	106.10
1	B	75	ASP	N-CA-C	-5.37	106.23	112.89
1	D	205	THR	CA-CB-OG1	-5.36	101.56	109.60
1	B	58	GLN	CB-CA-C	5.33	119.83	109.33
1	C	117	HIS	CB-CG-CD2	-5.27	124.35	131.20
1	C	159	PHE	N-CA-C	5.26	119.17	112.34
1	C	214	PRO	CA-C-O	-5.26	115.60	122.12
1	A	59	PHE	CA-CB-CG	-5.24	108.56	113.80
1	B	101	HIS	CA-CB-CG	-5.21	108.59	113.80
1	A	44	THR	CA-C-N	-5.19	114.42	119.76
1	A	44	THR	C-N-CA	-5.19	114.42	119.76
1	B	255	ARG	N-CA-CB	-5.15	103.33	110.38
1	C	32	LEU	O-C-N	-5.09	117.00	123.05
1	C	120	HIS	CA-CB-CG	5.08	118.88	113.80
1	A	10	ASP	CA-C-N	5.07	128.79	121.54
1	A	10	ASP	C-N-CA	5.07	128.79	121.54
1	A	199	THR	O-C-N	5.06	125.65	121.35
1	D	228	ALA	CA-C-O	-5.04	113.71	119.60
1	C	57	LYS	N-CA-C	-5.03	103.08	110.52
1	C	152	ASN	CA-C-O	5.03	125.01	120.09
1	C	155	TYR	O-C-N	-5.03	115.69	122.43
1	B	164	HIS	N-CA-C	5.02	119.56	113.38
1	A	261	PHE	CA-C-N	-5.01	113.75	122.36
1	A	261	PHE	C-N-CA	-5.01	113.75	122.36
1	D	78	ILE	O-C-N	5.01	128.59	123.03

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	262	SER	Peptide
1	C	158	ILE	Mainchain

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	2150	0	2027	16	0
1	B	2126	0	2005	36	0
1	C	2108	0	1980	16	0
1	D	2117	0	1986	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	48	0	0	1	0
3	B	48	0	0	0	0
3	C	24	0	0	0	0
3	D	24	0	0	0	0
4	A	8	0	12	0	0
4	B	16	0	24	7	0
4	C	4	0	5	0	0
4	D	20	0	30	9	0
5	A	7	0	10	1	0
5	D	7	0	10	0	0
6	A	284	0	0	9	0
6	B	278	0	0	10	0
6	C	212	0	0	3	0
6	D	262	0	0	7	0
All	All	9747	0	8089	89	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 (89) 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:252:PHE:CZ	1:B:255:ARG:HB3	1.81	1.16
6:A:633:HOH:O	1:C:234:MET:HE2	1.47	1.13
1:B:252:PHE:CZ	1:B:255:ARG:CB	2.38	1.06
1:B:252:PHE:CE2	1:B:255:ARG:HB2	1.91	1.04
1:D:34:SER:H	4:D:303:EDO:H11	1.22	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:PHE:CE2	1:B:255:ARG:CB	2.48	0.95
1:B:252:PHE:CD2	1:B:255:ARG:HB2	2.05	0.90
1:C:253[A]:ASP:OD2	6:C:401:HOH:O	1.93	0.85
1:B:252:PHE:CE2	1:B:255:ARG:NE	2.50	0.80
1:B:252:PHE:CE1	1:B:255:ARG:C	2.59	0.80
1:B:252:PHE:CE2	1:B:255:ARG:CD	2.64	0.79
1:B:252:PHE:CZ	1:B:255:ARG:HB2	2.12	0.79
1:B:252:PHE:CD1	1:B:255:ARG:O	2.36	0.78
1:A:194:ARG:NE	1:A:207:LEU:HD13	2.00	0.77
1:A:148[B]:MET:HE3	6:A:501:HOH:O	1.87	0.74
1:D:34:SER:N	4:D:303:EDO:H11	2.01	0.71
1:A:164:HIS:HD2	6:A:424:HOH:O	1.73	0.71
1:B:255:ARG:CD	6:B:510:HOH:O	2.38	0.71
1:C:7:PHE:CD1	1:C:8:GLY:N	2.60	0.70
1:B:252:PHE:CE2	1:B:255:ARG:HD2	2.28	0.69
1:D:108:SER:OG	4:D:303:EDO:H12	1.93	0.69
1:D:34:SER:H	4:D:303:EDO:C1	2.04	0.69
1:B:252:PHE:CD2	1:B:255:ARG:NE	2.61	0.68
1:B:16:SER:OG	6:B:401:HOH:O	2.11	0.68
1:A:57:LYS:HD2	6:A:684:HOH:O	1.94	0.67
1:B:252:PHE:CE1	1:B:255:ARG:CB	2.78	0.66
1:B:255:ARG:HG2	6:B:510:HOH:O	1.94	0.66
1:B:3:LYS:HE3	1:B:18:LYS:HZ3	1.61	0.66
1:B:253:ASP:OD2	6:B:402:HOH:O	2.14	0.65
1:A:111:HIS:HE1	6:A:628:HOH:O	1.78	0.65
1:D:255:ARG:CD	6:D:532:HOH:O	2.44	0.65
1:A:219:GLN:NE2	6:A:403:HOH:O	2.30	0.64
1:B:3:LYS:HE3	1:B:18:LYS:NZ	2.13	0.64
1:C:3:LYS:N	6:C:402:HOH:O	2.32	0.63
1:C:170:GLN:HE22	1:C:234:MET:HE3	1.63	0.63
1:B:252:PHE:HE2	1:B:255:ARG:HD2	1.63	0.63
1:A:219:GLN:HG3	1:A:220:GLU:N	2.14	0.62
1:A:9:PRO:HB2	6:A:419:HOH:O	2.00	0.61
1:B:255:ARG:CG	6:B:510:HOH:O	2.49	0.61
1:B:252:PHE:HE2	1:B:255:ARG:CD	2.14	0.58
1:C:8:GLY:HA2	1:D:25[B]:LEU:HD21	1.85	0.58
1:A:148[A]:MET:HE2	1:A:219:GLN:HA	1.88	0.56
1:B:252:PHE:CG	1:B:255:ARG:HB2	2.40	0.56
1:B:64:ASN:HD22	4:B:306:EDO:C2	2.18	0.56
1:D:252:PHE:H	4:D:308:EDO:C2	2.20	0.55
1:D:255:ARG:HG2	6:D:532:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:PHE:HD1	1:C:8:GLY:N	2.04	0.53
4:D:308:EDO:H11	6:D:461:HOH:O	2.08	0.53
1:B:252:PHE:CE1	1:B:255:ARG:O	2.60	0.53
1:B:252:PHE:CE1	1:B:255:ARG:HB2	2.43	0.53
1:B:186:ARG:HH11	1:B:186:ARG:HG3	1.74	0.53
1:B:185:GLU:HG2	4:B:303:EDO:O2	2.09	0.53
3:A:302[A]:EM5:O17	6:A:401:HOH:O	2.19	0.52
1:C:167:TYR:CE2	1:C:234:MET:HG3	2.45	0.52
4:B:305:EDO:H11	6:B:564:HOH:O	2.08	0.51
1:D:255:ARG:CG	6:D:532:HOH:O	2.59	0.51
1:A:49:GLN:NE2	6:A:408:HOH:O	2.44	0.50
1:B:186:ARG:HG3	1:B:186:ARG:NH1	2.26	0.50
1:C:18[A]:LYS:NZ	6:C:404:HOH:O	2.37	0.48
1:B:64:ASN:HD22	4:B:306:EDO:H21	1.79	0.48
1:A:133:SER:OG	5:A:304:PEG:C1	2.62	0.48
1:D:47:GLU:HB2	1:D:79:GLN:HB2	1.95	0.48
1:B:252:PHE:HE2	1:B:255:ARG:NE	2.06	0.48
1:A:166:LYS:HB2	1:A:166:LYS:HE2	1.77	0.47
1:C:49:GLN:OE1	1:C:79:GLN:NE2	2.48	0.47
4:B:305:EDO:H11	6:B:510:HOH:O	2.15	0.46
1:C:58:GLN:HG3	1:C:173:PHE:CD1	2.51	0.46
1:B:252:PHE:CD1	1:B:255:ARG:C	2.90	0.46
1:B:252:PHE:CE1	1:B:255:ARG:HB3	2.40	0.45
1:A:231:CYS:SG	1:A:240:ARG:NH1	2.90	0.45
1:C:110:GLN:NE2	1:D:110:GLN:NE2	2.66	0.44
1:D:3:LYS:N	6:D:406:HOH:O	2.52	0.43
1:C:54:SER:C	1:C:56:ASN:H	2.26	0.43
1:D:252:PHE:HB2	4:D:308:EDO:H11	2.00	0.43
1:C:7:PHE:CD1	1:C:7:PHE:C	2.96	0.43
1:B:252:PHE:CD2	1:B:252:PHE:O	2.72	0.42
1:D:255:ARG:HD2	6:D:532:HOH:O	2.11	0.42
4:B:305:EDO:C1	6:B:564:HOH:O	2.65	0.42
1:A:52:ASN:HA	1:A:178:ASN:HA	2.02	0.42
1:D:192:ARG:HD2	1:D:207:LEU:HD11	2.02	0.42
1:C:168:LYS:O	1:C:233:HIS:CD2	2.72	0.42
4:D:308:EDO:C1	6:D:461:HOH:O	2.68	0.42
4:B:303:EDO:C1	6:B:544:HOH:O	2.69	0.41
1:B:252:PHE:CD1	1:B:255:ARG:HB2	2.54	0.41
1:B:255:ARG:HD2	6:B:510:HOH:O	2.10	0.41
1:A:219:GLN:HG3	1:A:220:GLU:CD	2.46	0.41
1:A:103:SER:O	1:A:111:HIS:HD2	2.05	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:MET:HE2	1:C:148:MET:HB3	1.81	0.40
1:D:251:LYS:HA	4:D:308:EDO:H22	2.02	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	266/263 (101%)	260 (98%)	6 (2%)	0	100	100
1	B	265/263 (101%)	259 (98%)	6 (2%)	0	100	100
1	C	263/263 (100%)	251 (95%)	12 (5%)	0	100	100
1	D	264/263 (100%)	257 (97%)	7 (3%)	0	100	100
All	All	1058/1052 (101%)	1027 (97%)	31 (3%)	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	238/235 (101%)	234 (98%)	4 (2%)	53	17
1	B	235/235 (100%)	232 (99%)	3 (1%)	61	25
1	C	230/235 (98%)	227 (99%)	3 (1%)	61	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	233/235 (99%)	230 (99%)	3 (1%)	61	25
All	All	936/940 (100%)	923 (99%)	13 (1%)	59	24

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	89	GLN
1	A	156	ASP
1	A	219	GLN
1	B	3	LYS
1	B	89	GLN
1	B	156	ASP
1	C	54	SER
1	C	89	GLN
1	C	156	ASP
1	D	58	GLN
1	D	89	GLN
1	D	156	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	33	HIS
1	A	58	GLN
1	A	110	GLN
1	A	111	HIS
1	A	164	HIS
1	A	213	ASN
1	A	219	GLN
1	B	101	HIS
1	B	111	HIS
1	B	219	GLN
1	B	250	GLN
1	C	13	ASN
1	C	79	GLN
1	C	110	GLN
1	C	161	HIS
1	C	170	GLN
1	C	233	HIS

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Mol	Chain	Res	Type
1	D	101	HIS
1	D	110	GLN
1	D	219	GLN
1	D	250	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 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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$
4	EDO	B	304	-	3,3,3	1.28	0	2,2,2	0.19	0
4	EDO	B	306	-	3,3,3	2.93	2 (66%)	2,2,2	3.03	1 (50%)
4	EDO	A	303	-	3,3,3	0.42	0	2,2,2	0.67	0
3	EM5	B	302[B]	2	25,25,25	0.97	1 (4%)	35,35,35	1.52	9 (25%)
3	EM5	D	302	2	25,25,25	1.29	3 (12%)	35,35,35	1.34	3 (8%)
5	PEG	A	304	-	6,6,6	1.26	0	5,5,5	2.55	2 (40%)
3	EM5	C	302	2	25,25,25	1.78	5 (20%)	35,35,35	2.03	15 (42%)
4	EDO	D	303	-	3,3,3	0.88	0	2,2,2	0.76	0
4	EDO	D	306	-	3,3,3	0.94	0	2,2,2	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	C	303	-	3,3,3	0.68	0	2,2,2	1.07	0
4	EDO	B	303	-	3,3,3	1.61	1 (33%)	2,2,2	0.46	0
5	PEG	D	307	-	6,6,6	0.92	0	5,5,5	1.72	2 (40%)
3	EM5	A	302[A]	2	25,25,25	1.30	3 (12%)	35,35,35	1.24	4 (11%)
4	EDO	D	305	-	3,3,3	0.65	0	2,2,2	0.66	0
4	EDO	D	304	-	3,3,3	1.38	1 (33%)	2,2,2	1.08	0
4	EDO	D	308	-	3,3,3	1.06	0	2,2,2	2.13	1 (50%)
4	EDO	B	305	-	3,3,3	1.23	0	2,2,2	1.20	0
3	EM5	A	302[B]	2	25,25,25	1.23	2 (8%)	35,35,35	1.37	7 (20%)
4	EDO	A	305	-	3,3,3	0.48	0	2,2,2	2.23	2 (100%)
3	EM5	B	302[A]	2	25,25,25	1.04	1 (4%)	35,35,35	1.43	7 (20%)

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
4	EDO	B	304	-	-	1/1/1/1	-
4	EDO	B	306	-	-	1/1/1/1	-
4	EDO	A	303	-	-	1/1/1/1	-
3	EM5	B	302[B]	2	-	1/18/26/26	0/2/2/2
3	EM5	D	302	2	-	1/18/26/26	0/2/2/2
5	PEG	A	304	-	-	1/4/4/4	-
3	EM5	C	302	2	-	3/18/26/26	0/2/2/2
4	EDO	D	303	-	-	0/1/1/1	-
4	EDO	D	306	-	-	1/1/1/1	-
4	EDO	C	303	-	-	0/1/1/1	-
4	EDO	B	303	-	-	1/1/1/1	-
5	PEG	D	307	-	-	3/4/4/4	-
3	EM5	A	302[A]	2	-	1/18/26/26	0/2/2/2
4	EDO	D	305	-	-	1/1/1/1	-
4	EDO	D	304	-	-	0/1/1/1	-
4	EDO	D	308	-	-	1/1/1/1	-
4	EDO	B	305	-	-	1/1/1/1	-
3	EM5	A	302[B]	2	-	1/18/26/26	0/2/2/2
4	EDO	A	305	-	-	0/1/1/1	-
3	EM5	B	302[A]	2	-	1/18/26/26	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	EM5	O3-S1	-4.92	1.35	1.43
4	B	306	EDO	O1-C1	4.18	1.63	1.42
3	C	302	EM5	C12-N14	-3.50	1.26	1.33
3	A	302[A]	EM5	C12-N14	-3.02	1.27	1.33
3	C	302	EM5	O13-C12	3.01	1.30	1.23
3	C	302	EM5	C7-C8	2.90	1.44	1.39
3	A	302[B]	EM5	C12-N14	-2.52	1.28	1.33
3	D	302	EM5	C10-C9	-2.49	1.35	1.39
3	A	302[A]	EM5	O13-C12	2.46	1.29	1.23
4	B	303	EDO	O1-C1	2.29	1.53	1.42
3	D	302	EM5	C8-N18	2.28	1.42	1.37
3	A	302[B]	EM5	O13-C12	2.15	1.28	1.23
4	B	306	EDO	C2-C1	2.10	1.64	1.48
3	D	302	EM5	C12-N14	-2.08	1.29	1.33
3	C	302	EM5	C15-N14	2.05	1.50	1.46
3	B	302[B]	EM5	C23-C19	2.03	1.56	1.52
4	D	304	EDO	O1-C1	2.02	1.52	1.42
3	B	302[A]	EM5	C23-C19	2.02	1.56	1.52
3	A	302[A]	EM5	C10-C2	-2.01	1.36	1.39

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	EM5	C2-C6-CL1	-4.42	118.32	121.52
3	C	302	EM5	C16-C15-N14	4.32	121.79	111.60
5	A	304	PEG	O2-C2-C1	4.17	128.50	110.11
4	B	306	EDO	O1-C1-C2	4.10	143.63	112.39
3	C	302	EM5	C7-C6-C2	3.76	125.00	121.36
3	B	302[A]	EM5	C9-C8-N18	-3.53	117.96	121.08
5	A	304	PEG	O1-C1-C2	3.38	131.72	111.82
3	D	302	EM5	C23-C19-N18	-3.25	105.54	110.77
3	B	302[B]	EM5	O17-C16-C15	-3.18	99.82	111.50
3	C	302	EM5	O3-S1-O4	-3.18	113.91	118.80
3	D	302	EM5	C10-C2-S1	2.99	121.84	118.26
4	D	308	EDO	O2-C2-C1	2.95	134.83	112.39
3	C	302	EM5	C10-C2-C6	-2.87	115.32	118.33
3	B	302[B]	EM5	C9-C8-N18	-2.85	118.57	121.08
3	B	302[B]	EM5	C10-C2-S1	2.80	121.61	118.26
3	C	302	EM5	C24-C23-C19	-2.73	106.20	111.09
3	C	302	EM5	O13-C12-N14	-2.72	117.29	122.59
3	B	302[A]	EM5	C10-C2-S1	2.66	121.44	118.26
5	D	307	PEG	O2-C3-C4	2.65	121.80	110.11
3	C	302	EM5	C8-N18-C19	2.63	128.92	124.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	307	PEG	O1-C1-C2	-2.63	96.34	111.82
3	A	302[B]	EM5	C24-C23-C19	2.48	115.54	111.09
3	A	302[B]	EM5	C15-N14-C12	2.47	127.69	122.11
3	C	302	EM5	C15-N14-C12	2.46	127.67	122.11
3	A	302[B]	EM5	C9-C8-N18	-2.45	118.92	121.08
3	A	302[A]	EM5	C9-C8-N18	-2.45	118.92	121.08
3	C	302	EM5	O4-S1-N5	2.44	110.88	107.35
3	B	302[A]	EM5	O4-S1-N5	2.41	110.83	107.35
3	B	302[B]	EM5	C7-C6-CL1	-2.36	114.58	118.45
3	B	302[B]	EM5	C8-N18-C19	-2.33	120.78	124.60
4	A	305	EDO	O2-C2-C1	2.30	129.91	112.39
3	C	302	EM5	C8-C7-C6	-2.28	116.45	120.05
3	B	302[A]	EM5	C7-C6-CL1	-2.26	114.75	118.45
3	A	302[B]	EM5	O4-S1-N5	2.22	110.55	107.35
3	C	302	EM5	C21-C20-C19	-2.21	107.13	111.09
3	B	302[B]	EM5	C7-C6-C2	2.21	123.50	121.36
3	C	302	EM5	C9-C12-N14	2.20	121.59	117.32
3	B	302[B]	EM5	C23-C19-N18	-2.20	107.24	110.77
3	B	302[B]	EM5	O4-S1-N5	2.19	110.51	107.35
3	B	302[A]	EM5	C7-C6-C2	2.17	123.46	121.36
4	A	305	EDO	O1-C1-C2	-2.15	95.98	112.39
3	A	302[A]	EM5	O13-C12-N14	-2.13	118.44	122.59
3	C	302	EM5	C20-C19-N18	-2.12	107.35	110.77
3	C	302	EM5	C10-C2-S1	2.09	120.77	118.26
3	A	302[B]	EM5	O13-C12-N14	-2.08	118.53	122.59
3	B	302[A]	EM5	C16-C15-N14	-2.07	106.71	111.60
3	A	302[B]	EM5	C8-N18-C19	-2.06	121.23	124.60
3	B	302[A]	EM5	O3-S1-N5	2.05	110.31	107.35
3	D	302	EM5	O3-S1-N5	2.05	110.30	107.35
3	A	302[A]	EM5	C10-C2-S1	2.04	120.70	118.26
3	B	302[B]	EM5	O3-S1-N5	2.02	110.26	107.35
3	A	302[B]	EM5	C10-C2-S1	2.01	120.66	118.26
3	A	302[A]	EM5	O3-S1-C2	-2.00	104.35	107.26

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	302	EM5	C16-C15-N14-C12
4	A	303	EDO	O1-C1-C2-O2
5	A	304	PEG	O2-C3-C4-O4
4	B	306	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	D	305	EDO	O1-C1-C2-O2
5	D	307	PEG	C4-C3-O2-C2
4	B	303	EDO	O1-C1-C2-O2
4	D	306	EDO	O1-C1-C2-O2
4	D	308	EDO	O1-C1-C2-O2
5	D	307	PEG	O1-C1-C2-O2
5	D	307	PEG	C1-C2-O2-C3
4	B	304	EDO	O1-C1-C2-O2
3	A	302[A]	EM5	C6-C2-S1-N5
3	A	302[B]	EM5	C6-C2-S1-N5
3	B	302[A]	EM5	C6-C2-S1-N5
3	B	302[B]	EM5	C6-C2-S1-N5
3	D	302	EM5	C6-C2-S1-N5
3	C	302	EM5	C6-C2-S1-N5
4	B	305	EDO	O1-C1-C2-O2
3	C	302	EM5	C10-C2-S1-N5

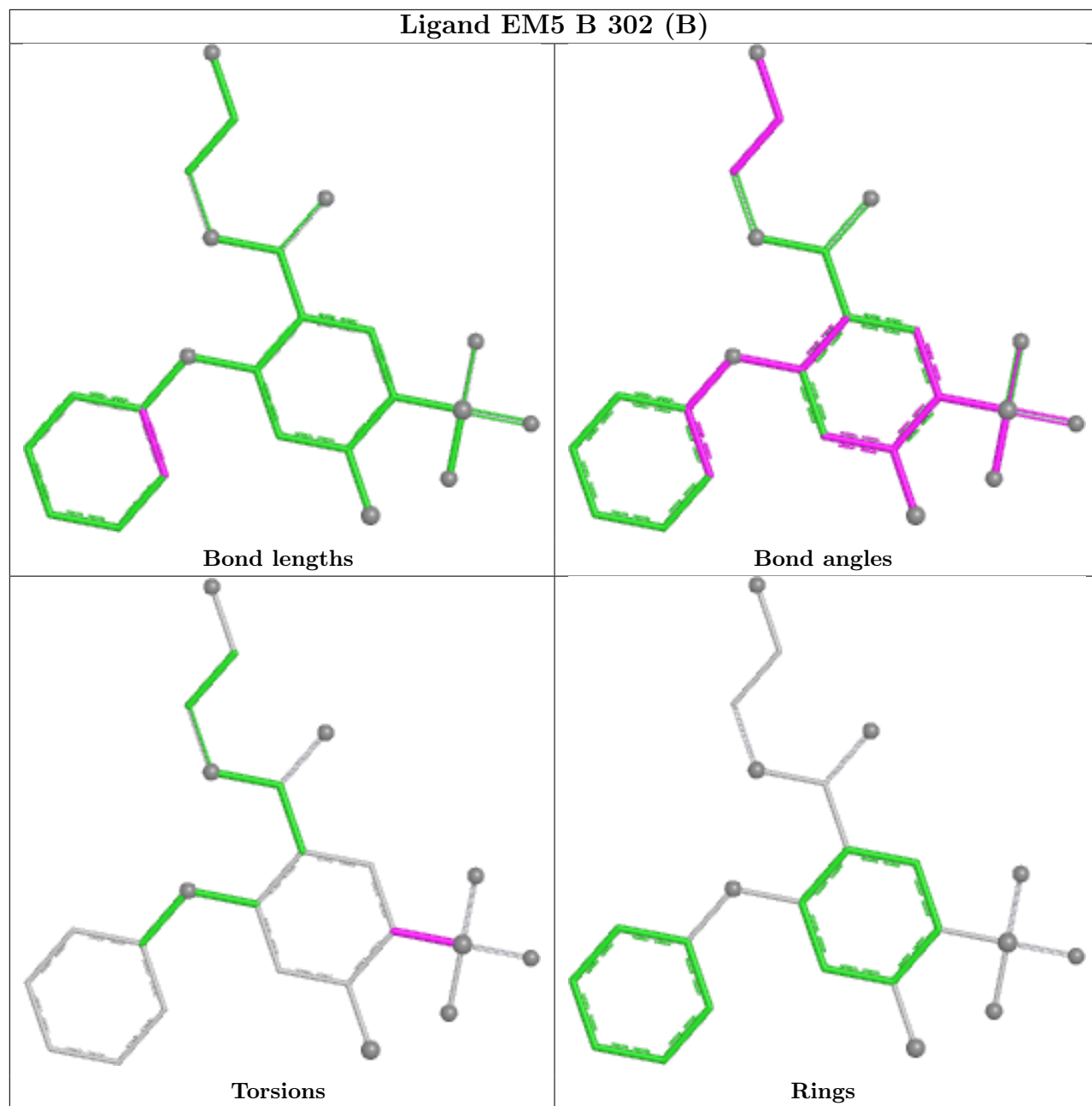
There are no ring outliers.

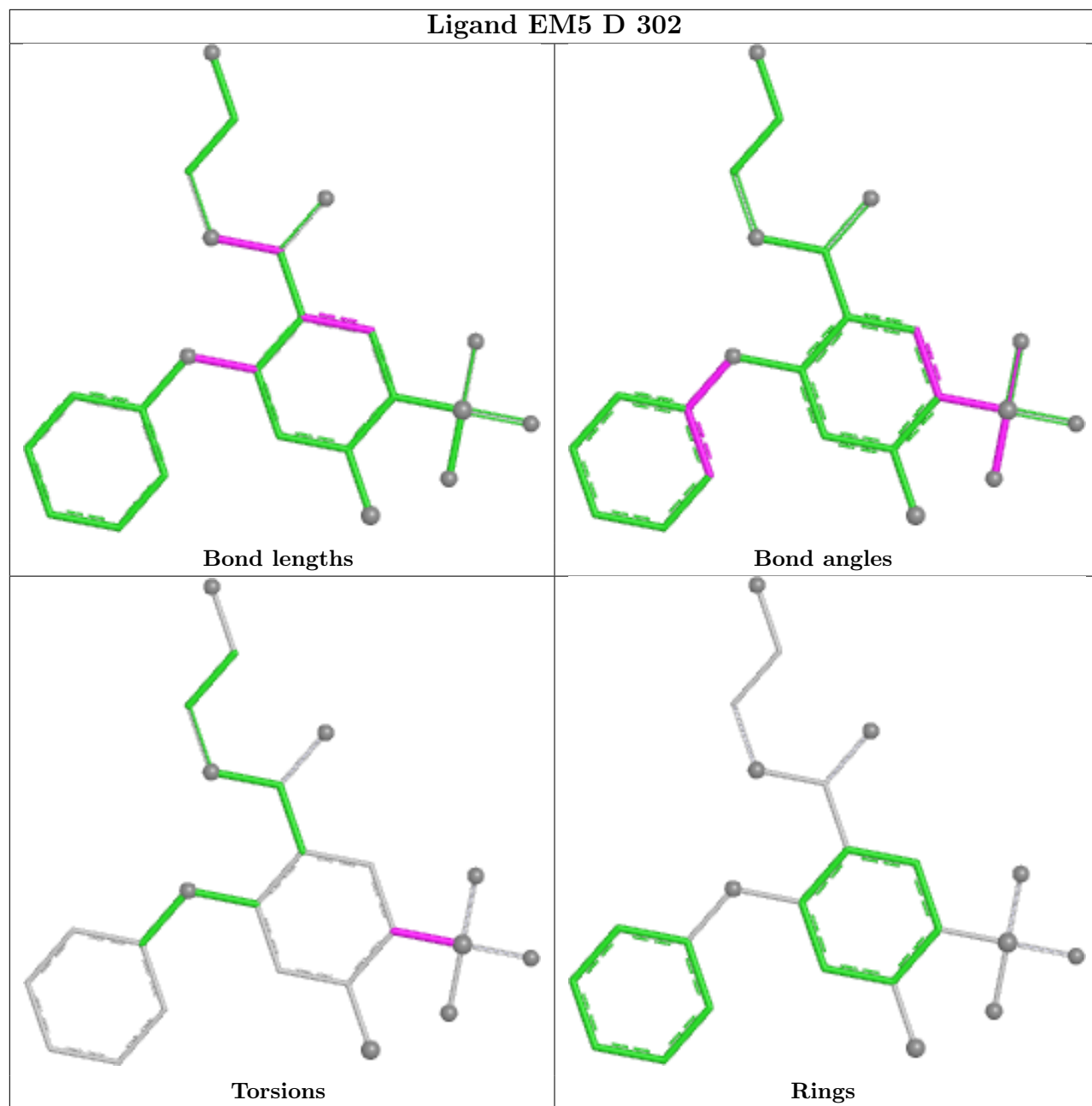
7 monomers are involved in 18 short contacts:

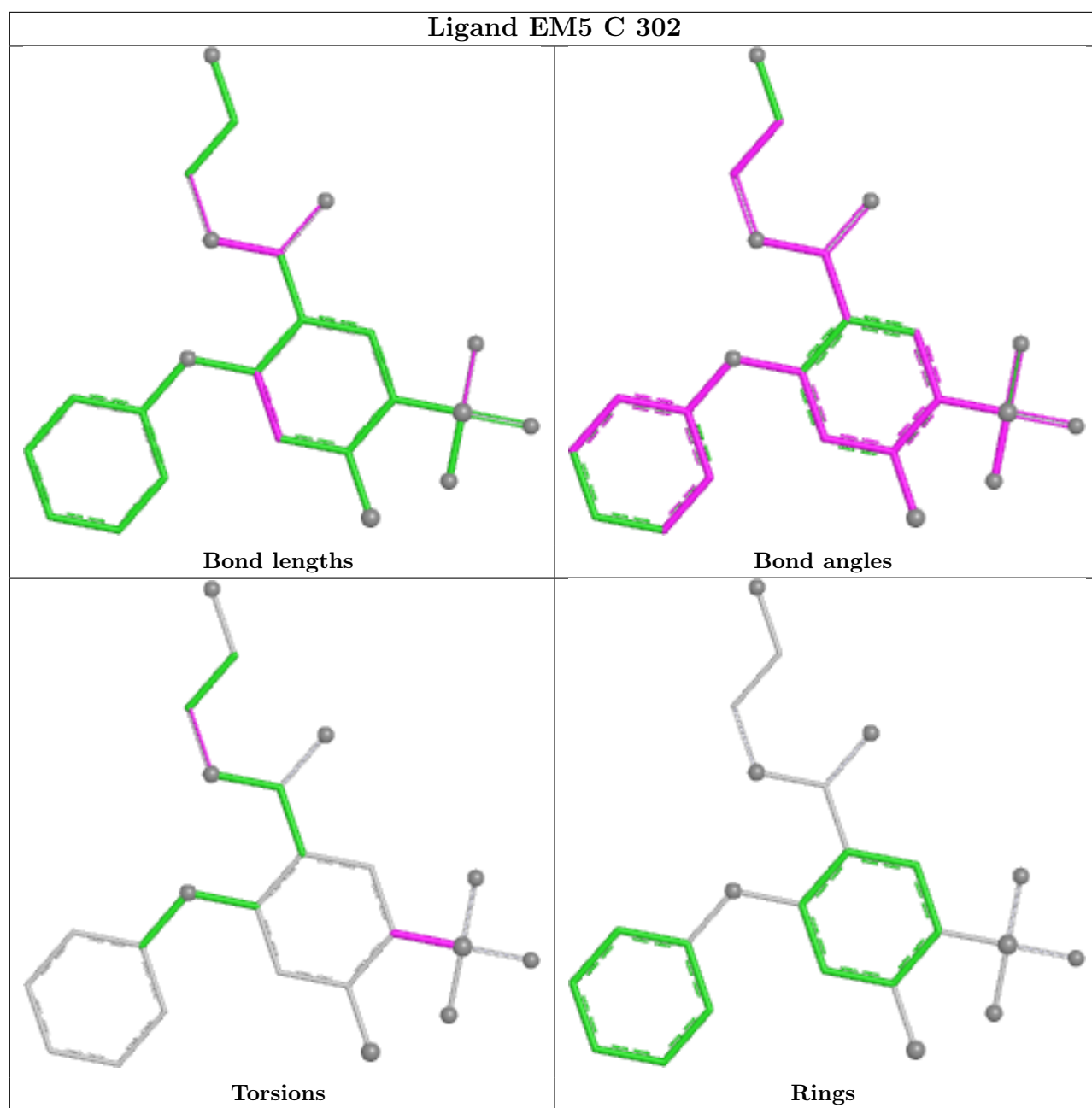
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	306	EDO	2	0
5	A	304	PEG	1	0
4	D	303	EDO	4	0
4	B	303	EDO	2	0
3	A	302[A]	EM5	1	0
4	D	308	EDO	5	0
4	B	305	EDO	3	0

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.

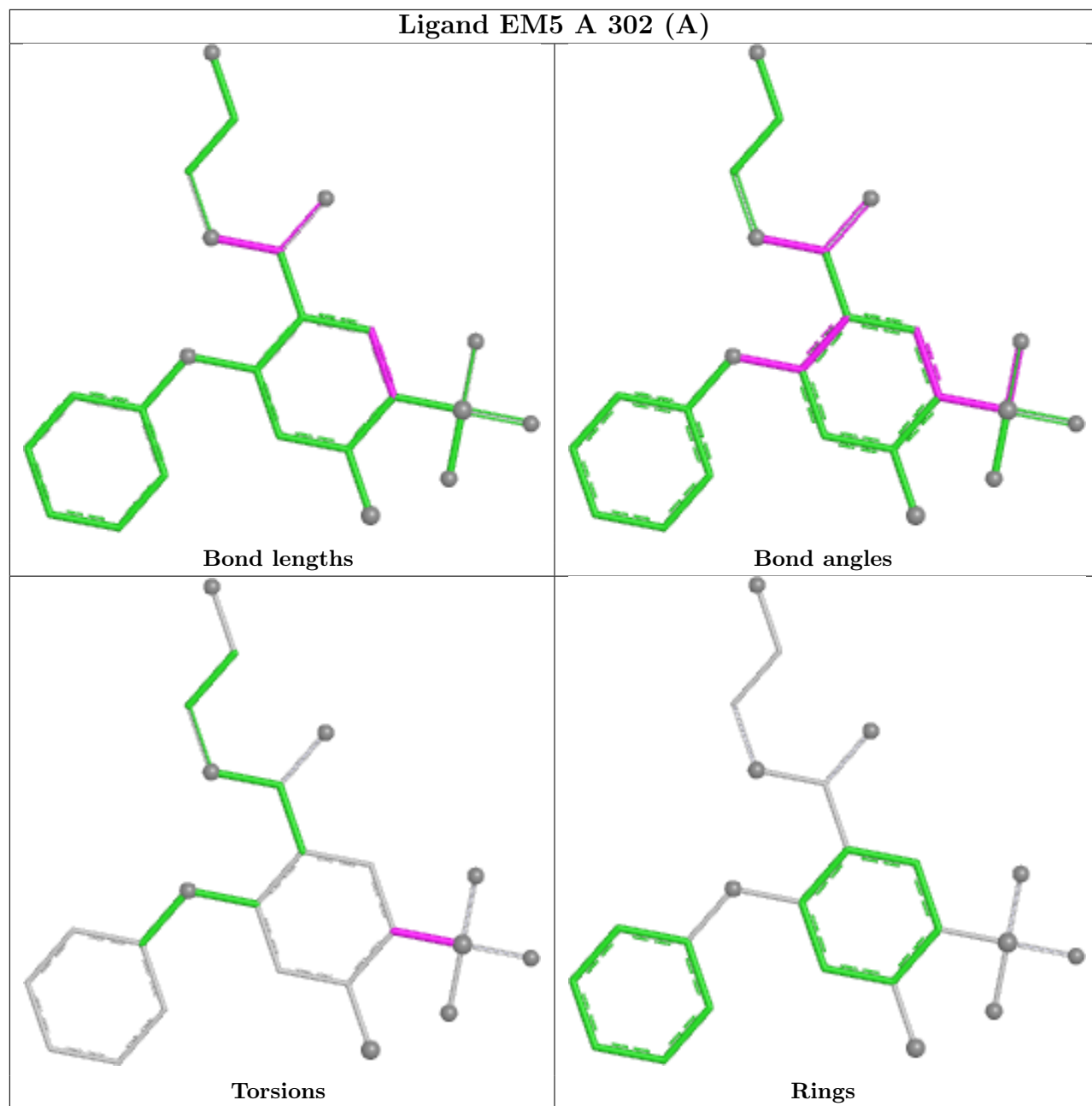
Ligand EM5 B 302 (B)



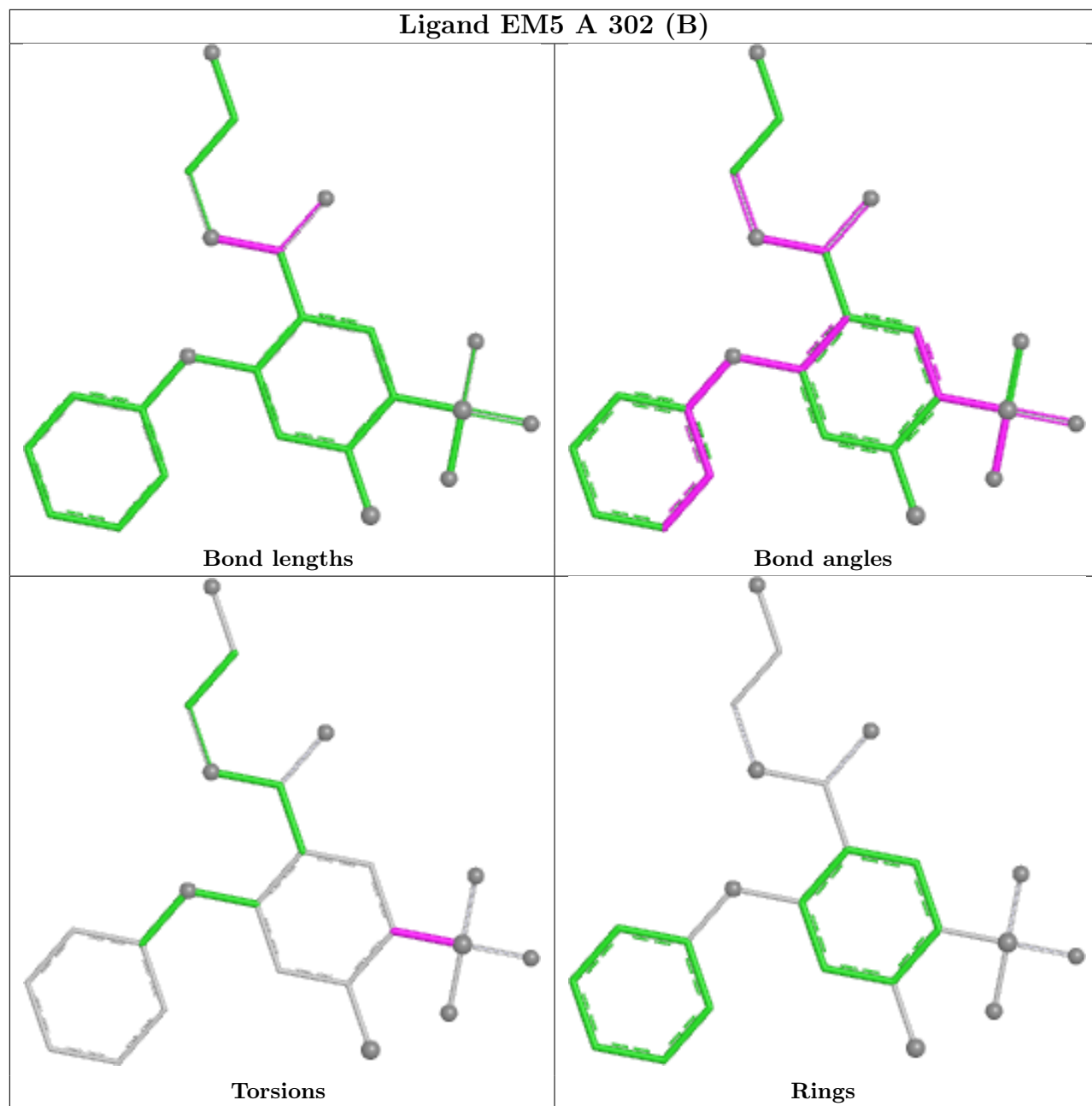


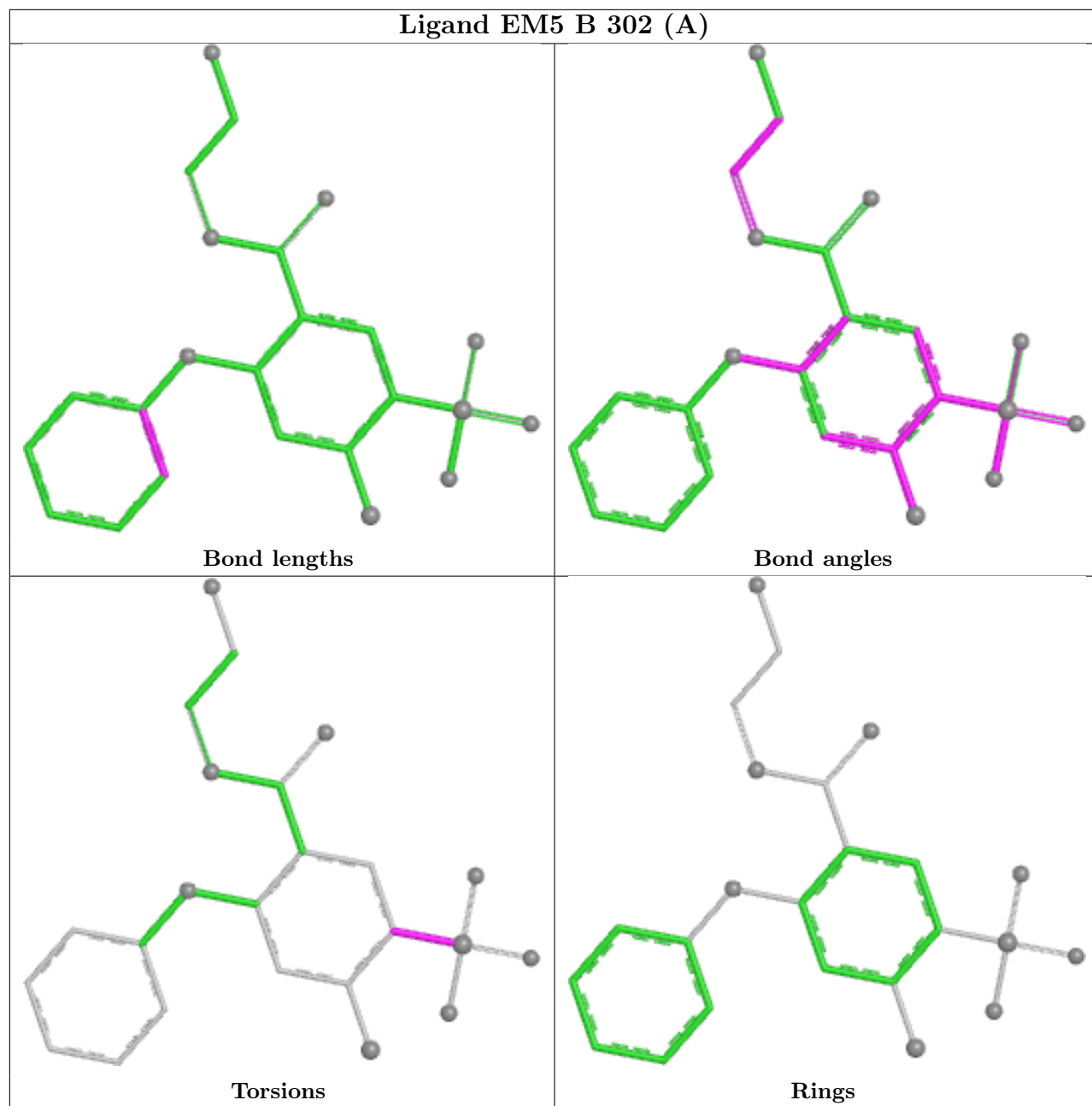


Ligand EM5 A 302 (A)



Ligand EM5 A 302 (B)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	261/263 (99%)	-0.01	4 (1%) 72 73	7, 16, 33, 61	7 (2%)
1	B	261/263 (99%)	-0.02	7 (2%) 56 57	6, 14, 28, 58	6 (2%)
1	C	261/263 (99%)	0.61	23 (8%) 15 16	7, 21, 41, 70	4 (1%)
1	D	261/263 (99%)	-0.01	5 (1%) 66 67	8, 16, 31, 66	5 (1%)
All	All	1044/1052 (99%)	0.14	39 (3%) 45 46	6, 17, 34, 70	22 (2%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	252	PHE	9.3
1	D	252	PHE	5.1
1	B	253	ASP	5.0
1	C	55	ALA	4.6
1	C	8	GLY	4.1
1	D	253	ASP	3.9
1	C	3	LYS	3.9
1	C	54	SER	3.3
1	C	262	SER	3.3
1	C	228	ALA	3.3
1	C	173	PHE	3.2
1	C	165	VAL	3.1
1	C	7	PHE	3.0
1	A	263	GLN	2.9
1	C	61	LEU	2.8
1	C	230	TYR	2.8
1	B	263	GLN	2.7
1	D	263	GLN	2.7
1	A	253	ASP	2.7
1	A	7	PHE	2.5
1	B	3	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	158	ILE	2.5
1	C	235	ASP	2.5
1	C	162	LEU	2.5
1	C	159	PHE	2.4
1	C	156	ASP	2.4
1	B	136	SER	2.4
1	B	7	PHE	2.4
1	C	153	PRO	2.3
1	C	57	LYS	2.2
1	C	50	GLY	2.2
1	A	8	GLY	2.2
1	B	167	TYR	2.1
1	D	3	LYS	2.1
1	D	25[A]	LEU	2.1
1	C	59	PHE	2.1
1	C	51	TYR	2.1
1	C	58	GLN	2.1
1	C	53	LEU	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 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(Å ²)	Q<0.9
4	EDO	D	304	4/4	0.85	0.15	21,26,37,37	0
4	EDO	D	306	4/4	0.87	0.16	31,44,44,64	0
4	EDO	D	303	4/4	0.88	0.14	18,22,37,58	0
5	PEG	A	304	7/7	0.89	0.13	27,41,75,76	0
4	EDO	B	305	4/4	0.90	0.11	21,28,30,62	0

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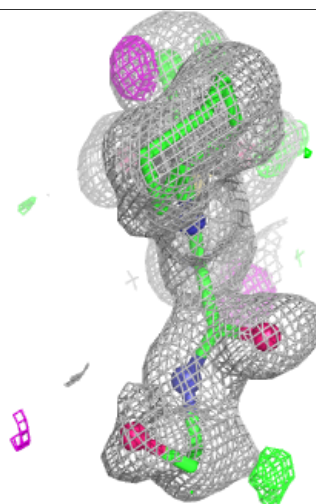
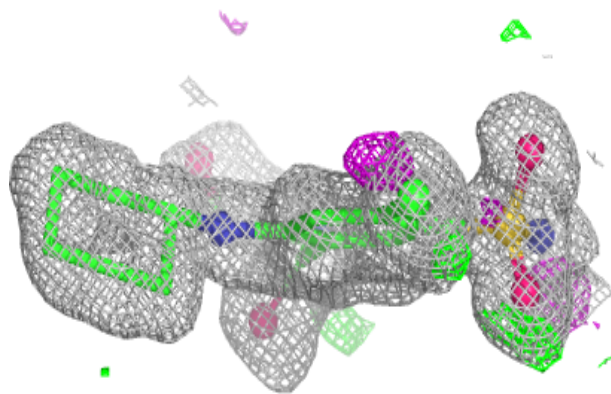
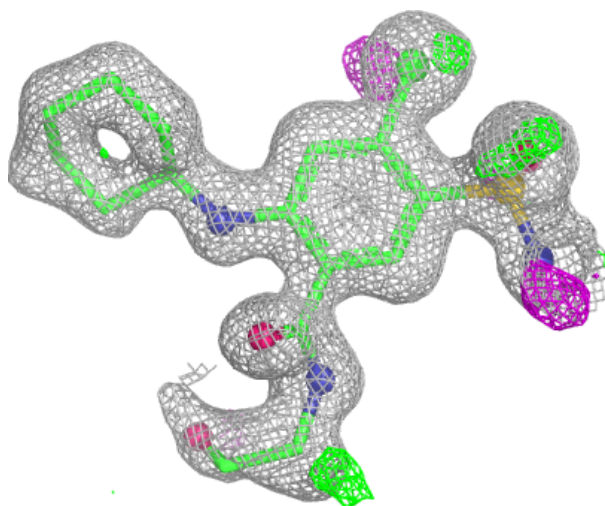
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	C	303	4/4	0.90	0.11	20,25,32,37	0
4	EDO	A	305	4/4	0.90	0.10	22,25,29,42	0
4	EDO	D	305	4/4	0.91	0.12	25,37,42,58	0
5	PEG	D	307	7/7	0.91	0.13	27,48,59,63	0
4	EDO	D	308	4/4	0.92	0.10	26,28,31,34	0
4	EDO	B	303	4/4	0.92	0.11	22,23,31,51	0
4	EDO	B	304	4/4	0.92	0.18	22,49,50,68	0
4	EDO	A	303	4/4	0.93	0.10	45,49,57,62	0
4	EDO	B	306	4/4	0.94	0.09	24,25,26,40	0
3	EM5	C	302	24/24	0.98	0.07	12,17,29,47	0
3	EM5	D	302	24/24	0.99	0.05	9,13,22,34	0
3	EM5	A	302[B]	24/24	0.99	0.05	9,15,24,30	24
3	EM5	B	302[A]	24/24	0.99	0.04	8,12,18,23	24
3	EM5	B	302[B]	24/24	0.99	0.04	7,13,21,27	24
3	EM5	A	302[A]	24/24	0.99	0.05	9,12,20,29	24
2	ZN	A	301	1/1	1.00	0.01	9,9,9,9	0
2	ZN	B	301	1/1	1.00	0.01	7,7,7,7	0
2	ZN	C	301	1/1	1.00	0.02	13,13,13,13	0
2	ZN	D	301	1/1	1.00	0.01	9,9,9,9	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.

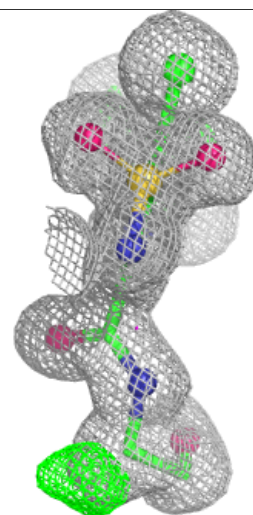
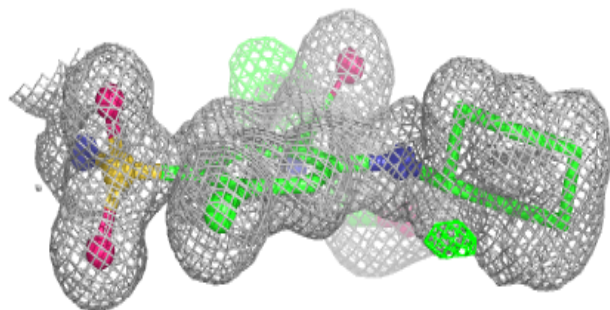
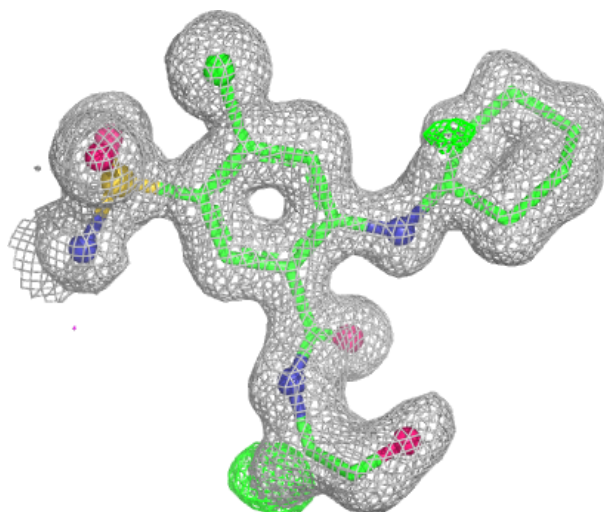
Electron density around EM5 C 302:

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



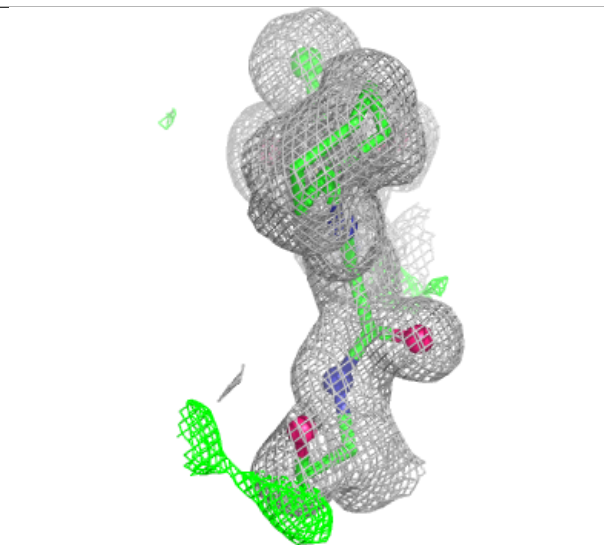
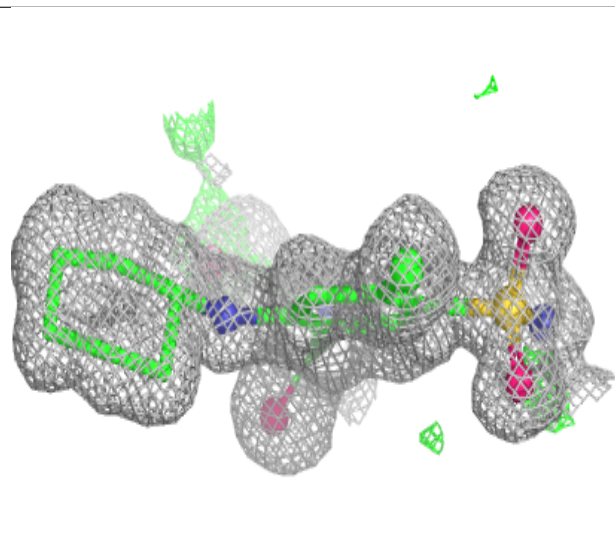
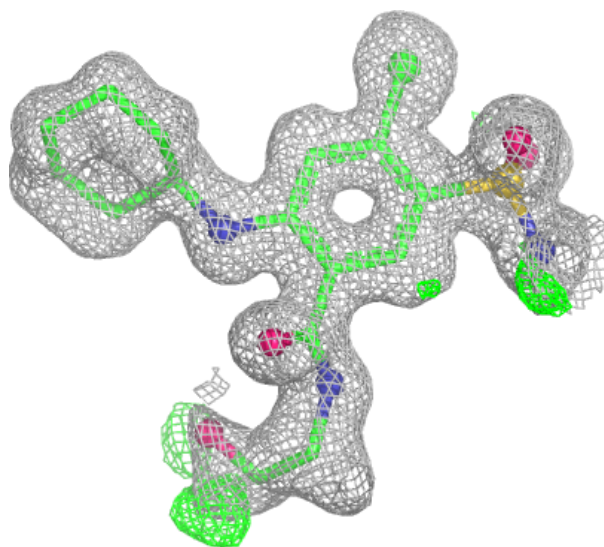
Electron density around EM5 D 302:

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



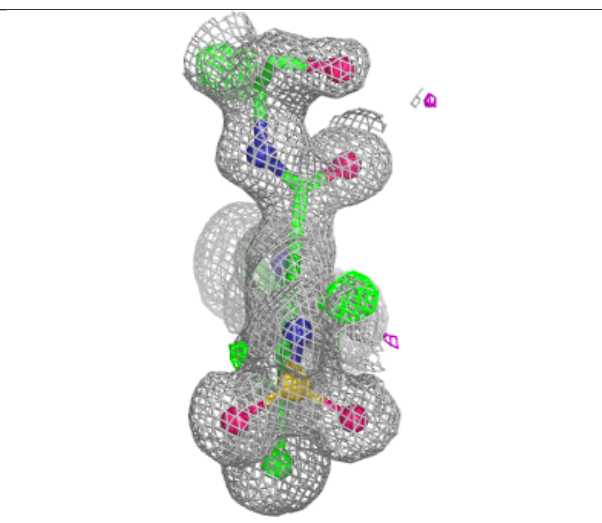
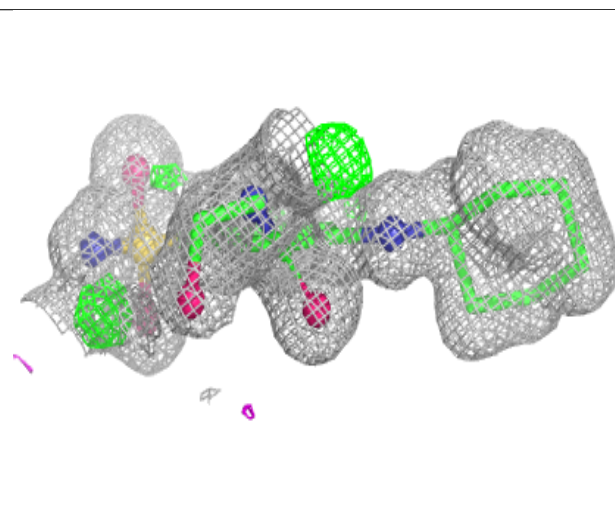
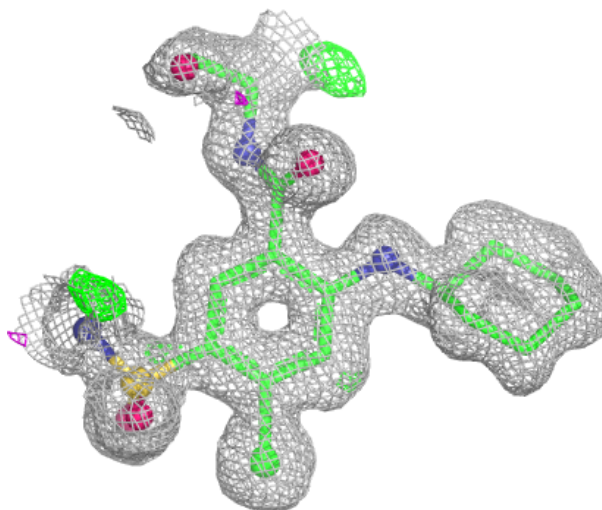
Electron density around EM5 A 302 (B):

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



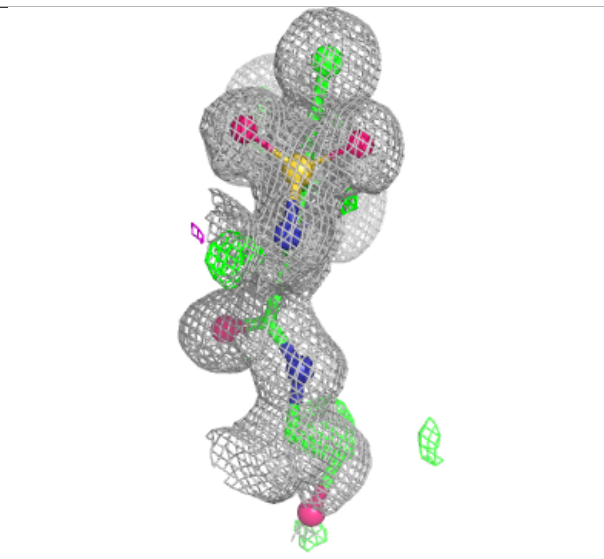
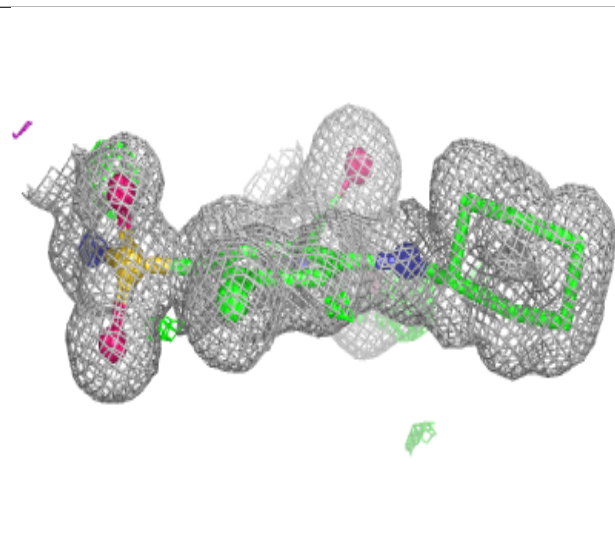
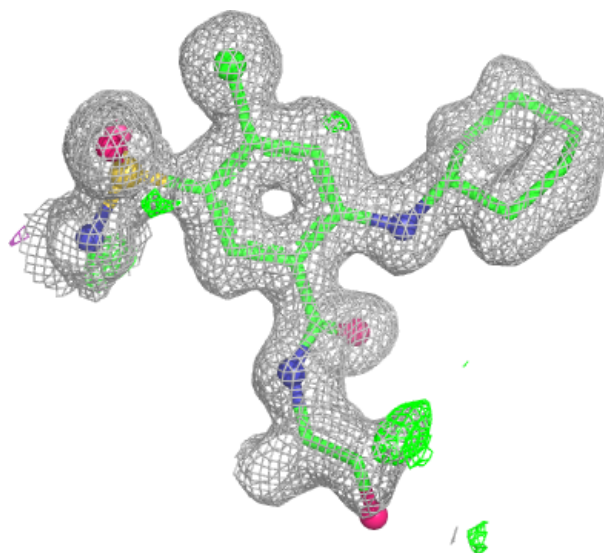
Electron density around EM5 B 302 (A):

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



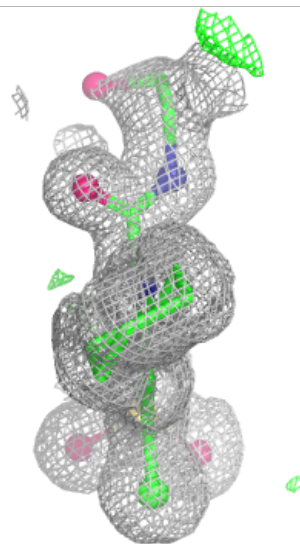
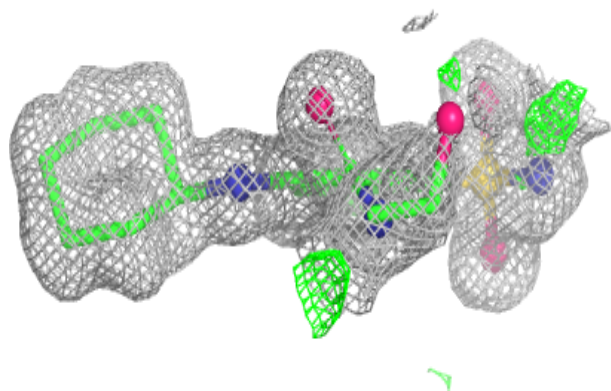
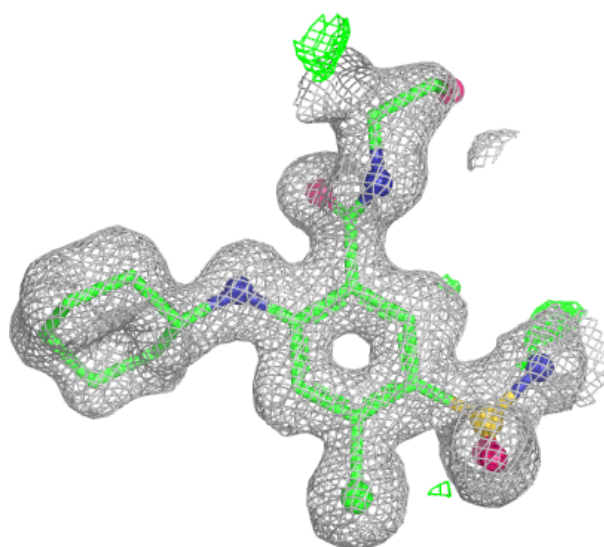
Electron density around EM5 B 302 (B):

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



Electron density around EM5 A 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.