



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:44 PM EDT

PDB ID : 6C7F / pdb_00006c7f
Title : Crystal structure of human phosphodiesterase 2A with 1-(2-chloro-5-isobutoxy-phenyl)-N,4-dimethyl-[1,2,4]triazolo[4,3-a]quinoxaline-8-carboxamide
Authors : Xu, R.; Aertgeerts, K.
Deposited on : 2018-01-22
Resolution : 1.82 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

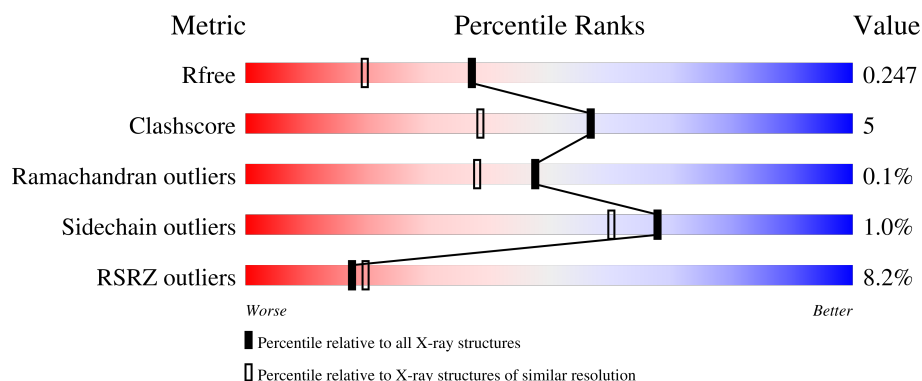
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	342	7% 88% 10% ..
1	B	342	8% 87% 11% .
1	C	342	9% 81% 12% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8814 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.

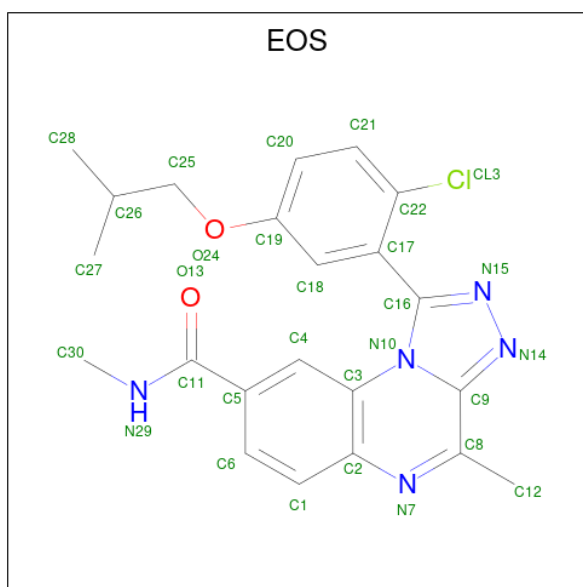
- Molecule 1 is a protein called cGMP-dependent 3',5'-cyclic phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2775	1767	475	508	25			
1	B	336	Total	C	N	O	S	0	0	0
			2750	1754	472	499	25			
1	C	319	Total	C	N	O	S	0	0	0
			2625	1675	451	474	25			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	576	SER	-	expression tag	UNP O00408
A	577	ALA	-	expression tag	UNP O00408
A	578	MET	-	expression tag	UNP O00408
B	576	SER	-	expression tag	UNP O00408
B	577	ALA	-	expression tag	UNP O00408
B	578	MET	-	expression tag	UNP O00408
C	576	SER	-	expression tag	UNP O00408
C	577	ALA	-	expression tag	UNP O00408
C	578	MET	-	expression tag	UNP O00408

- Molecule 2 is 1-[2-chloro-5-(2-methylpropoxy)phenyl]-N,4-dimethyl[1,2,4]triazolo[4,3-a]quin oxaline-8-carboxamide (CCD ID: EOS) (formula: C₂₂H₂₂ClN₅O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			30	22	1	5	2		
2	B	1	Total	C	Cl	N	O	0	0
			30	22	1	5	2		
2	C	1	Total	C	Cl	N	O	0	0
			30	22	1	5	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	214	Total 214	O 214	0	0
5	B	196	Total 196	O 196	0	0
5	C	158	Total 158	O 158	0	0

- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.25Å 73.00Å 91.95Å 90.00° 110.33° 90.00°	Depositor
Resolution (Å)	71.73 – 1.82 71.73 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.3 (71.73-1.82) 99.4 (71.73-1.82)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.82Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.195 , 0.246 0.198 , 0.247	Depositor DCC
R_{free} test set	4553 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8814	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.40% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EOS, ZN, MG

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	0.48	0/2842	0.76	0/3835
1	B	0.46	0/2817	0.72	0/3801
1	C	0.46	0/2689	0.73	2/3626 (0.1%)
All	All	0.47	0/8348	0.74	2/11262 (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	C	652	ASP	CA-C-N	-5.15	115.07	120.38
1	C	652	ASP	C-N-CA	-5.15	115.07	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2775	0	2713	23	0
1	B	2750	0	2699	24	0
1	C	2625	0	2571	29	0
2	A	30	0	0	1	0
2	B	30	0	0	0	0
2	C	30	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	214	0	0	3	0
5	B	196	0	0	3	0
5	C	158	0	0	3	0
All	All	8814	0	7983	75	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 (75) 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:591:GLN:HG2	1:B:595:ALA:HB3	1.74	0.67
1:B:633:LYS:NZ	5:B:1102:HOH:O	2.28	0.67
1:B:782:LYS:O	1:B:786:VAL:HG13	1.95	0.65
1:B:784:ALA:HA	1:B:877:LEU:HD11	1.79	0.65
1:C:864:GLU:OE2	1:C:892:ARG:NH1	2.32	0.63
1:C:859:GLN:HG2	1:C:895:TRP:CE2	2.34	0.63
1:B:676:GLU:N	1:B:676:GLU:OE1	2.35	0.59
1:B:775:ARG:NH1	5:B:1104:HOH:O	2.30	0.59
1:A:579:ASP:N	5:A:1103:HOH:O	2.35	0.59
1:C:676:GLU:OE1	5:C:1101:HOH:O	2.16	0.57
1:B:875:GLN:HG3	1:B:882:ALA:HA	1.85	0.57
1:C:830:PHE:HA	1:C:848:MET:HE2	1.85	0.57
1:A:830:PHE:O	1:A:848:MET:HG3	2.05	0.56
1:B:859:GLN:O	1:B:863:MET:HG3	2.06	0.55
1:C:617:MET:HG3	5:C:1140:HOH:O	2.06	0.54
1:C:826:ILE:HD13	2:C:1001:EOS:C8	2.39	0.53
1:B:845:MET:HG3	1:B:847:MET:HG2	1.91	0.52
1:C:707:PHE:CG	1:C:708:GLN:N	2.76	0.52
1:C:880:LYS:O	1:C:880:LYS:HG3	2.11	0.51
1:A:859:GLN:HG2	1:A:895:TRP:CE2	2.46	0.50
1:A:723:GLY:O	1:A:728:ARG:NH1	2.45	0.50
1:C:593:VAL:O	1:C:596:ILE:HG12	2.12	0.50
1:B:875:GLN:HE21	1:B:882:ALA:HA	1.78	0.49
1:A:809:LEU:HD22	1:A:862:PHE:HZ	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:MET:SD	1:A:648:LYS:HE3	2.52	0.48
1:A:651:ARG:NH1	1:C:786:VAL:O	2.47	0.48
1:B:892:ARG:NH1	5:B:1113:HOH:O	2.45	0.48
1:C:703:THR:HG21	1:C:707:PHE:HE2	1.78	0.48
1:A:664:VAL:HG13	1:A:807:CYS:HB3	1.96	0.48
1:B:590:ILE:HG23	1:B:621:SER:HA	1.95	0.48
1:A:682:GLU:OE1	1:A:756:ARG:NH2	2.30	0.47
1:C:833:GLN:OE1	1:C:848:MET:HE1	2.14	0.47
1:C:707:PHE:O	1:C:709:VAL:N	2.47	0.47
1:C:675:LEU:HD23	1:C:880:LYS:HG2	1.97	0.47
1:A:844:PRO:HB2	1:A:848:MET:HB3	1.97	0.47
1:C:692:SER:O	1:C:696:HIS:HB3	2.15	0.46
1:A:582:TYR:CZ	1:A:586:LEU:HD11	2.51	0.46
1:A:676:GLU:O	1:A:679:ASN:HB2	2.15	0.46
1:A:826:ILE:HD12	2:A:1001:EOS:C8	2.47	0.45
1:A:872:LYS:NZ	5:A:1113:HOH:O	2.48	0.45
1:A:671:LEU:HD13	1:A:803:LEU:HD22	1.99	0.44
1:A:872:LYS:HE2	1:A:885:TYR:CZ	2.53	0.44
1:B:626:MET:HG2	1:B:672:TYR:CD1	2.52	0.44
1:B:778:LYS:O	1:B:782:LYS:HG3	2.18	0.44
1:C:675:LEU:HD13	1:C:878:PHE:CG	2.53	0.44
1:A:862:PHE:HD1	1:A:866:ILE:HD12	1.82	0.44
1:A:793:LYS:HA	1:A:793:LYS:HD3	1.67	0.44
1:C:746:PHE:CE1	1:C:757:MET:HE3	2.53	0.43
1:A:617:MET:HE2	1:A:617:MET:HA	2.01	0.43
1:B:910:ASN:O	1:B:911:ASN:HB2	2.19	0.43
1:B:675:LEU:HD13	1:B:878:PHE:CG	2.54	0.42
1:B:605:TYR:HD2	1:B:666:HIS:CE1	2.37	0.42
1:A:701:ARG:HG2	5:A:1172:HOH:O	2.20	0.42
1:C:593:VAL:HG13	1:C:600:PHE:CD2	2.54	0.42
1:C:835:ASP:OD2	1:C:850:ARG:NH2	2.48	0.42
1:C:817:LYS:N	1:C:817:LYS:HD2	2.35	0.41
1:B:644:LEU:HA	1:B:644:LEU:HD23	1.83	0.41
1:B:778:LYS:HB3	1:B:778:LYS:HE3	1.78	0.41
1:C:703:THR:HG21	1:C:707:PHE:CE2	2.56	0.41
1:A:864:GLU:OE2	1:A:892:ARG:NH2	2.51	0.41
1:C:856:PRO:HG3	1:C:902:PHE:CD1	2.54	0.41
1:C:610:LEU:HD12	1:C:611:PRO:HD2	2.03	0.41
1:C:824:GLU:HG2	1:C:828:LYS:HE2	2.01	0.41
1:A:910:ASN:HB3	1:A:912:SER:HB3	2.02	0.41
1:B:707:PHE:HB2	1:B:833:GLN:NE2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:824:GLU:O	1:C:828:LYS:HG3	2.21	0.41
1:B:582:TYR:HA	1:B:644:LEU:HD11	2.01	0.41
1:B:852:LYS:HA	1:B:852:LYS:HD3	1.92	0.40
1:B:746:PHE:CE2	1:B:757:MET:HG2	2.56	0.40
1:C:729:HIS:O	1:C:733:GLN:HG2	2.21	0.40
1:C:826:ILE:CD1	2:C:1001:EOS:C12	2.99	0.40
1:C:843:ARG:HA	1:C:844:PRO:HD3	1.81	0.40
1:A:603:PHE:HA	1:A:670:LEU:HD13	2.02	0.40
1:B:819:THR:CG2	1:B:895:TRP:HE1	2.34	0.40
1:C:794:GLN:OE1	5:C:1102:HOH:O	2.22	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	337/342 (98%)	334 (99%)	3 (1%)	0	100	100
1	B	334/342 (98%)	328 (98%)	6 (2%)	0	100	100
1	C	315/342 (92%)	308 (98%)	6 (2%)	1 (0%)	36	26
All	All	986/1026 (96%)	970 (98%)	15 (2%)	1 (0%)	48	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	708	GLN

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	306/308 (99%)	303 (99%)	3 (1%)	68	60
1	B	303/308 (98%)	300 (99%)	3 (1%)	68	60
1	C	290/308 (94%)	287 (99%)	3 (1%)	68	60
All	All	899/924 (97%)	890 (99%)	9 (1%)	68	60

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	793	LYS
1	A	826	ILE
1	A	893	GLU
1	B	785	GLU
1	B	786	VAL
1	B	887	ARG
1	C	596	ILE
1	C	840	MET
1	C	897	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	591	GLN
1	B	624	GLN
1	B	630	ASN
1	B	739	ASN
1	B	781	GLN
1	B	865	HIS
1	B	875	GLN
1	B	900	HIS
1	C	755	GLN
1	C	781	GLN
1	C	900	HIS

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 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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
2	EOS	B	1001	-	32,33,33	1.20	3 (9%)	45,48,48	1.59	11 (24%)
2	EOS	C	1001	-	32,33,33	1.07	3 (9%)	45,48,48	1.68	6 (13%)
2	EOS	A	1001	-	32,33,33	1.07	2 (6%)	45,48,48	1.51	6 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EOS	B	1001	-	-	2/15/15/15	0/4/4/4
2	EOS	C	1001	-	-	5/15/15/15	0/4/4/4
2	EOS	A	1001	-	-	1/15/15/15	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	EOS	C11-N29	3.04	1.37	1.33
2	B	1001	EOS	C11-N29	3.02	1.37	1.33
2	A	1001	EOS	C11-N29	2.87	1.37	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	EOS	C3-N10	-2.62	1.39	1.42
2	B	1001	EOS	C17-C16	-2.62	1.44	1.47
2	A	1001	EOS	C17-C16	-2.19	1.44	1.47
2	C	1001	EOS	C3-N10	-2.18	1.39	1.42
2	C	1001	EOS	C17-C16	-2.18	1.44	1.47

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001	EOS	C5-C11-N29	-5.60	110.01	117.01
2	C	1001	EOS	C25-O24-C19	-4.85	107.18	117.85
2	A	1001	EOS	C25-O24-C19	-4.74	107.42	117.85
2	C	1001	EOS	C22-C17-C16	-4.48	118.34	122.37
2	A	1001	EOS	C5-C11-N29	-4.19	111.78	117.01
2	B	1001	EOS	C5-C11-N29	-3.92	112.11	117.01
2	C	1001	EOS	O13-C11-N29	3.79	128.26	122.67
2	A	1001	EOS	C22-C17-C16	-3.66	119.09	122.37
2	B	1001	EOS	C25-O24-C19	-3.62	109.87	117.85
2	B	1001	EOS	O13-C11-N29	3.52	127.88	122.67
2	B	1001	EOS	C6-C5-C4	3.28	123.04	119.25
2	A	1001	EOS	C6-C5-C4	2.92	122.63	119.25
2	B	1001	EOS	C18-C17-C22	2.79	120.92	117.84
2	B	1001	EOS	C18-C17-C16	-2.50	115.62	121.83
2	B	1001	EOS	C12-C8-N7	2.47	122.07	119.62
2	C	1001	EOS	C6-C5-C4	2.41	122.03	119.25
2	B	1001	EOS	C9-C8-N7	-2.34	120.22	123.13
2	A	1001	EOS	O13-C11-N29	2.33	126.12	122.67
2	A	1001	EOS	C1-C6-C5	-2.27	118.38	120.80
2	B	1001	EOS	C17-C16-N15	-2.27	120.06	124.62
2	C	1001	EOS	N10-C16-N15	-2.13	108.68	109.94
2	B	1001	EOS	C1-C6-C5	-2.11	118.55	120.80
2	B	1001	EOS	C21-C22-C17	-2.03	119.11	121.36

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1001	EOS	C5-C11-N29-C30
2	C	1001	EOS	O13-C11-N29-C30
2	C	1001	EOS	C26-C25-O24-C19
2	B	1001	EOS	O13-C11-N29-C30
2	C	1001	EOS	O24-C25-C26-C27

Continued on next page...

Continued from previous page...

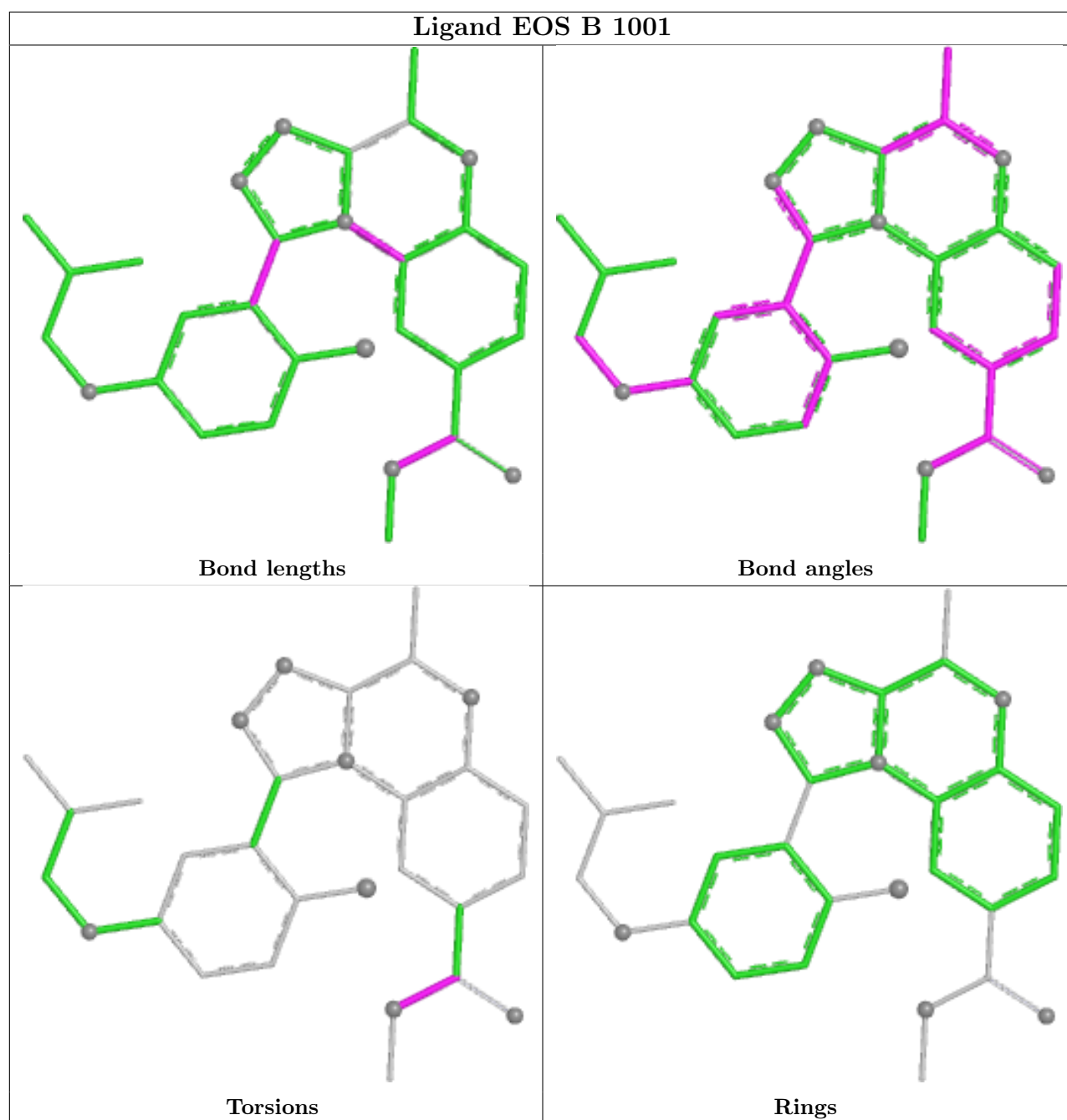
Mol	Chain	Res	Type	Atoms
2	C	1001	EOS	O24-C25-C26-C28
2	B	1001	EOS	C5-C11-N29-C30
2	A	1001	EOS	C26-C25-O24-C19

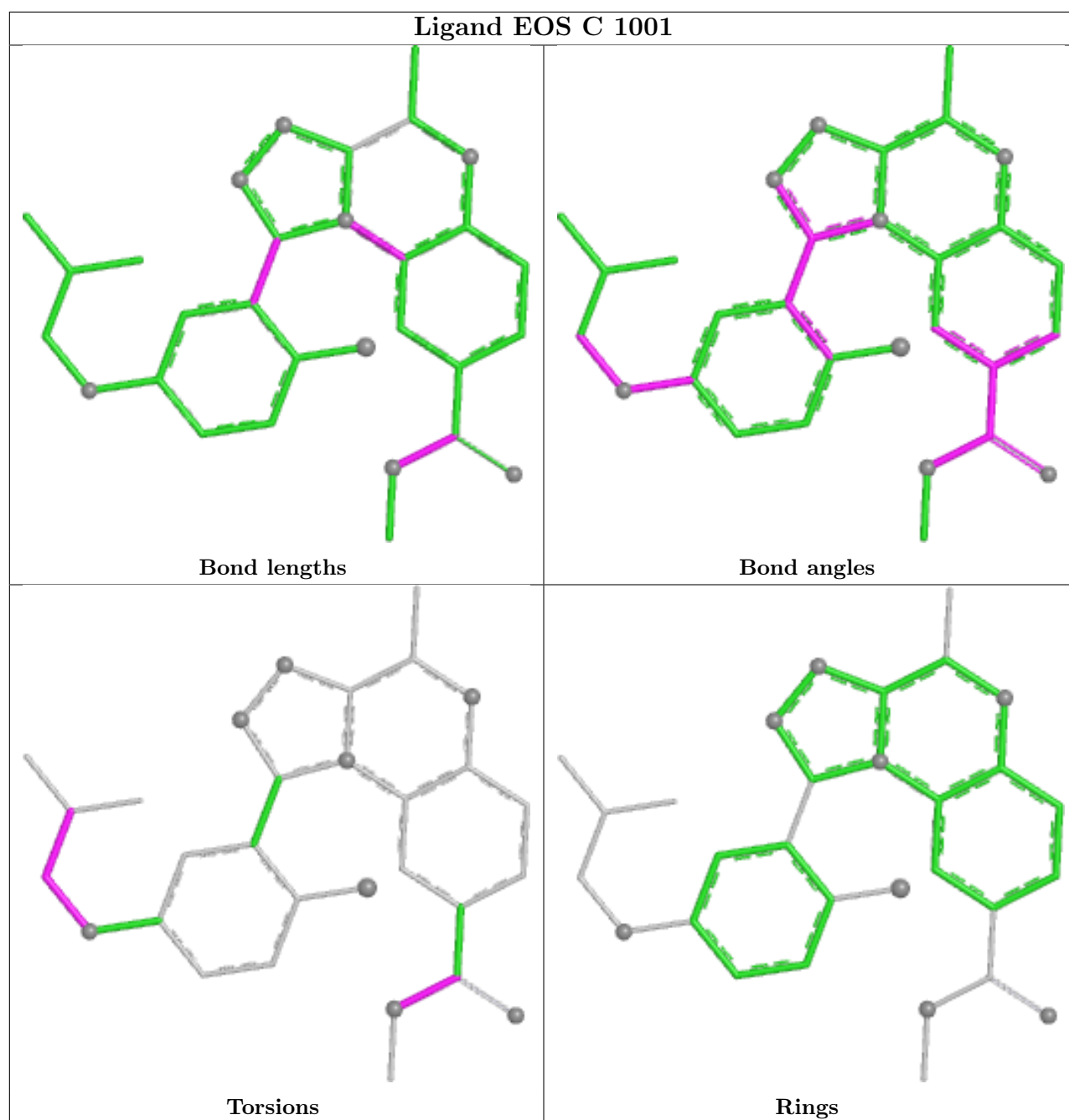
There are no ring outliers.

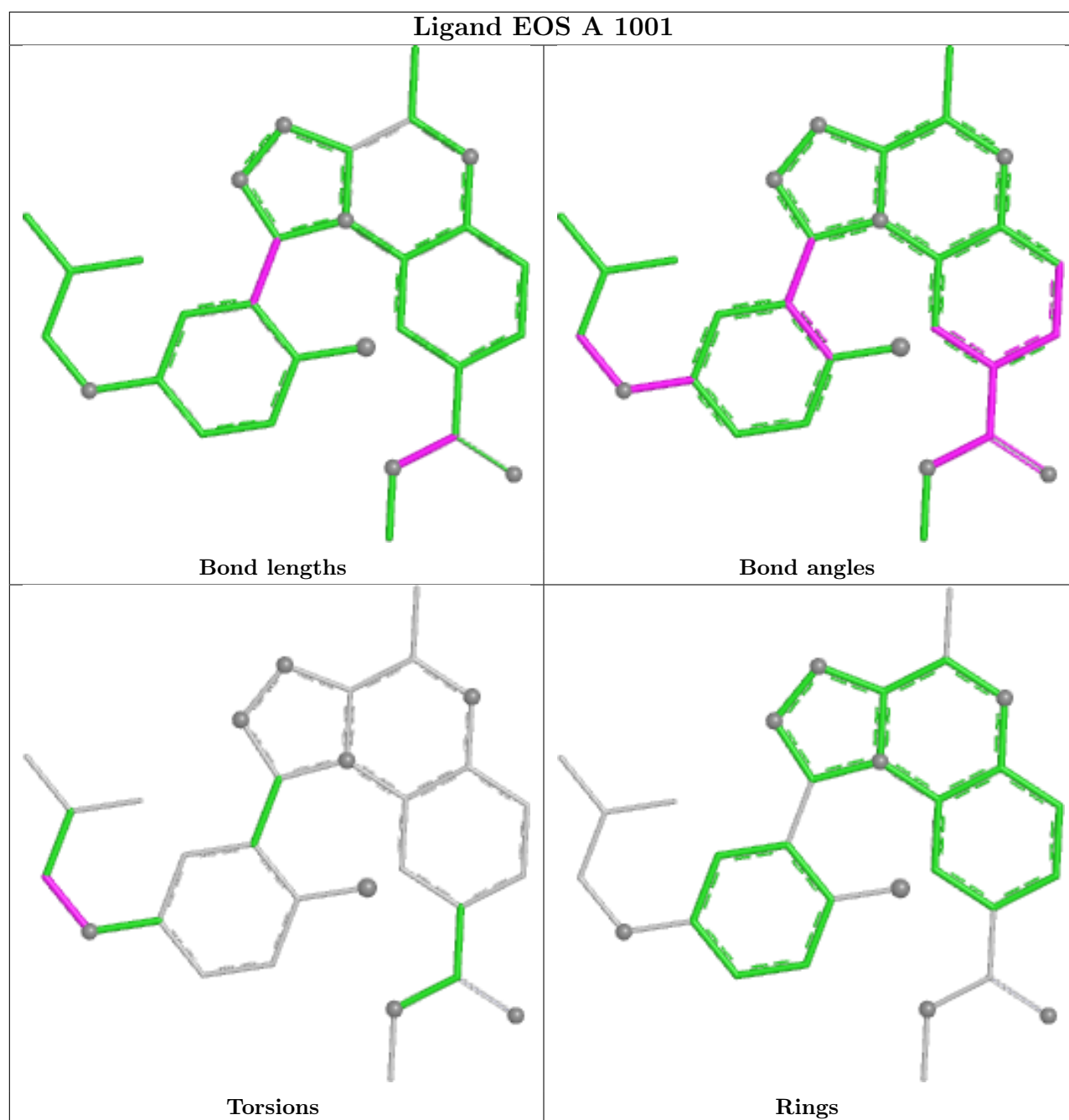
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	EOS	2	0
2	A	1001	EOS	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.







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	339/342 (99%)	0.33	23 (6%) 23 27	15, 32, 55, 72	0
1	B	336/342 (98%)	0.57	28 (8%) 17 20	16, 35, 62, 72	0
1	C	319/342 (93%)	0.64	31 (9%) 13 15	19, 38, 60, 80	0
All	All	994/1026 (96%)	0.51	82 (8%) 17 20	15, 35, 59, 80	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	786	VAL	6.8
1	C	707	PHE	6.6
1	C	719	TYR	6.4
1	C	718	LEU	6.2
1	B	784	ALA	5.6
1	C	709	VAL	5.5
1	C	708	GLN	4.6
1	B	785	GLU	4.5
1	C	840	MET	4.5
1	B	680	TYR	4.4
1	B	910	ASN	4.2
1	C	596	ILE	4.1
1	C	720	SER	3.9
1	C	841	GLY	3.9
1	C	590	ILE	3.8
1	A	841	GLY	3.6
1	C	836	LEU	3.6
1	B	787	GLY	3.6
1	B	617	MET	3.2
1	B	790	ARG	3.2
1	B	783	MET	3.1
1	A	709	VAL	3.1
1	C	790	ARG	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	780	LEU	3.0
1	A	848	MET	2.9
1	C	721	SER	2.9
1	C	786	VAL	2.9
1	B	588	ASP	2.9
1	C	599	ASN	2.8
1	B	675	LEU	2.8
1	A	909	SER	2.7
1	C	706	SER	2.7
1	A	794	GLN	2.7
1	A	712	LYS	2.7
1	A	910	ASN	2.7
1	C	916	LEU	2.7
1	A	917	ASP	2.6
1	C	880	LYS	2.6
1	B	591	GLN	2.6
1	C	897	LYS	2.6
1	A	706	SER	2.5
1	C	909	SER	2.5
1	A	842	ASN	2.5
1	B	909	SER	2.5
1	B	676	GLU	2.5
1	B	613	ASP	2.5
1	C	778	LYS	2.4
1	B	593	VAL	2.4
1	B	582	TYR	2.4
1	A	710	ALA	2.4
1	C	613	ASP	2.3
1	C	591	GLN	2.3
1	A	790	ARG	2.3
1	C	843	ARG	2.3
1	A	643	CYS	2.3
1	B	595	ALA	2.3
1	A	785	GLU	2.3
1	A	678	THR	2.3
1	A	839	ALA	2.2
1	A	793	LYS	2.2
1	C	598	SER	2.2
1	B	877	LEU	2.2
1	C	594	ALA	2.2
1	A	746	PHE	2.2
1	C	705	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	788	TYR	2.1
1	B	598	SER	2.1
1	C	751	ARG	2.1
1	A	679	ASN	2.1
1	A	786	VAL	2.1
1	C	839	ALA	2.1
1	A	579	ASP	2.1
1	B	772	HIS	2.0
1	C	879	PRO	2.0
1	B	585	LEU	2.0
1	A	717	ALA	2.0
1	B	594	ALA	2.0
1	B	882	ALA	2.0
1	B	590	ILE	2.0
1	C	741	HIS	2.0
1	A	879	PRO	2.0
1	B	879	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
2	EOS	C	1001	30/30	0.94	0.10	22,28,36,39	0
2	EOS	B	1001	30/30	0.95	0.09	15,25,38,43	0
2	EOS	A	1001	30/30	0.96	0.08	17,24,43,47	0
4	MG	B	1003	1/1	0.98	0.04	16,16,16,16	0
4	MG	A	1003	1/1	0.99	0.03	18,18,18,18	0
4	MG	C	1003	1/1	0.99	0.04	18,18,18,18	0

Continued on next page...

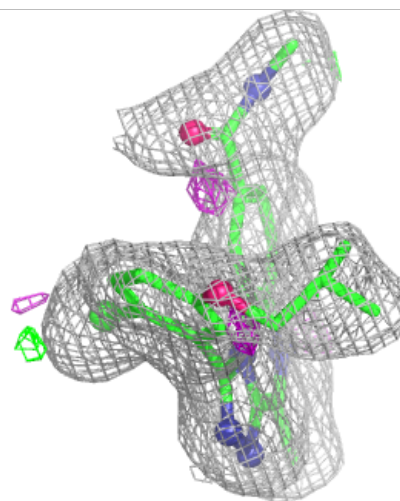
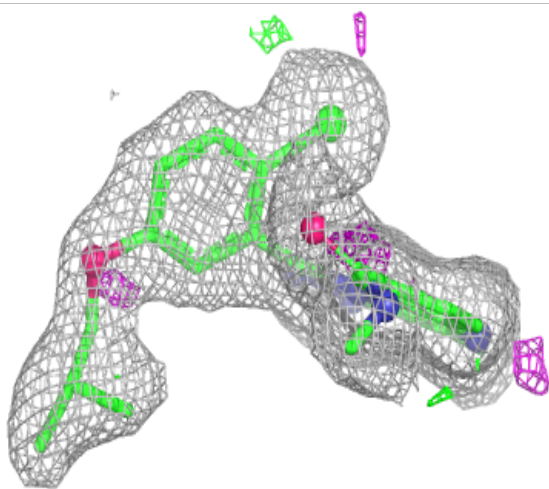
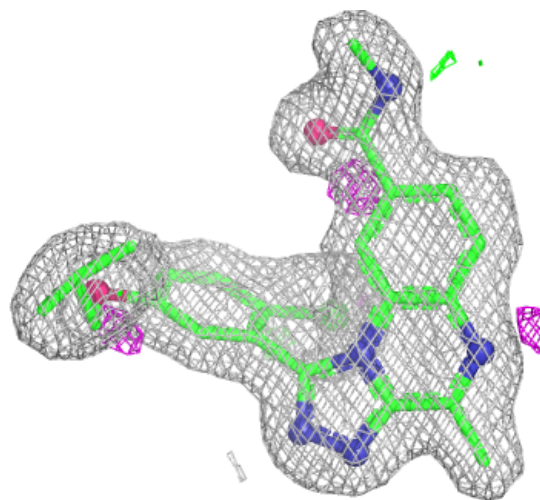
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	A	1002	1/1	1.00	0.01	20,20,20,20	0
3	ZN	B	1002	1/1	1.00	0.01	21,21,21,21	0
3	ZN	C	1002	1/1	1.00	0.02	23,23,23,23	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.

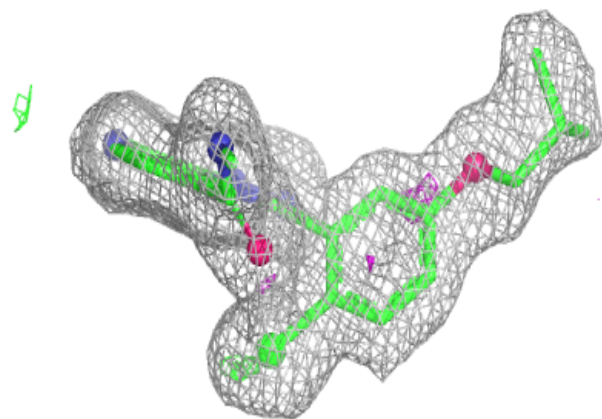
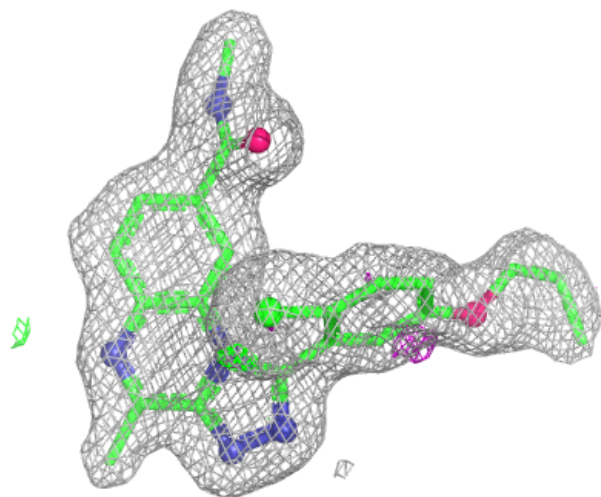
Electron density around EOS C 1001:

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



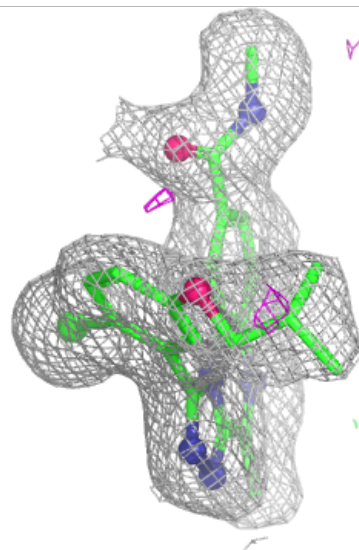
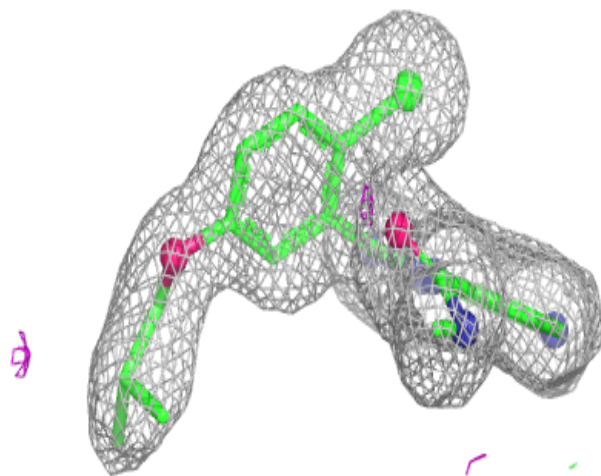
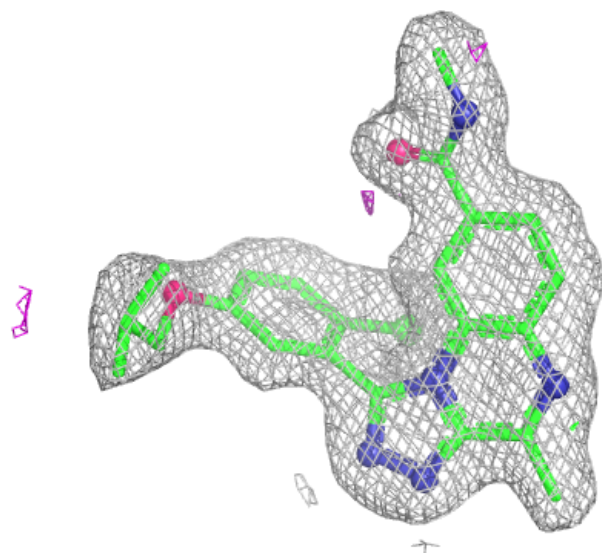
Electron density around EOS B 1001:

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



Electron density around EOS A 1001:

$2mF_o-DF_c$ (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.