



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:34 AM UTC

PDB ID : 6C7G / pdb_00006c7g
Title : Crystal structure of human phosphodiesterase 2A with N-(1-adamantyl)-1-(2-chloro-5-isobutoxy-phenyl)-4-methyl-[1,2,4]triazolo[4,3-a]quinoxaline-8-carboxamide
Authors : Xu, R.; Aertgeerts, K.
Deposited on : 2018-01-22
Resolution : 1.68 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

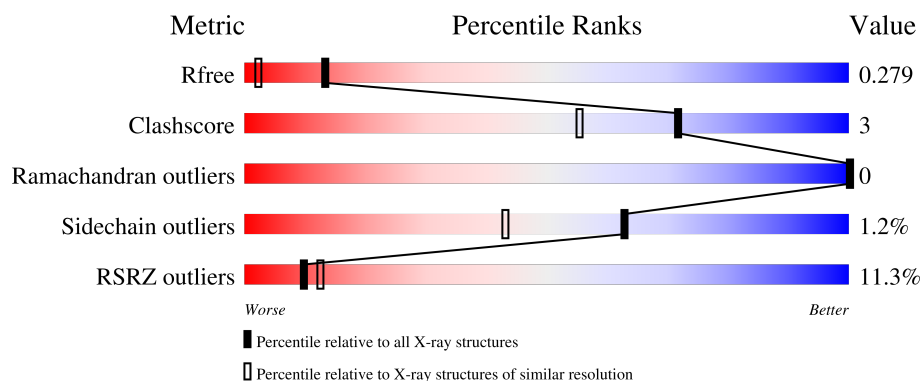
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	
1	B	342	
1	C	342	
1	D	342	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11803 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.

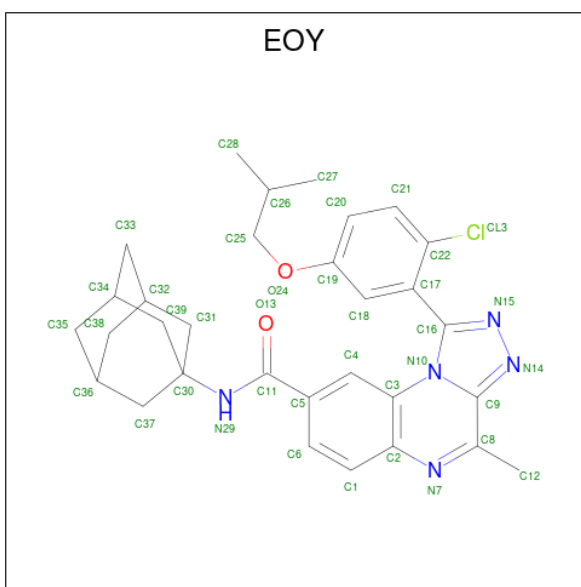
- Molecule 1 is a protein called cGMP-dependent 3',5'-cyclic phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2786	1774	477	509	26			
1	B	338	Total	C	N	O	S	0	0	0
			2767	1763	474	505	25			
1	C	326	Total	C	N	O	S	0	0	0
			2668	1701	459	483	25			
1	D	335	Total	C	N	O	S	0	0	0
			2742	1750	471	496	25			

There are 12 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
D	576	SER	-	expression tag	UNP O00408
D	577	ALA	-	expression tag	UNP O00408
D	578	MET	-	expression tag	UNP O00408

- Molecule 2 is 1-[2-chloro-5-(2-methylpropoxy)phenyl]-4-methyl-N-[(3s,5s,7s)-tricyclo[3.3.1.1 3,7]decan-1-yl][1,2,4]triazolo[4,3-a]quinoxaline-8-carboxamide (CCD ID: EOY) (formula: C₃₁H₃₄ClN₅O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	9	0
			39	31	1	5	2		
2	B	1	Total	C	Cl	N	O	9	0
			39	31	1	5	2		
2	C	1	Total	C	Cl	N	O	9	0
			39	31	1	5	2		
2	D	1	Total	C	Cl	N	O	9	0
			39	31	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		
3	D	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		

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

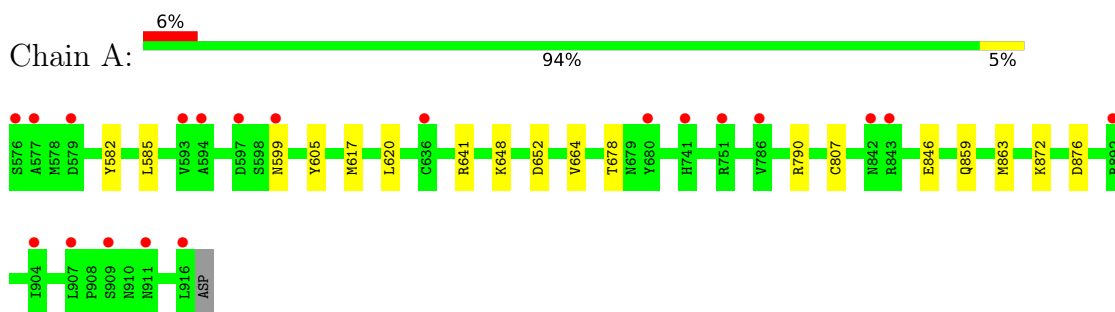
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	212	Total 212	O 212	0	0
5	B	173	Total 173	O 173	0	0
5	C	143	Total 143	O 143	0	0
5	D	148	Total 148	O 148	0	0

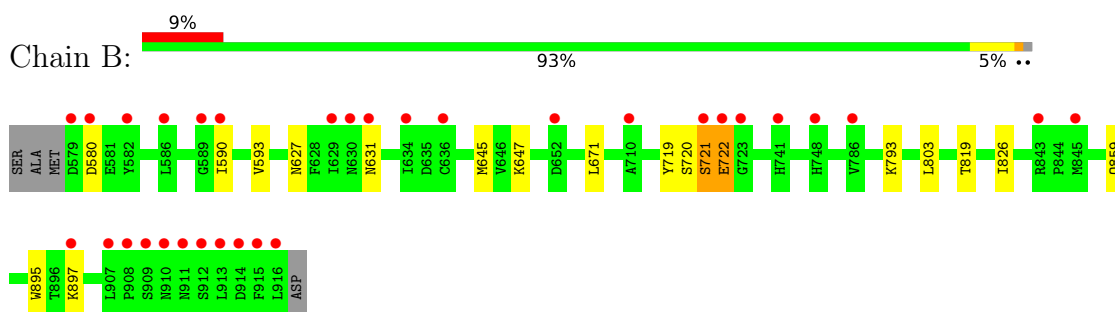
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

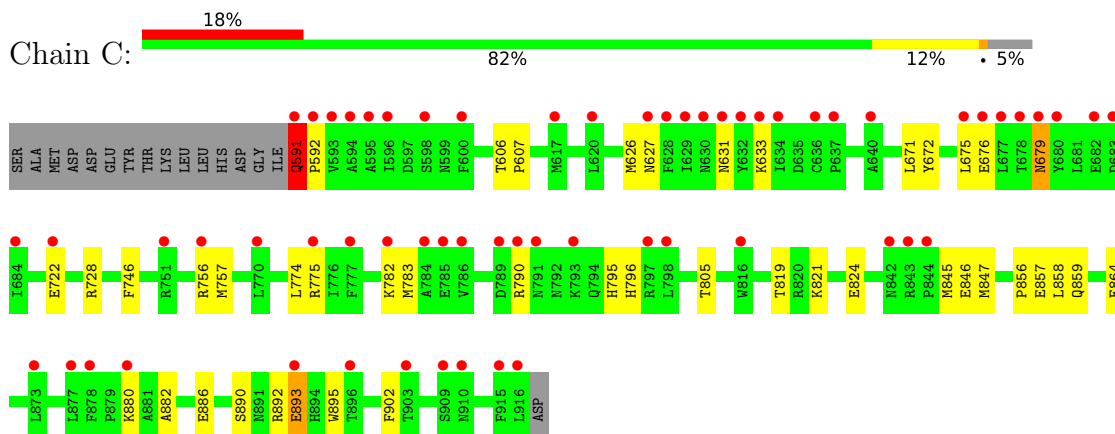
- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase



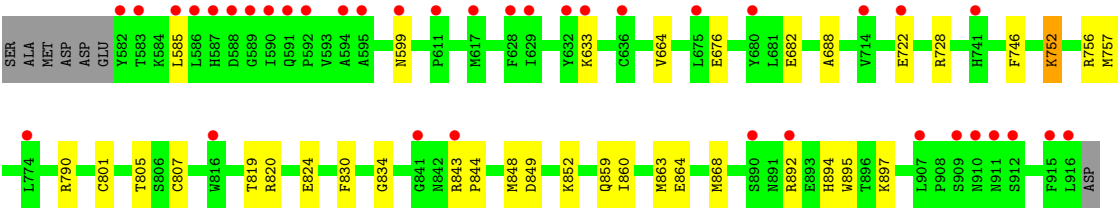
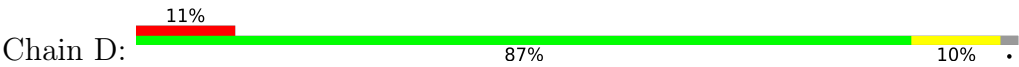
- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.14Å 73.99Å 91.74Å 109.48° 91.49° 91.04°	Depositor
Resolution (Å)	66.13 – 1.68 66.13 – 1.68	Depositor EDS
% Data completeness (in resolution range)	92.3 (66.13-1.68) 92.4 (66.13-1.68)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 1.68Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.197 , 0.234 (Not available) , 0.279	Depositor DCC
R_{free} test set	7096 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	12.8	Xtriage
Anisotropy	0.858	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11803	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.56% 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: EOY, MG, ZN

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	0.50	0/2853	0.72	2/3849 (0.1%)
1	B	0.47	0/2834	0.71	1/3824 (0.0%)
1	C	0.44	0/2733	0.74	2/3687 (0.1%)
1	D	0.47	0/2809	0.71	0/3790
All	All	0.47	0/11229	0.72	5/15150 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	721	SER	N-CA-C	-7.20	104.65	113.50
1	C	591	GLN	CA-C-N	-6.76	113.00	119.76
1	C	591	GLN	C-N-CA	-6.76	113.00	119.76
1	A	652	ASP	CA-C-N	-5.60	114.61	120.38
1	A	652	ASP	C-N-CA	-5.60	114.61	120.38

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	721	SER	Peptide

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Mol	Chain	Res	Type	Group
1	B	722	GLU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2786	0	2728	9	0
1	B	2767	0	2709	10	0
1	C	2668	0	2619	28	0
1	D	2742	0	2695	30	0
2	A	39	0	0	0	0
2	B	39	0	0	1	0
2	C	39	0	0	1	0
2	D	39	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	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
4	D	1	0	0	0	0
5	A	212	0	0	0	0
5	B	173	0	0	2	0
5	C	143	0	0	0	0
5	D	148	0	0	0	0
All	All	11803	0	10751	73	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 3.

All (73) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:843:ARG:NH1	1:D:849:ASP:OD2	2.06	0.89
1:D:864:GLU:HG2	1:D:892:ARG:HE	1.36	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:627:ASN:O	1:C:631:ASN:ND2	2.18	0.76
1:D:894:HIS:HA	1:D:897:LYS:HD2	1.77	0.67
1:B:719:TYR:O	1:B:722:GLU:HB3	1.97	0.65
1:D:859:GLN:HG2	1:D:895:TRP:CE2	2.33	0.64
1:C:859:GLN:HG2	1:C:895:TRP:CE2	2.33	0.63
1:C:722:GLU:OE1	1:D:728:ARG:NH1	2.33	0.62
1:B:859:GLN:HG2	1:B:895:TRP:CE2	2.36	0.60
1:C:728:ARG:NH1	1:D:722:GLU:OE2	2.35	0.59
1:C:676:GLU:HG2	1:C:679:ASN:HB2	1.85	0.58
1:D:633:LYS:N	1:D:633:LYS:HD2	2.19	0.57
1:A:859:GLN:O	1:A:863:MET:HG3	2.04	0.56
1:D:819:THR:CG2	1:D:895:TRP:HE1	2.18	0.56
1:A:872:LYS:NZ	1:A:876:ASP:OD1	2.37	0.54
1:C:633:LYS:N	1:C:633:LYS:HD2	2.23	0.54
1:A:582:TYR:CE1	1:A:641:ARG:HG3	2.43	0.53
1:C:819:THR:CG2	1:C:895:TRP:HE1	2.22	0.53
1:C:882:ALA:O	1:C:886:GLU:HG2	2.09	0.52
1:D:864:GLU:OE2	1:D:892:ARG:NH2	2.44	0.51
1:C:864:GLU:OE2	1:C:892:ARG:NH2	2.42	0.50
1:B:671:LEU:HD13	1:B:803:LEU:HD22	1.92	0.50
1:A:585:LEU:HD12	1:A:617:MET:HE2	1.94	0.49
1:D:820:ARG:NH1	1:D:824:GLU:OE2	2.46	0.49
1:D:843:ARG:NH2	1:D:852:LYS:HD2	2.28	0.48
1:A:585:LEU:HG	1:A:620:LEU:HD11	1.96	0.47
1:A:678:THR:O	1:A:790:ARG:NH2	2.48	0.46
1:B:819:THR:CG2	1:B:895:TRP:HE1	2.27	0.46
1:D:819:THR:HG21	1:D:895:TRP:HE1	1.79	0.46
1:D:843:ARG:HD2	1:D:844:PRO:HD2	1.97	0.46
1:C:880:LYS:HE2	1:C:880:LYS:HB3	1.66	0.46
1:B:647:LYS:NZ	5:B:1111:HOH:O	2.47	0.45
1:D:843:ARG:HH12	1:D:849:ASP:CG	2.17	0.45
1:C:845:MET:HG3	1:C:847:MET:HG2	1.98	0.45
1:D:746:PHE:CZ	1:D:757:MET:HE2	2.52	0.45
1:D:859:GLN:O	1:D:863:MET:HG3	2.16	0.44
1:A:648:LYS:HG3	1:D:790:ARG:HD2	1.98	0.44
1:C:805:THR:HB	2:C:1001:EOY:C28	2.46	0.44
1:D:664:VAL:HG13	1:D:807:CYS:HB3	2.00	0.44
1:D:864:GLU:CD	1:D:892:ARG:HH21	2.25	0.44
1:A:599:ASN:O	1:A:605:TYR:HB2	2.18	0.44
1:A:664:VAL:HG13	1:A:807:CYS:HB3	1.99	0.44
1:C:606:THR:HA	1:C:607:PRO:HD2	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:783:MET:HG3	1:C:795:HIS:CE1	2.52	0.44
1:B:720:SER:C	1:B:722:GLU:HG2	2.43	0.43
1:D:682:GLU:OE1	1:D:756:ARG:NH2	2.32	0.43
1:C:675:LEU:O	1:C:676:GLU:HB3	2.18	0.43
1:B:645:MET:HG2	5:B:1253:HOH:O	2.19	0.43
1:D:819:THR:HG22	1:D:895:TRP:HE1	1.82	0.43
1:C:626:MET:HG2	1:C:672:TYR:CD2	2.53	0.43
1:C:890:SER:O	1:C:893:GLU:HG2	2.18	0.43
1:D:830:PHE:HB3	1:D:848:MET:HG2	2.01	0.43
1:C:746:PHE:CE2	1:C:757:MET:HG2	2.53	0.42
1:D:801:CYS:O	1:D:805:THR:HG23	2.18	0.42
1:D:860:ILE:O	1:D:864:GLU:HG3	2.19	0.42
1:C:790:ARG:O	1:C:796:HIS:NE2	2.25	0.42
1:C:821:LYS:NZ	1:C:824:GLU:OE2	2.36	0.42
1:D:834:GLY:HA3	1:D:848:MET:O	2.19	0.42
1:C:857:GLU:HG3	1:C:858:LEU:N	2.35	0.42
1:D:688:ALA:HA	1:D:757:MET:HE1	2.02	0.42
1:D:868:MET:SD	1:D:892:ARG:HD2	2.60	0.42
1:D:752:LYS:HB2	1:D:752:LYS:HE3	1.96	0.41
1:B:590:ILE:O	1:C:774:LEU:HD13	2.20	0.41
1:C:782:LYS:HB2	1:C:782:LYS:HE3	1.81	0.41
1:B:627:ASN:O	1:B:631:ASN:HB2	2.21	0.41
1:C:591:GLN:N	1:C:592:PRO:HD2	2.35	0.41
1:D:585:LEU:HD23	1:D:585:LEU:HA	1.91	0.41
1:C:671:LEU:O	1:C:675:LEU:HB2	2.21	0.41
1:C:819:THR:HG22	1:C:895:TRP:HE1	1.84	0.41
1:C:856:PRO:HG3	1:C:902:PHE:CD1	2.56	0.41
1:C:676:GLU:HG2	1:C:679:ASN:CB	2.50	0.40
1:D:864:GLU:HG2	1:D:892:ARG:NE	2.19	0.40
1:B:826:ILE:HD13	2:B:1001:EOY:C9	2.50	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	339/342 (99%)	337 (99%)	2 (1%)	0	100	100
1	B	336/342 (98%)	332 (99%)	4 (1%)	0	100	100
1	C	324/342 (95%)	319 (98%)	5 (2%)	0	100	100
1	D	333/342 (97%)	331 (99%)	2 (1%)	0	100	100
All	All	1332/1368 (97%)	1319 (99%)	13 (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	307/308 (100%)	306 (100%)	1 (0%)	86	81
1	B	305/308 (99%)	301 (99%)	4 (1%)	61	39
1	C	294/308 (96%)	288 (98%)	6 (2%)	48	23
1	D	302/308 (98%)	299 (99%)	3 (1%)	68	52
All	All	1208/1232 (98%)	1194 (99%)	14 (1%)	63	43

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	846	GLU
1	B	580	ASP
1	B	593	VAL
1	B	793	LYS
1	B	897	LYS
1	C	591	GLN
1	C	679	ASN
1	C	756	ARG
1	C	775	ARG
1	C	846	GLU

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Mol	Chain	Res	Type
1	C	893	GLU
1	D	599	ASN
1	D	676	GLU
1	D	752	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	859	GLN
1	A	894	HIS
1	B	791	ASN
1	C	591	GLN
1	C	624	GLN
1	C	631	ASN
1	C	679	ASN
1	C	781	GLN
1	C	875	GLN
1	C	894	HIS
1	D	875	GLN
1	D	894	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	EOY	A	1001	-	44,45,45	0.89	0	66,69,69	1.48	10 (15%)
2	EOY	B	1001	-	44,45,45	1.06	2 (4%)	66,69,69	1.40	6 (9%)
2	EOY	D	1001	-	44,45,45	0.95	0	66,69,69	1.34	8 (12%)
2	EOY	C	1001	-	44,45,45	0.99	2 (4%)	66,69,69	1.29	5 (7%)

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	EOY	A	1001	-	-	5/18/45/45	0/8/7/7
2	EOY	B	1001	-	-	3/18/45/45	0/8/7/7
2	EOY	D	1001	-	-	5/18/45/45	0/8/7/7
2	EOY	C	1001	-	-	4/18/45/45	0/8/7/7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	EOY	C17-C16	-2.78	1.43	1.47
2	C	1001	EOY	C17-C16	-2.31	1.44	1.47
2	C	1001	EOY	C30-N29	-2.09	1.44	1.47
2	B	1001	EOY	C30-N29	-2.05	1.44	1.47

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	EOY	C25-O24-C19	-6.36	103.86	117.85
2	C	1001	EOY	C30-N29-C11	-5.36	114.93	125.89
2	A	1001	EOY	C25-O24-C19	-5.27	106.25	117.85
2	B	1001	EOY	C30-N29-C11	-4.69	116.31	125.89
2	C	1001	EOY	C25-O24-C19	-4.59	107.75	117.85
2	A	1001	EOY	N10-C16-N15	-4.00	107.57	109.94
2	D	1001	EOY	C25-O24-C19	-3.89	109.29	117.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	EOY	C5-C11-N29	-3.84	109.83	116.87
2	A	1001	EOY	C9-N10-C16	3.59	106.44	104.78
2	D	1001	EOY	N10-C16-N15	-3.58	107.82	109.94
2	D	1001	EOY	C6-C5-C4	3.57	123.37	119.25
2	D	1001	EOY	C9-N10-C16	3.46	106.38	104.78
2	B	1001	EOY	C22-C17-C16	-3.43	119.29	122.37
2	D	1001	EOY	C5-C11-N29	-3.34	110.75	116.87
2	A	1001	EOY	C6-C5-C4	3.25	123.01	119.25
2	C	1001	EOY	C6-C5-C4	3.17	122.91	119.25
2	A	1001	EOY	C1-C6-C5	-3.11	117.48	120.80
2	B	1001	EOY	C12-C8-N7	3.05	122.65	119.62
2	D	1001	EOY	O13-C11-N29	2.88	128.26	122.59
2	D	1001	EOY	C30-N29-C11	-2.65	120.47	125.89
2	A	1001	EOY	O13-C11-N29	2.64	127.79	122.59
2	D	1001	EOY	C17-C16-N10	2.57	131.53	126.62
2	A	1001	EOY	C17-C16-N10	2.49	131.39	126.62
2	B	1001	EOY	C6-C5-C4	2.36	121.98	119.25
2	A	1001	EOY	C2-C3-N10	2.25	117.96	116.28
2	A	1001	EOY	C30-N29-C11	-2.17	121.45	125.89
2	B	1001	EOY	C1-C6-C5	-2.14	118.51	120.80
2	C	1001	EOY	C22-C17-C16	-2.08	120.50	122.37
2	C	1001	EOY	C17-C16-N15	-2.03	120.53	124.62

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	EOY	C39-C30-N29-C11
2	A	1001	EOY	C31-C30-N29-C11
2	A	1001	EOY	C37-C30-N29-C11
2	B	1001	EOY	C39-C30-N29-C11
2	B	1001	EOY	C31-C30-N29-C11
2	B	1001	EOY	C37-C30-N29-C11
2	C	1001	EOY	C39-C30-N29-C11
2	C	1001	EOY	C31-C30-N29-C11
2	C	1001	EOY	C37-C30-N29-C11
2	D	1001	EOY	C39-C30-N29-C11
2	D	1001	EOY	C31-C30-N29-C11
2	D	1001	EOY	C37-C30-N29-C11
2	A	1001	EOY	C20-C19-O24-C25
2	D	1001	EOY	C20-C19-O24-C25
2	A	1001	EOY	C18-C19-O24-C25

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Mol	Chain	Res	Type	Atoms
2	D	1001	EOY	C18-C19-O24-C25
2	C	1001	EOY	N29-C11-C5-C4

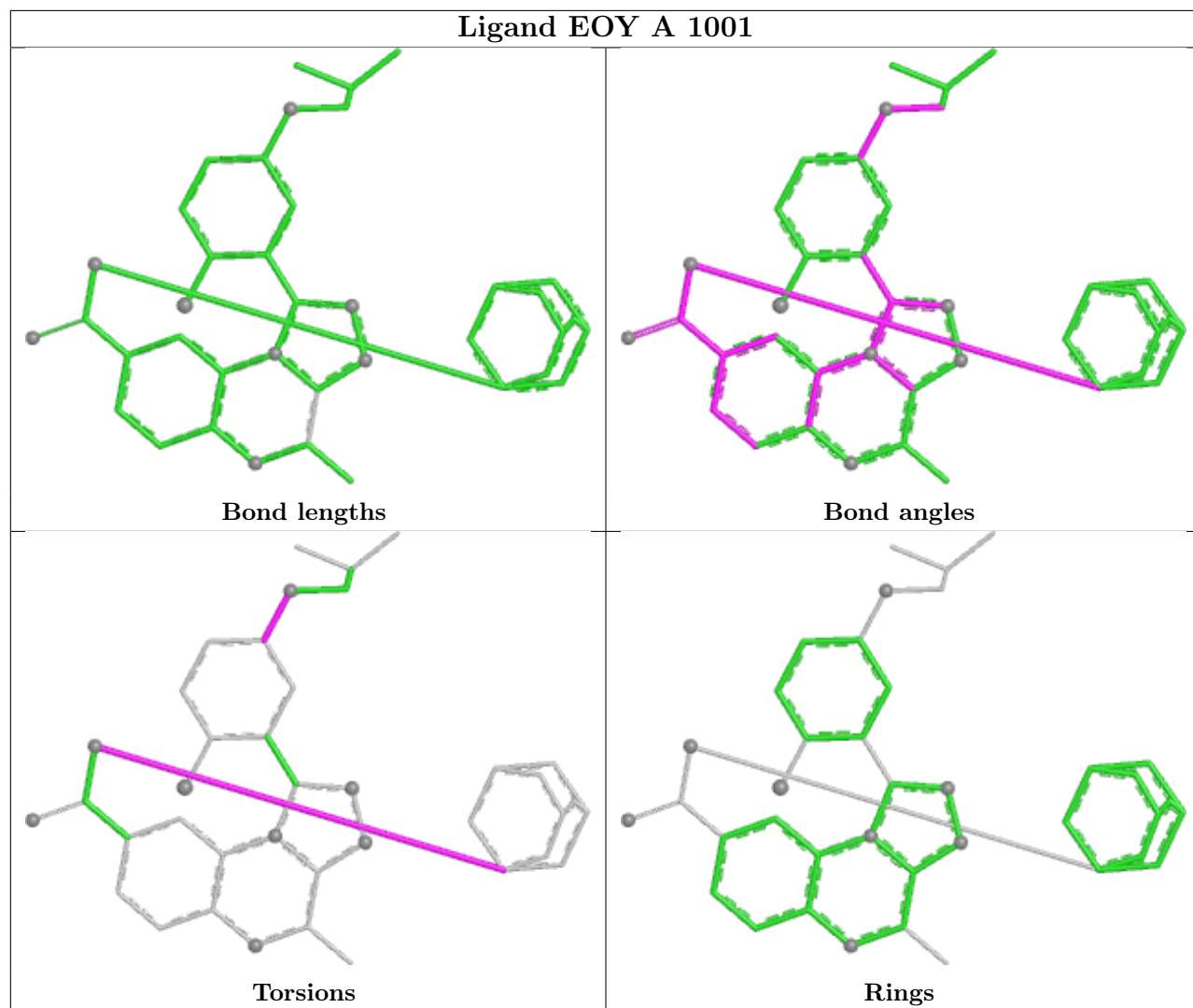
There are no ring outliers.

2 monomers are involved in 2 short contacts:

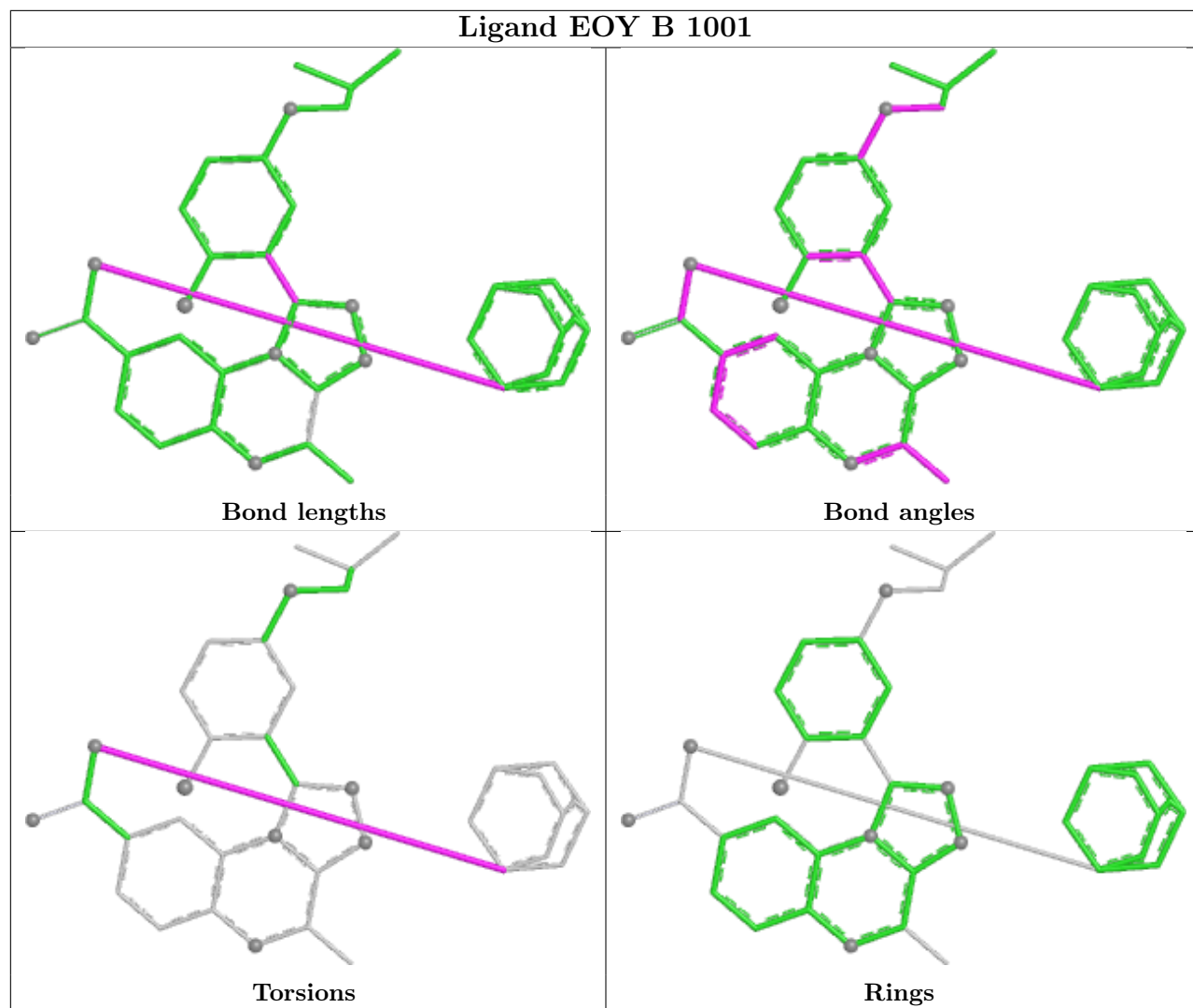
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	EOY	1	0
2	C	1001	EOY	1	0

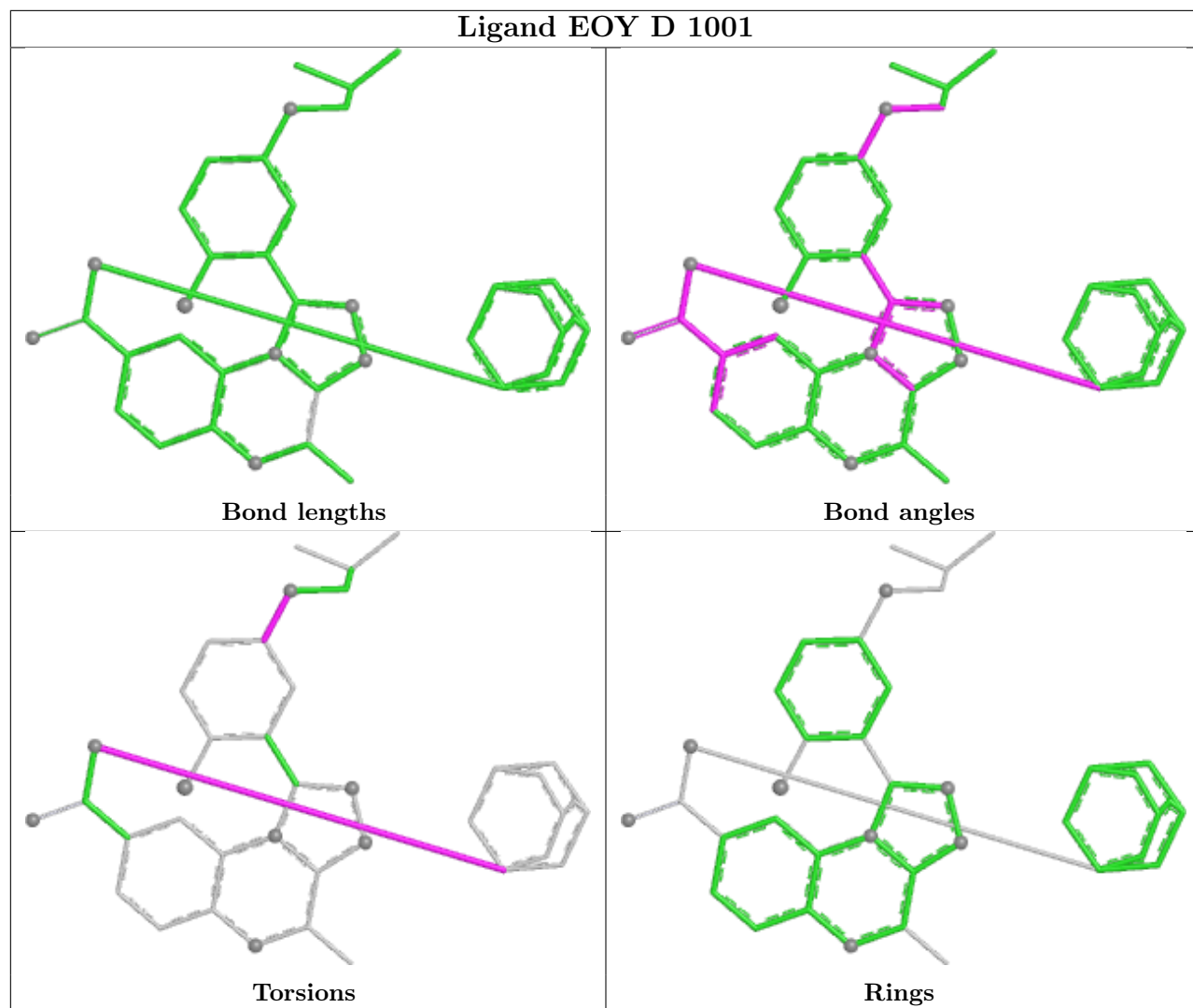
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

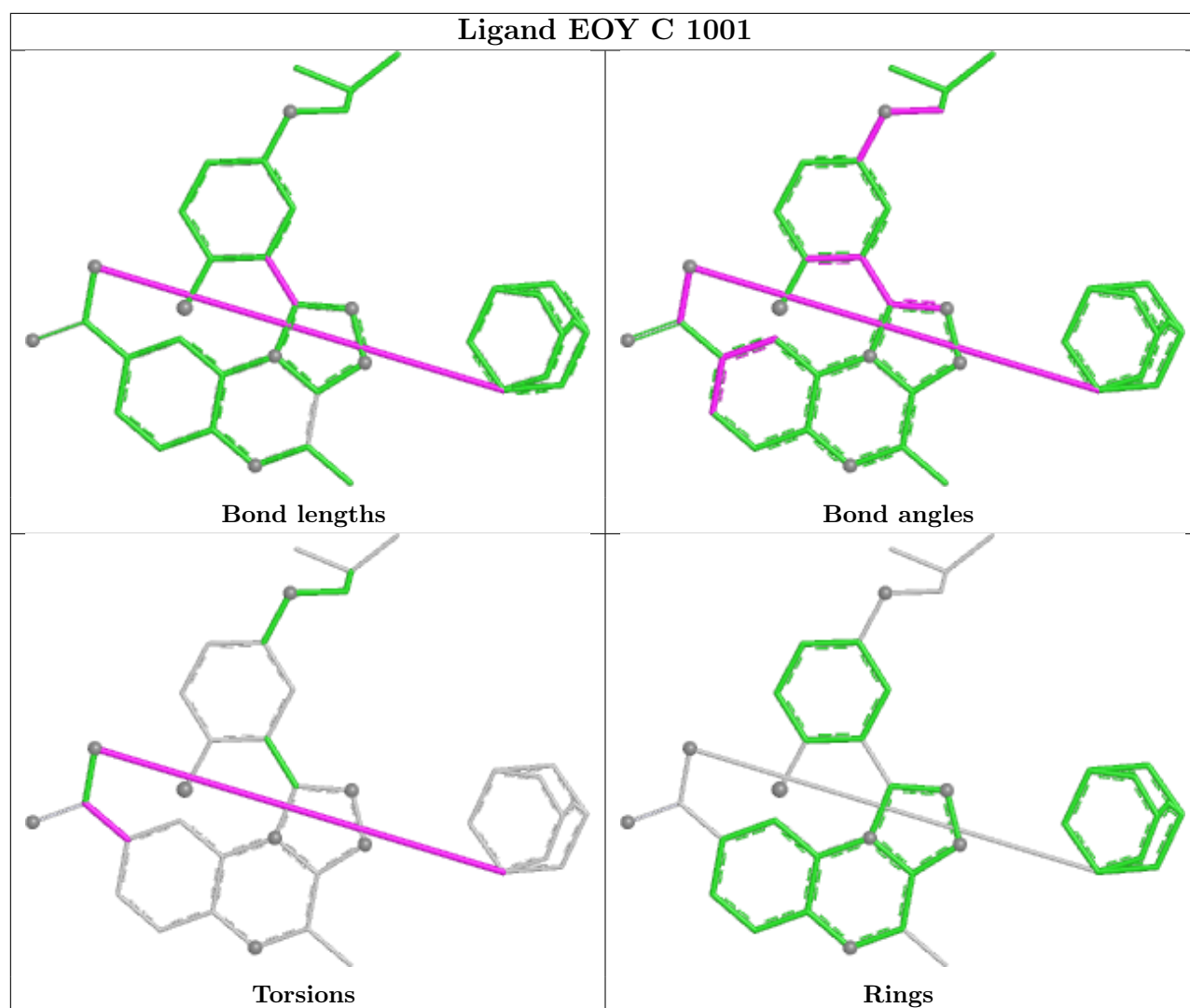
Ligand EOY A 1001



Ligand EOY B 1001







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	341/342 (99%)	0.53	20 (5%)	28 36	7, 19, 34, 44	0
1	B	338/342 (98%)	0.76	32 (9%)	14 16	7, 21, 38, 52	0
1	C	326/342 (95%)	1.18	61 (18%)	3 4	9, 27, 49, 59	0
1	D	335/342 (97%)	0.92	38 (11%)	10 12	9, 23, 40, 49	0
All	All	1340/1368 (97%)	0.84	151 (11%)	10 12	7, 22, 42, 59	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	680	TYR	5.6
1	C	594	ALA	5.3
1	C	593	VAL	5.1
1	C	595	ALA	5.1
1	B	915	PHE	5.0
1	B	579	ASP	5.0
1	D	583	THR	4.8
1	B	721	SER	4.8
1	C	786	VAL	4.8
1	C	791	ASN	4.4
1	D	632	TYR	4.2
1	D	911	ASN	4.0
1	B	748	HIS	3.9
1	D	586	LEU	3.9
1	B	630	ASN	3.9
1	D	916	LEU	3.9
1	C	784	ALA	3.9
1	B	741	HIS	3.8
1	C	596	ILE	3.8
1	C	591	GLN	3.7
1	D	591	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	676	GLU	3.6
1	C	640	ALA	3.6
1	D	915	PHE	3.6
1	C	793	LYS	3.6
1	B	910	ASN	3.5
1	C	675	LEU	3.5
1	B	634	ILE	3.5
1	C	592	PRO	3.5
1	C	878	PHE	3.4
1	B	636	CYS	3.4
1	C	636	CYS	3.4
1	A	576	SER	3.4
1	D	636	CYS	3.3
1	A	916	LEU	3.3
1	C	843	ARG	3.3
1	B	916	LEU	3.3
1	C	756	ARG	3.2
1	B	722	GLU	3.2
1	C	915	PHE	3.2
1	C	909	SER	3.2
1	C	628	PHE	3.1
1	C	751	ARG	3.1
1	C	633	LYS	3.1
1	C	916	LEU	3.0
1	D	774	LEU	3.0
1	B	909	SER	3.0
1	C	631	ASN	3.0
1	C	785	GLU	3.0
1	C	679	ASN	3.0
1	C	777	PHE	2.9
1	C	797	ARG	2.9
1	A	911	ASN	2.9
1	D	582	TYR	2.9
1	D	585	LEU	2.9
1	D	909	SER	2.8
1	C	634	ILE	2.8
1	D	590	ILE	2.8
1	B	631	ASN	2.8
1	C	877	LEU	2.8
1	C	790	ARG	2.8
1	D	589	GLY	2.8
1	C	632	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	579	ASP	2.8
1	C	630	ASN	2.7
1	D	722	GLU	2.7
1	B	723	GLY	2.7
1	B	582	TYR	2.7
1	D	599	ASN	2.7
1	D	912	SER	2.6
1	C	678	THR	2.6
1	D	629	ILE	2.6
1	C	873	LEU	2.6
1	D	843	ARG	2.6
1	B	580	ASP	2.6
1	A	593	VAL	2.6
1	D	680	TYR	2.6
1	D	595	ALA	2.6
1	B	897	LYS	2.6
1	A	599	ASN	2.6
1	B	913	LEU	2.6
1	C	629	ILE	2.6
1	C	842	ASN	2.6
1	C	775	ARG	2.6
1	C	677	LEU	2.5
1	B	590	ILE	2.5
1	D	594	ALA	2.5
1	D	741	HIS	2.5
1	C	598	SER	2.5
1	D	617	MET	2.5
1	C	682	GLU	2.5
1	B	586	LEU	2.5
1	B	907	LEU	2.5
1	C	620	LEU	2.5
1	D	675	LEU	2.5
1	B	843	ARG	2.4
1	C	637	PRO	2.4
1	A	636	CYS	2.4
1	C	627	ASN	2.4
1	C	903	THR	2.4
1	A	680	TYR	2.4
1	D	611	PRO	2.4
1	D	816	TRP	2.4
1	B	652	ASP	2.4
1	B	589	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	907	LEU	2.3
1	B	914	ASP	2.3
1	C	683	ASP	2.3
1	C	896	THR	2.3
1	A	892	ARG	2.3
1	D	587	HIS	2.2
1	B	911	ASN	2.2
1	C	798	LEU	2.2
1	C	684	ILE	2.2
1	B	908	PRO	2.2
1	C	844	PRO	2.2
1	B	710	ALA	2.2
1	C	782	LYS	2.2
1	A	907	LEU	2.2
1	B	786	VAL	2.2
1	D	890	SER	2.2
1	A	594	ALA	2.2
1	C	617	MET	2.2
1	C	816	TRP	2.2
1	C	770	LEU	2.2
1	D	841	GLY	2.2
1	D	628	PHE	2.2
1	D	633	LYS	2.2
1	D	592	PRO	2.2
1	D	714	VAL	2.1
1	A	842	ASN	2.1
1	D	910	ASN	2.1
1	A	597	ASP	2.1
1	A	909	SER	2.1
1	C	600	PHE	2.1
1	D	588	ASP	2.1
1	C	722	GLU	2.1
1	A	904	ILE	2.1
1	C	910	ASN	2.1
1	B	912	SER	2.1
1	C	789	ASP	2.1
1	A	843	ARG	2.1
1	D	892	ARG	2.1
1	B	629	ILE	2.1
1	B	845	MET	2.1
1	C	893	GLU	2.1
1	A	741	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	786	VAL	2.0
1	A	751	ARG	2.0
1	A	577	ALA	2.0
1	C	880	LYS	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](#)

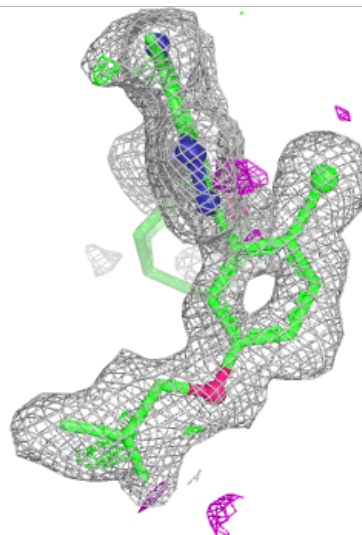
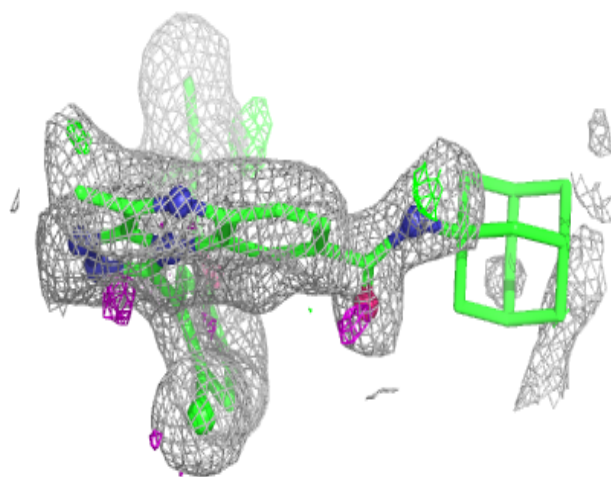
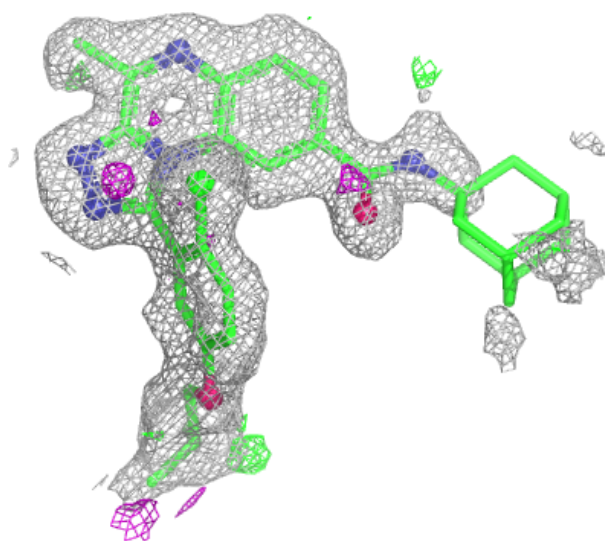
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	EOY	B	1001	39/39	0.90	0.12	11,20,34,34	9
2	EOY	A	1001	39/39	0.91	0.12	10,19,32,34	9
2	EOY	C	1001	39/39	0.92	0.12	13,22,35,37	9
2	EOY	D	1001	39/39	0.92	0.11	11,21,32,36	9
4	MG	D	1003	1/1	0.97	0.03	8,8,8,8	0
3	ZN	D	1002	1/1	0.99	0.03	13,13,13,13	0
4	MG	A	1003	1/1	0.99	0.02	7,7,7,7	0
4	MG	B	1003	1/1	0.99	0.02	6,6,6,6	0
4	MG	C	1003	1/1	0.99	0.02	9,9,9,9	0
3	ZN	A	1002	1/1	0.99	0.02	10,10,10,10	0
3	ZN	C	1002	1/1	1.00	0.02	12,12,12,12	0
3	ZN	B	1002	1/1	1.00	0.01	11,11,11,11	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.

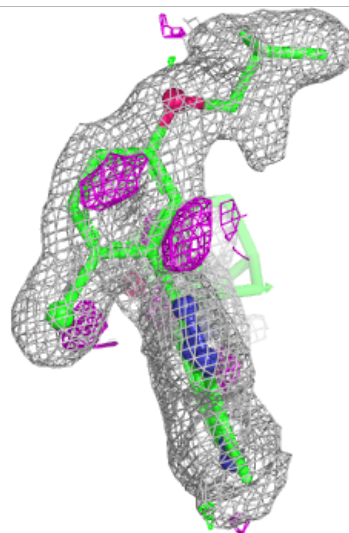
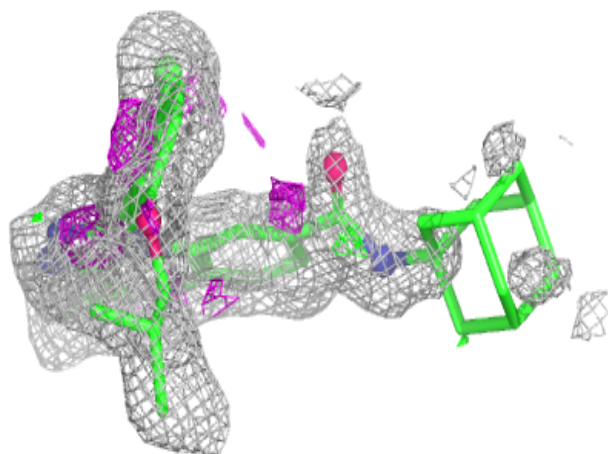
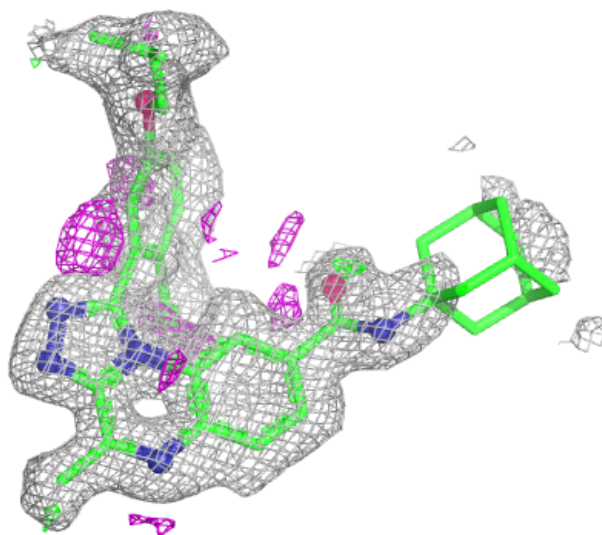
Electron density around EOY B 1001:

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



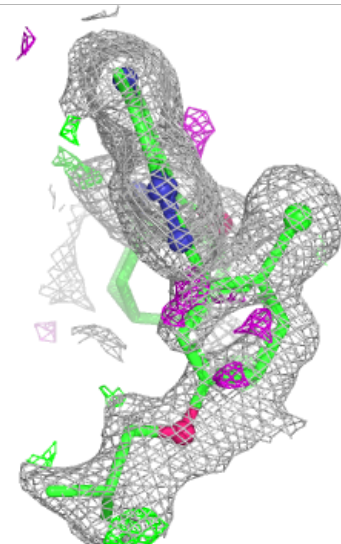
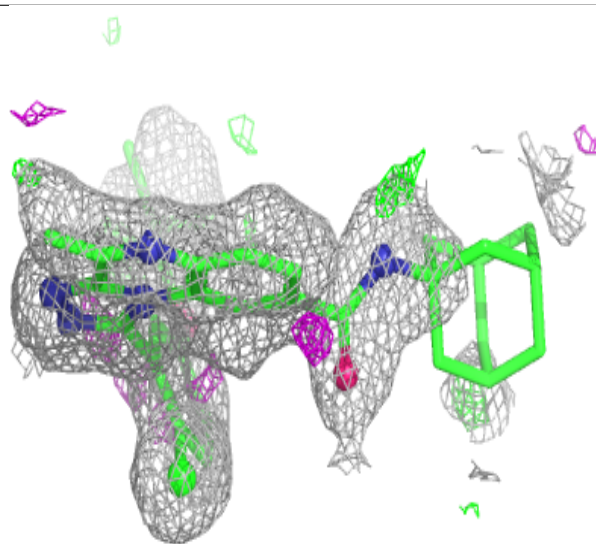
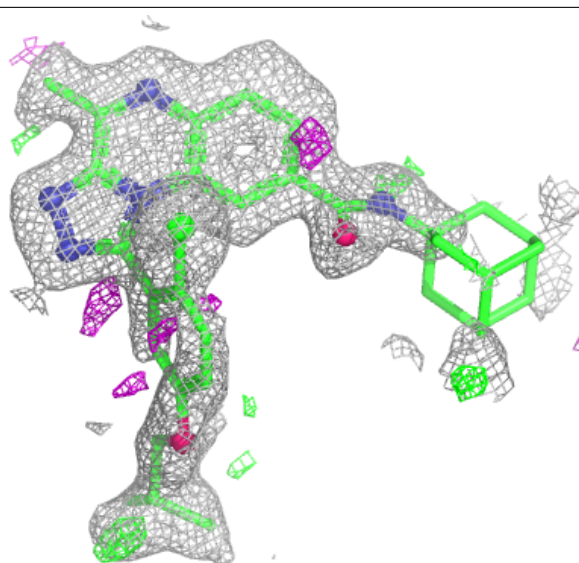
Electron density around EOY A 1001:

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



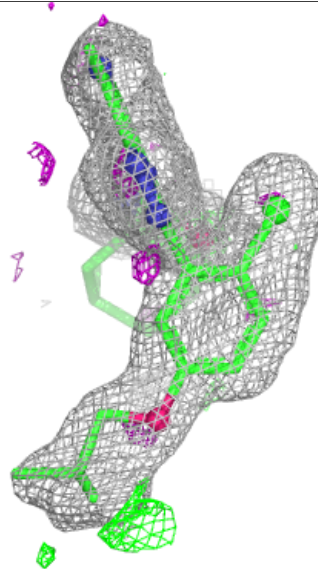
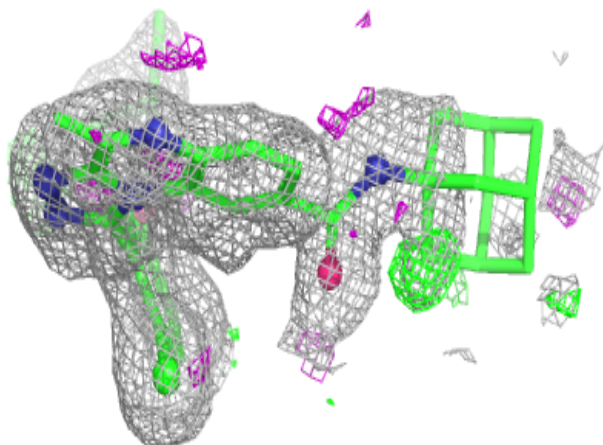
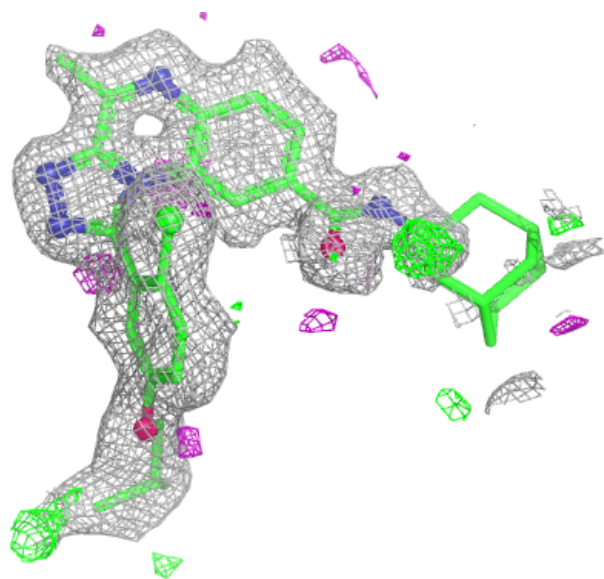
Electron density around EOY C 1001:

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



Electron density around EOY D 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.