



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:45 PM UTC

PDB ID : 9H4T / pdb_00009h4t
Title : Crystal Structure of TorA
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Deposited on : 2024-10-21
Resolution : 1.86 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

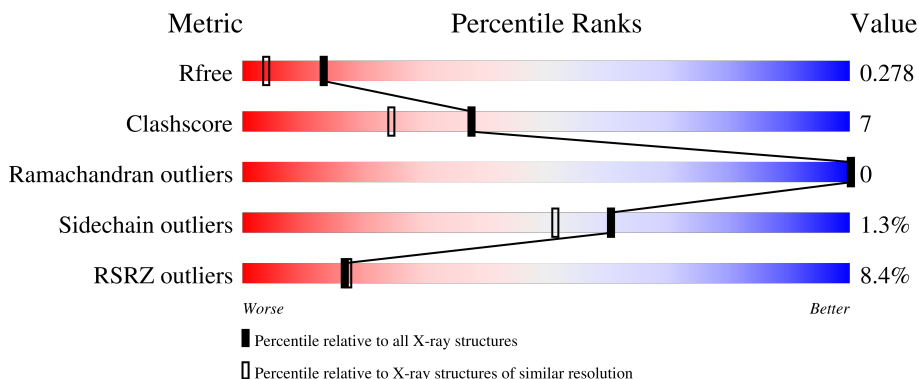
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	848	4% 82% 10% 7%
1	B	848	11% 80% 13% 6%

2 Entry composition [i](#)

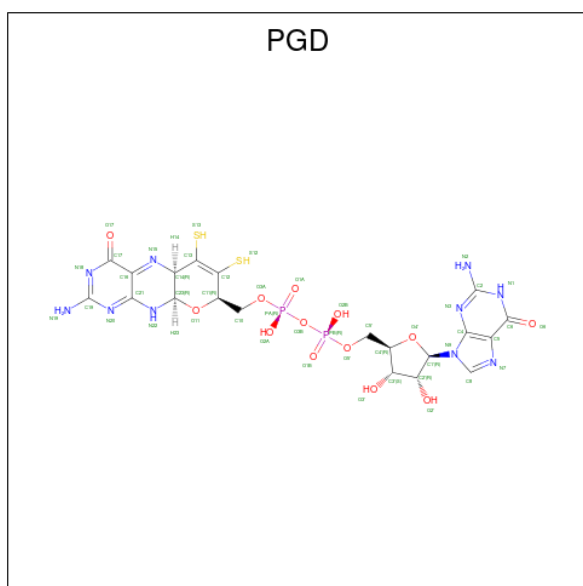
There are 8 unique types of molecules in this entry. The entry contains 14495 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Trimethylamine-N-oxide reductase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	790	Total	C	N	O	S	0	2	0
			6243	3958	1109	1150	26			
1	B	795	Total	C	N	O	S	0	2	0
			6284	3982	1115	1160	27			

- Molecule 2 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: PGD) (formula: $C_{20}H_{24}N_{10}O_{13}P_2S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	0
			47	20	10	13	2 2		
2	A	1	Total	C	N	O	P S	0	0
			47	20	10	13	2 2		
2	B	1	Total	C	N	O	P S	0	0
			47	20	10	13	2 2		

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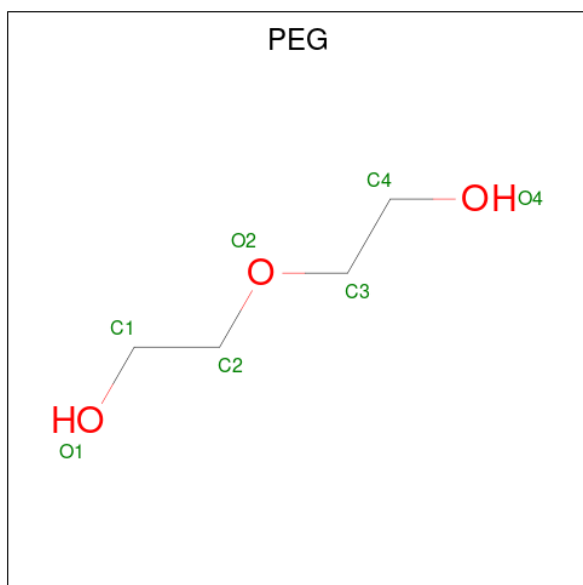
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	S	
			47	20	10	13	2	2	
									0
									0

- Molecule 3 is MOLYBDENUM(VI) ION (CCD ID: 6MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

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

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



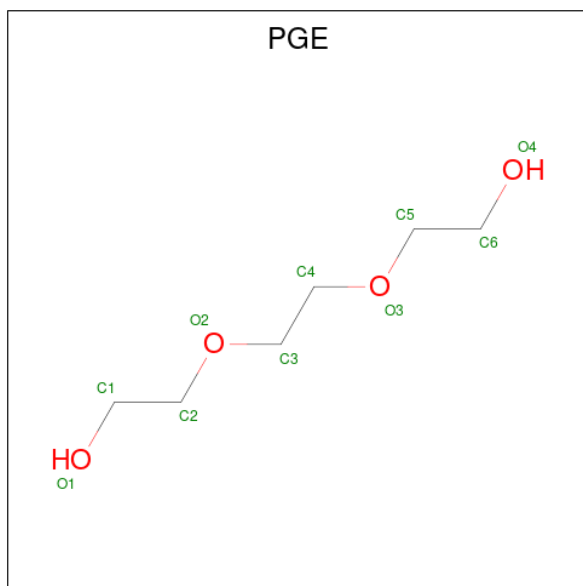
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



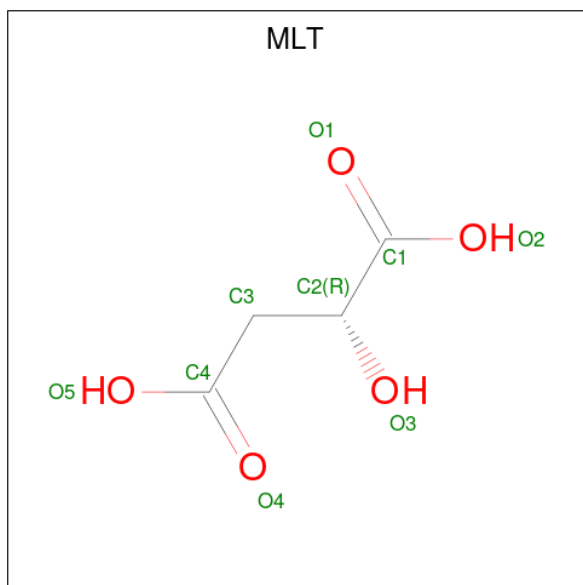
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	A	1	Total	C	O	0	0
			10	6	4		

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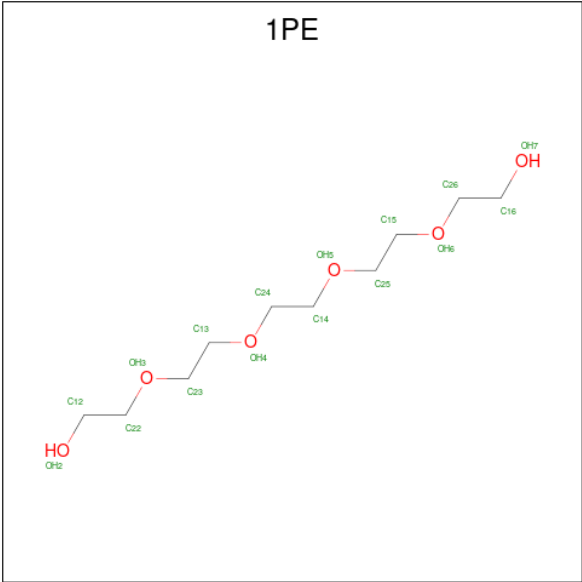
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is D-MALATE (CCD ID: MLT) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	4	5		
6	A	1	Total	C	O	0	0
			9	4	5		
6	A	1	Total	C	O	0	0
			9	4	5		
6	A	1	Total	C	O	0	0
			9	4	5		
6	B	1	Total	C	O	0	0
			9	4	5		
6	B	1	Total	C	O	0	0
			9	4	5		
6	B	1	Total	C	O	0	0
			9	4	5		

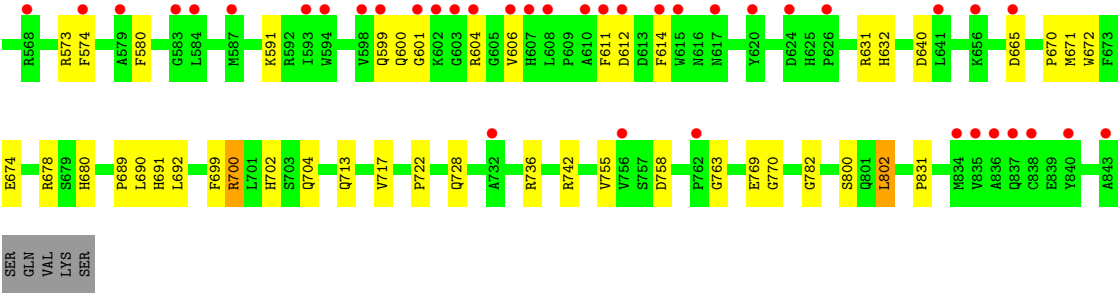
- Molecule 7 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	849	Total	O	0	0
			849	849		
8	B	695	Total	O	0	0
			695	695		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.66Å 117.47Å 100.05Å 90.00° 103.25° 90.00°	Depositor
Resolution (Å)	47.79 – 1.86 47.79 – 1.86	Depositor EDS
% Data completeness (in resolution range)	90.8 (47.79-1.86) 90.9 (47.79-1.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.87Å)	Xtriage
Refinement program	REFMAC v1.0	Depositor
R, R_{free}	0.235 , 0.289 (Not available) , 0.278	Depositor DCC
R_{free} test set	2101 reflections (1.32%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14495	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.64 % 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 6.7289e-03.*

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: MLT, PGE, PGD, 1PE, 6MO, PEG

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	0.54	0/6414	0.86	3/8709 (0.0%)
1	B	0.54	0/6457	0.87	7/8771 (0.1%)
All	All	0.54	0/12871	0.86	10/17480 (0.1%)

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	A	0	7
1	B	0	9
All	All	0	16

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	ASP	CA-CB-CG	7.46	120.06	112.60
1	B	511	ASP	CA-CB-CG	7.31	119.91	112.60
1	A	71	PHE	CA-CB-CG	6.24	120.04	113.80
1	B	123	ASP	CB-CA-C	-5.98	100.51	110.68
1	B	71	PHE	CA-CB-CG	5.87	119.67	113.80

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	111	ARG	Sidechain
1	A	573	ARG	Sidechain
1	A	604	ARG	Sidechain
1	A	631	ARG	Sidechain

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	6243	0	6067	87	0
1	B	6284	0	6096	87	0
2	A	94	0	40	0	0
2	B	94	0	40	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	84	0	120	4	0
4	B	21	0	30	0	0
5	A	30	0	42	2	0
5	B	20	0	28	1	0
6	A	36	0	16	5	0
6	B	27	0	12	2	0
7	B	16	0	22	0	0
8	A	849	0	0	33	0
8	B	695	0	0	30	0
All	All	14495	0	12513	178	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 7.

The worst 5 of 178 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ARG:HD3	8:A:1016:HOH:O	1.62	0.99
1:B:758:ASP:O	8:B:1001:HOH:O	1.82	0.96
1:B:167:HIS:CD2	1:B:533:ARG:HD3	2.00	0.95
1:B:690:LEU:HD23	8:B:1002:HOH:O	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LYS:NZ	8:A:1002:HOH:O	2.04	0.90

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	790/848 (93%)	765 (97%)	25 (3%)	0	100	100
1	B	795/848 (94%)	769 (97%)	26 (3%)	0	100	100
All	All	1585/1696 (94%)	1534 (97%)	51 (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	655/698 (94%)	650 (99%)	5 (1%)	73	67
1	B	660/698 (95%)	648 (98%)	12 (2%)	51	40
All	All	1315/1396 (94%)	1298 (99%)	17 (1%)	61	51

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	713	GLN
1	B	802	LEU
1	B	334	LYS
1	B	378	MET
1	B	382	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	713	GLN
1	B	728	GLN
1	B	829	ASN
1	B	96	ASN
1	A	809	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 34 ligands modelled in this entry, 2 are monoatomic - leaving 32 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
6	MLT	A	916	-	8,8,8	1.11	0	10,10,10	1.33	2 (20%)
4	PEG	B	904	-	6,6,6	0.15	0	5,5,5	0.14	0
4	PEG	A	906	-	6,6,6	0.14	0	5,5,5	0.08	0
5	PGE	A	912	-	9,9,9	0.19	0	8,8,8	0.16	0
7	1PE	B	906	-	15,15,15	0.20	0	14,14,14	0.10	0
4	PEG	A	920	-	6,6,6	0.14	0	5,5,5	0.11	0
2	PGD	A	902	3	46,52,52	1.18	5 (10%)	56,81,81	0.86	2 (3%)
4	PEG	A	908	-	6,6,6	0.14	0	5,5,5	0.08	0
4	PEG	A	917	-	6,6,6	0.15	0	5,5,5	0.08	0
4	PEG	A	904	-	6,6,6	0.19	0	5,5,5	0.12	0
5	PGE	A	910	-	9,9,9	0.15	0	8,8,8	0.17	0
4	PEG	A	909	-	6,6,6	0.13	0	5,5,5	0.08	0
4	PEG	B	911	-	6,6,6	0.13	0	5,5,5	0.10	0
6	MLT	B	908	-	8,8,8	1.16	0	10,10,10	1.46	2 (20%)
6	MLT	B	910	-	8,8,8	1.11	0	10,10,10	1.34	2 (20%)
5	PGE	B	907	-	9,9,9	0.17	0	8,8,8	0.13	0
5	PGE	A	911	-	9,9,9	0.16	0	8,8,8	0.14	0
4	PEG	A	919	-	6,6,6	0.14	0	5,5,5	0.08	0
4	PEG	A	907	-	6,6,6	0.14	0	5,5,5	0.06	0
4	PEG	A	922	-	6,6,6	0.21	0	5,5,5	0.12	0
6	MLT	A	914	-	8,8,8	1.06	0	10,10,10	1.39	2 (20%)
2	PGD	A	901	3	46,52,52	1.19	2 (4%)	56,81,81	0.80	2 (3%)
6	MLT	B	909	-	8,8,8	1.16	0	10,10,10	1.22	2 (20%)
2	PGD	B	902	3	46,52,52	1.21	3 (6%)	56,81,81	0.90	2 (3%)
4	PEG	A	918	-	6,6,6	0.13	0	5,5,5	0.07	0
4	PEG	A	905	-	6,6,6	0.13	0	5,5,5	0.08	0
6	MLT	A	915	-	8,8,8	1.14	0	10,10,10	1.40	2 (20%)
5	PGE	B	905	-	9,9,9	0.21	0	8,8,8	0.09	0
4	PEG	A	921	-	6,6,6	0.13	0	5,5,5	0.09	0
2	PGD	B	901	3	46,52,52	1.13	2 (4%)	56,81,81	0.76	1 (1%)
4	PEG	B	912	-	6,6,6	0.20	0	5,5,5	0.10	0
6	MLT	A	913	-	8,8,8	1.08	0	10,10,10	1.32	2 (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
6	MLT	A	916	-	-	4/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	B	904	-	-	1/4/4/4	-
4	PEG	A	906	-	-	2/4/4/4	-
5	PGE	A	912	-	-	3/7/7/7	-
7	1PE	B	906	-	-	9/13/13/13	-
4	PEG	A	920	-	-	2/4/4/4	-
2	PGD	A	902	3	-	3/22/82/82	0/6/6/6
4	PEG	A	908	-	-	0/4/4/4	-
4	PEG	A	917	-	-	2/4/4/4	-
4	PEG	A	904	-	-	2/4/4/4	-
5	PGE	A	910	-	-	2/7/7/7	-
4	PEG	A	909	-	-	1/4/4/4	-
4	PEG	B	911	-	-	2/4/4/4	-
6	MLT	B	908	-	-	1/8/8/8	-
6	MLT	B	910	-	-	4/8/8/8	-
5	PGE	B	907	-	-	4/7/7/7	-
5	PGE	A	911	-	-	4/7/7/7	-
4	PEG	A	919	-	-	2/4/4/4	-
4	PEG	A	907	-	-	2/4/4/4	-
4	PEG	A	922	-	-	4/4/4/4	-
6	MLT	A	914	-	-	3/8/8/8	-
2	PGD	A	901	3	-	5/22/82/82	0/6/6/6
6	MLT	B	909	-	-	6/8/8/8	-
2	PGD	B	902	3	-	3/22/82/82	0/6/6/6
4	PEG	A	918	-	-	2/4/4/4	-
4	PEG	A	905	-	-	2/4/4/4	-
6	MLT	A	915	-	-	4/8/8/8	-
5	PGE	B	905	-	-	4/7/7/7	-
4	PEG	A	921	-	-	1/4/4/4	-
2	PGD	B	901	3	-	10/22/82/82	0/6/6/6
4	PEG	B	912	-	-	1/4/4/4	-
6	MLT	A	913	-	-	0/8/8/8	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	902	PGD	C16-N15	5.71	1.33	1.28
2	A	901	PGD	C16-N15	5.29	1.33	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	PGD	C16-N15	4.48	1.32	1.28
2	B	901	PGD	C16-N15	4.47	1.32	1.28
2	B	901	PGD	C17-C16	-3.42	1.37	1.47

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	914	MLT	O1-C1-C2	-3.01	116.58	122.60
6	A	913	MLT	O1-C1-C2	-2.77	117.06	122.60
6	A	915	MLT	O1-C1-C2	-2.77	117.07	122.60
6	B	908	MLT	O2-C1-C2	2.69	118.44	112.74
6	B	910	MLT	O1-C1-C2	-2.69	117.23	122.60

There are no chirality outliers.

5 of 95 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	PGD	C5'-O5'-PB-O1B
2	A	901	PGD	C5'-O5'-PB-O2B
2	A	901	PGD	C5'-O5'-PB-O3B
2	A	902	PGD	PA-O3B-PB-O5'
2	A	902	PGD	O3A-C10-C11-O11

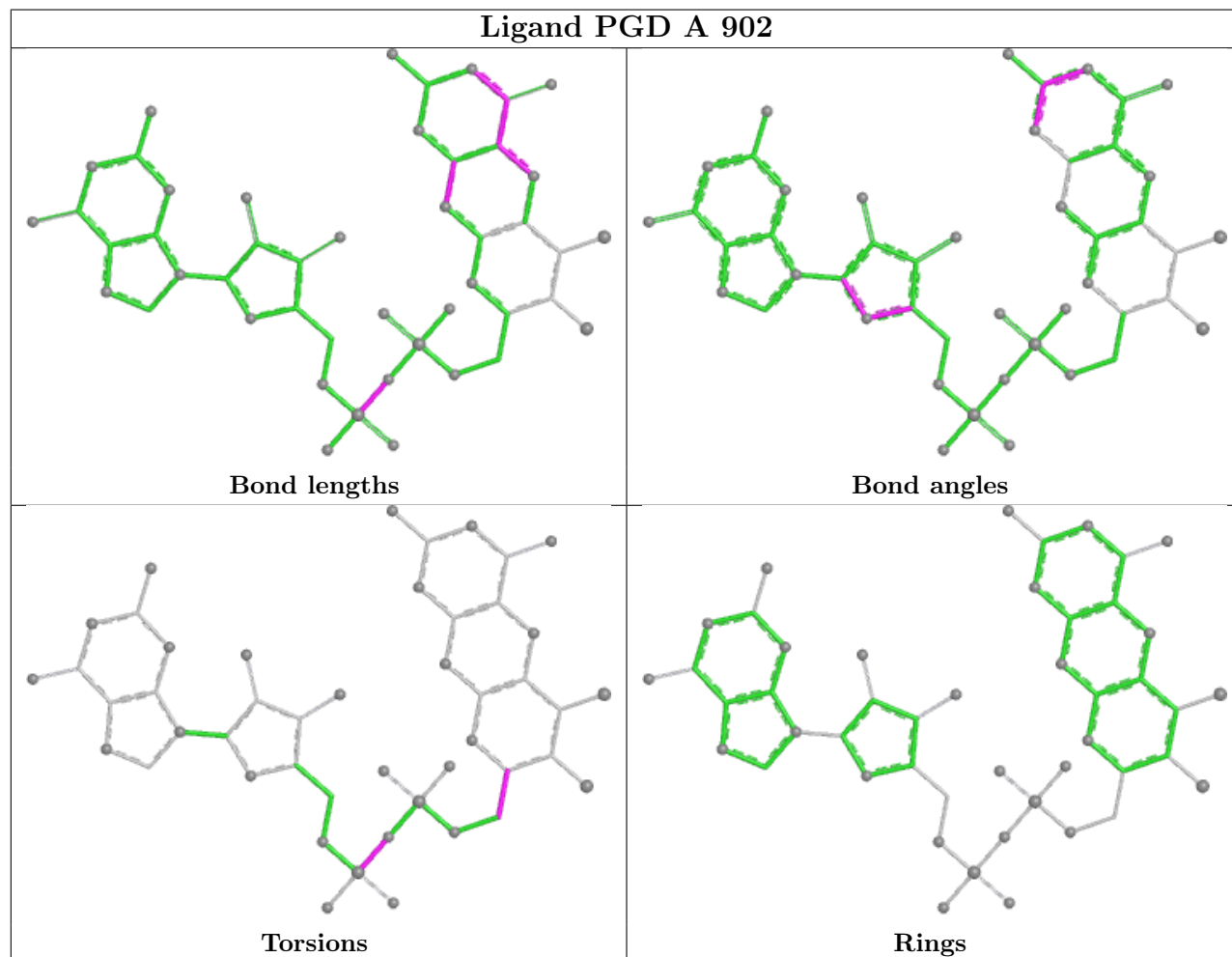
There are no ring outliers.

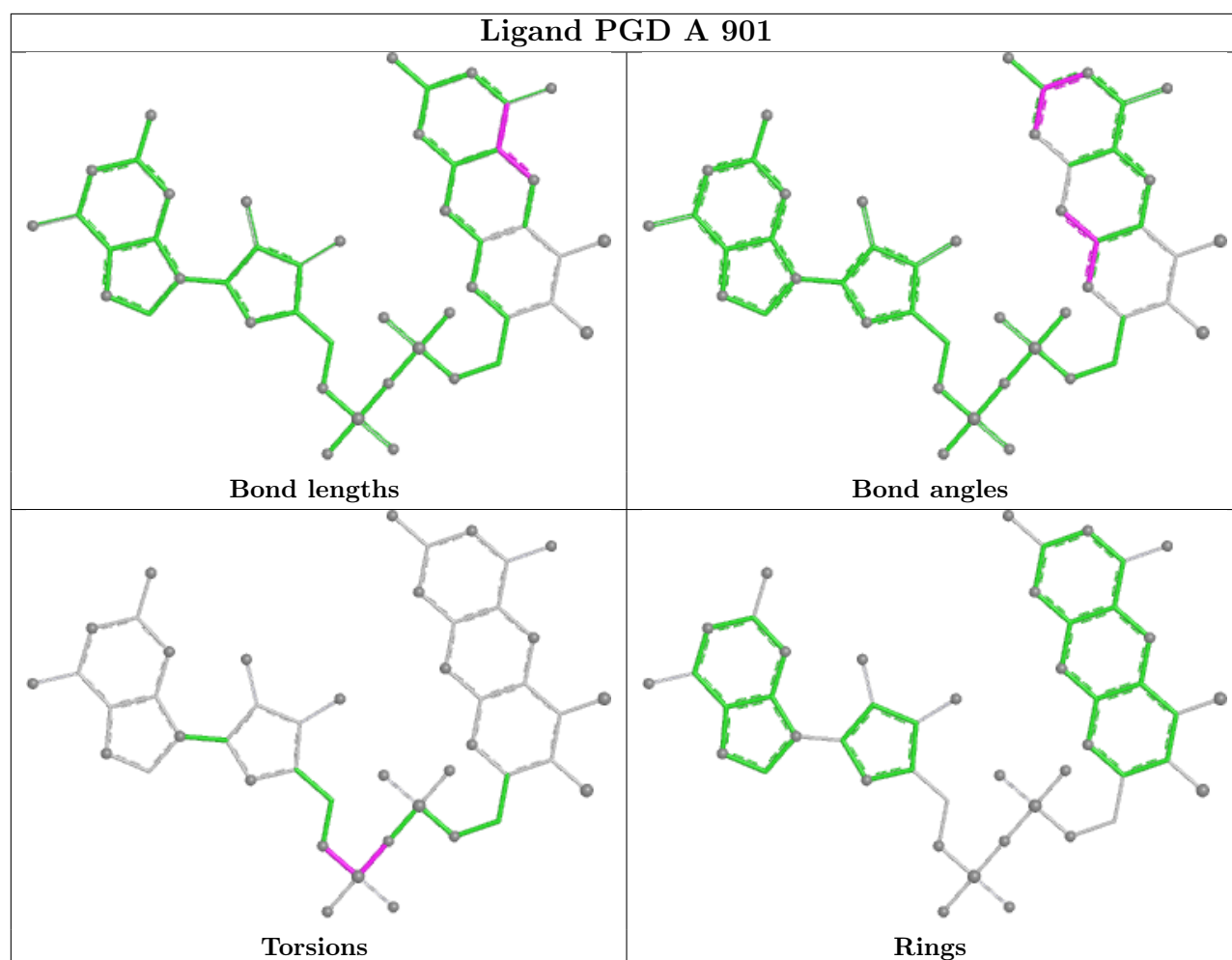
11 monomers are involved in 15 short contacts:

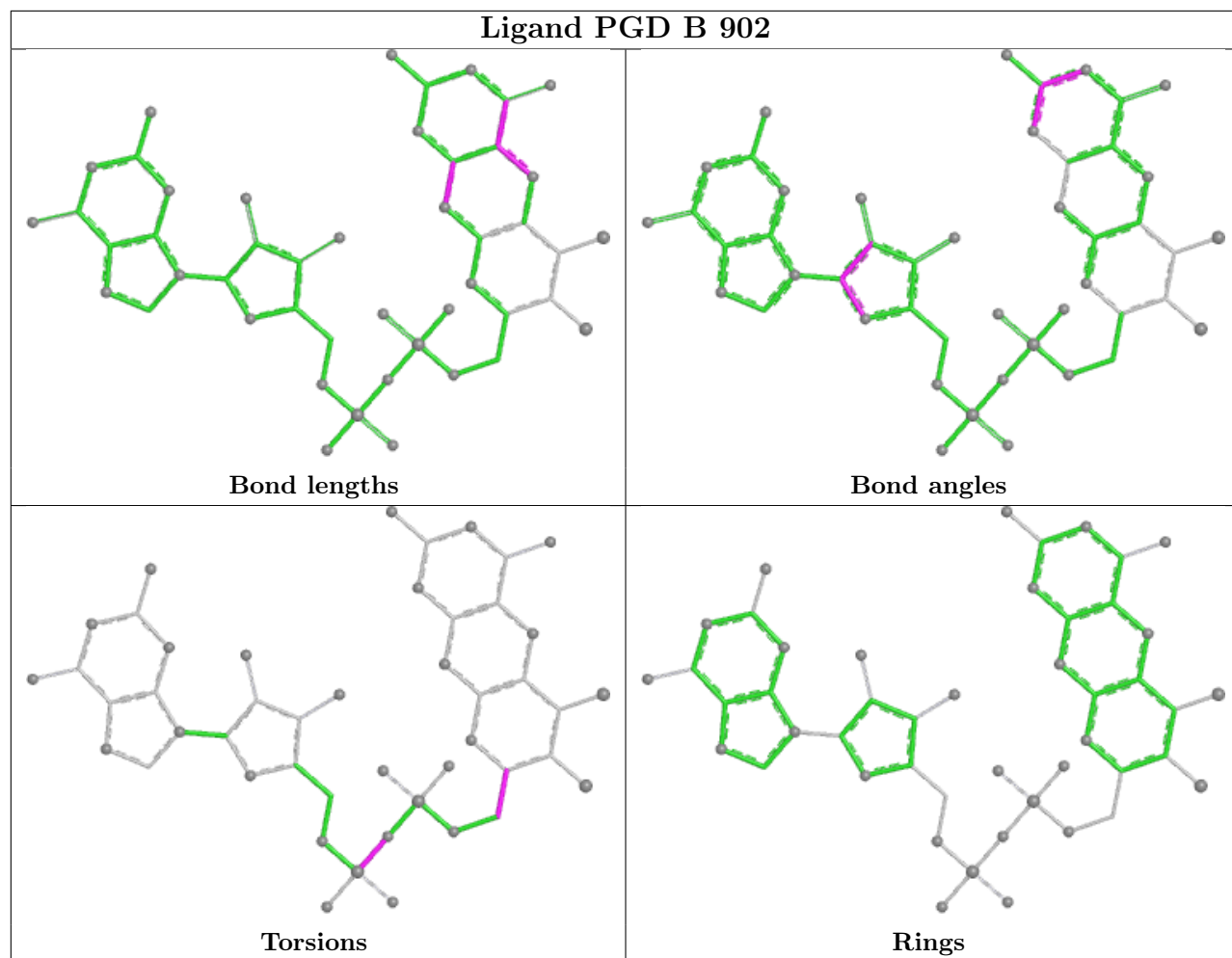
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	906	PEG	2	0
5	A	912	PGE	1	0
4	A	908	PEG	1	0
5	A	910	PGE	1	0
6	B	908	MLT	2	0
4	A	922	PEG	1	0
6	A	914	MLT	3	0
6	A	915	MLT	1	0
5	B	905	PGE	1	0
2	B	901	PGD	2	0
6	A	913	MLT	1	0

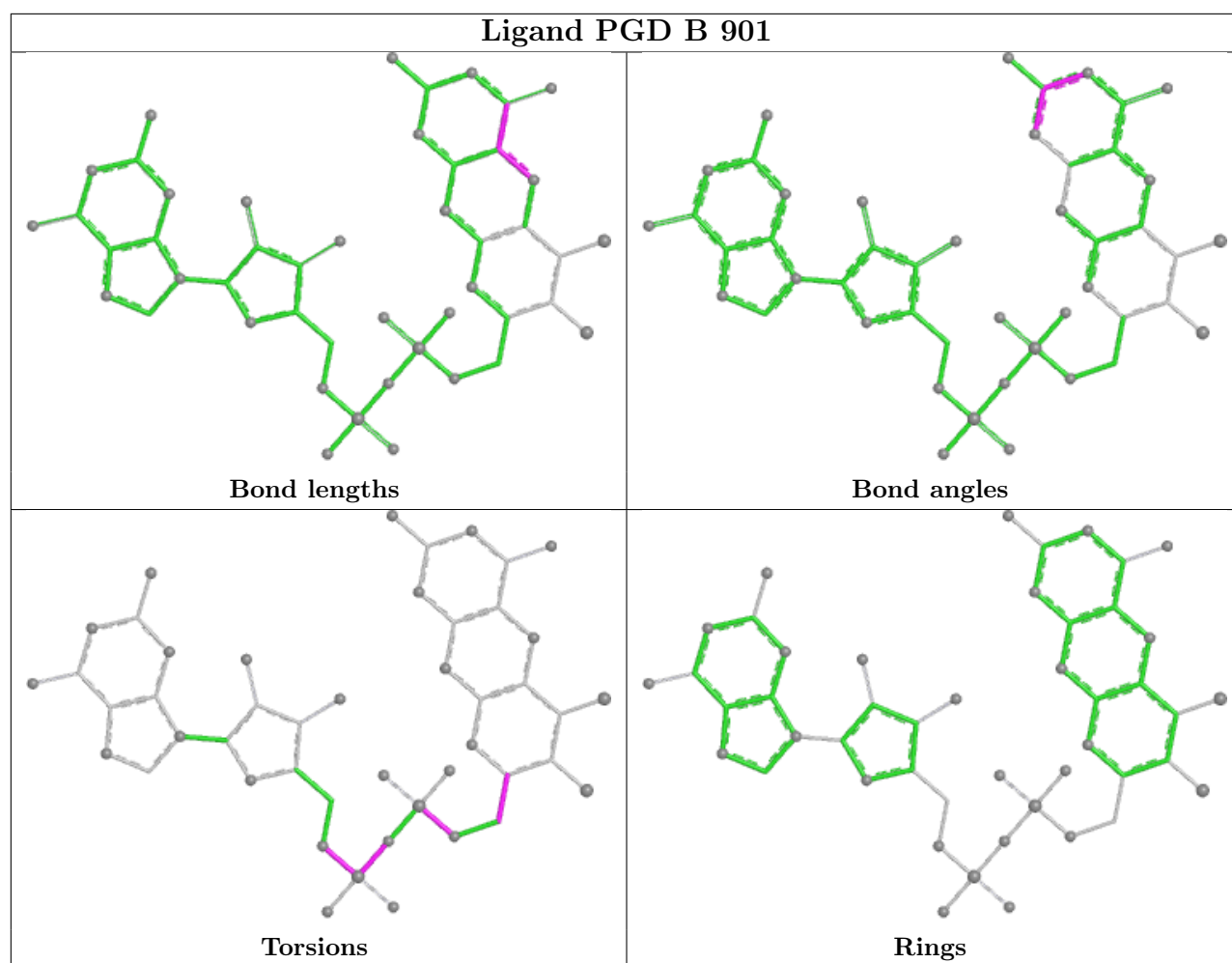
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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 [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	790/848 (93%)	0.64	38 (4%) 35 39	13, 24, 38, 71	2 (0%)
1	B	795/848 (93%)	0.92	95 (11%) 9 8	14, 26, 48, 70	2 (0%)
All	All	1585/1696 (93%)	0.78	133 (8%) 17 17	13, 25, 45, 71	4 (0%)

The worst 5 of 133 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	838	CYS	5.5
1	B	430	SER	4.6
1	B	641	LEU	4.5
1	B	836	ALA	4.3
1	B	429	GLY	4.3

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](#)

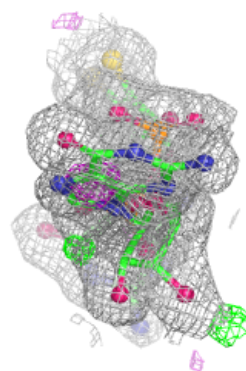
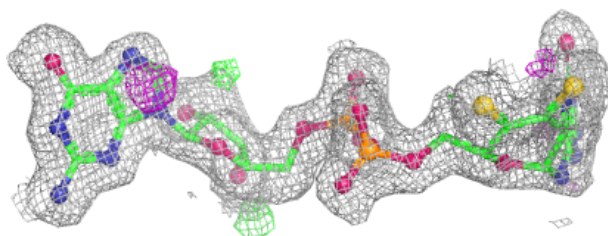
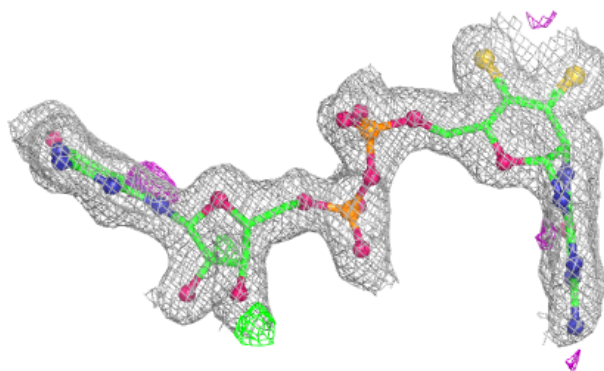
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
5	PGE	B	907	10/10	0.64	0.28	44,51,69,73	0
4	PEG	B	904	7/7	0.67	0.19	37,44,47,56	0
5	PGE	A	912	10/10	0.68	0.19	37,45,61,67	0
4	PEG	A	904	7/7	0.68	0.23	32,60,71,75	0
4	PEG	A	906	7/7	0.71	0.17	44,52,64,65	0
4	PEG	A	909	7/7	0.74	0.26	30,51,84,84	0
6	MLT	A	915	9/9	0.74	0.18	33,51,74,77	0
4	PEG	B	911	7/7	0.75	0.19	46,50,56,60	0
4	PEG	A	920	7/7	0.76	0.17	37,44,53,54	0
4	PEG	A	905	7/7	0.76	0.19	44,53,66,67	0
5	PGE	A	911	10/10	0.77	0.20	42,55,62,70	0
4	PEG	A	922	7/7	0.77	0.19	32,36,59,74	0
7	1PE	B	906	16/16	0.77	0.21	46,58,71,83	0
4	PEG	A	917	7/7	0.78	0.16	45,49,74,75	0
6	MLT	B	909	9/9	0.80	0.14	37,47,53,56	0
6	MLT	A	916	9/9	0.80	0.18	43,58,69,85	0
4	PEG	A	921	7/7	0.81	0.16	29,37,52,56	0
6	MLT	A	914	9/9	0.81	0.20	22,47,66,83	0
6	MLT	B	910	9/9	0.81	0.15	58,66,78,90	0
4	PEG	B	912	7/7	0.81	0.18	35,44,46,53	0
4	PEG	A	908	7/7	0.82	0.16	35,40,59,62	0
5	PGE	B	905	10/10	0.83	0.15	26,42,48,50	0
4	PEG	A	918	7/7	0.83	0.17	37,40,51,66	0
5	PGE	A	910	10/10	0.84	0.18	33,42,61,67	0
4	PEG	A	907	7/7	0.85	0.17	38,46,52,53	0
6	MLT	B	908	9/9	0.87	0.21	41,54,73,77	0
4	PEG	A	919	7/7	0.87	0.15	42,48,56,57	0
6	MLT	A	913	9/9	0.88	0.15	31,45,56,73	0
2	PGD	A	902	47/47	0.95	0.08	11,18,29,31	0
2	PGD	B	901	47/47	0.95	0.08	18,22,29,35	0
2	PGD	A	901	47/47	0.96	0.08	14,21,28,37	0
2	PGD	B	902	47/47	0.96	0.07	10,18,30,38	0
3	6MO	A	903	1/1	1.00	0.04	24,24,24,24	0
3	6MO	B	903	1/1	1.00	0.02	26,26,26,26	0

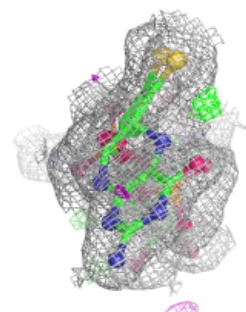
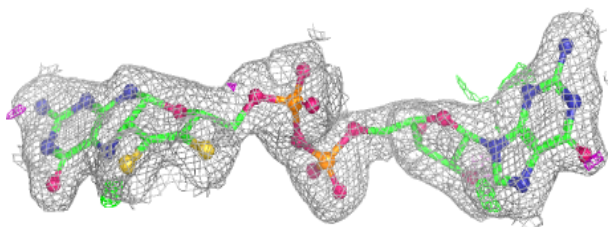
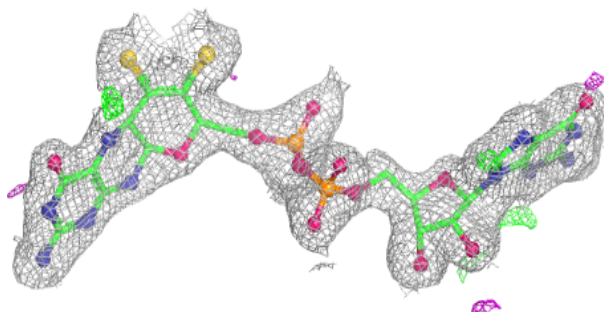
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PGD A 902:

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

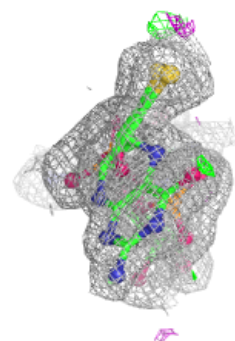
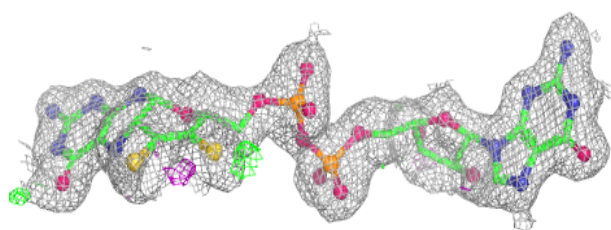
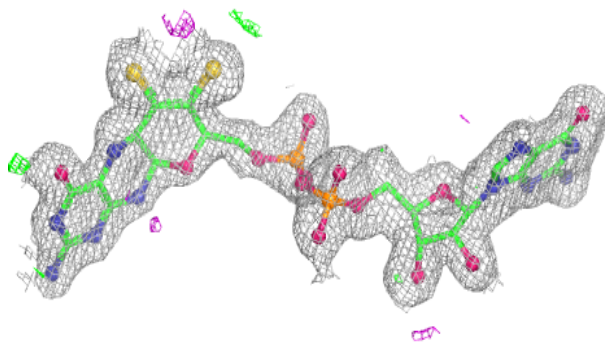
**Electron density around PGD B 901:**

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

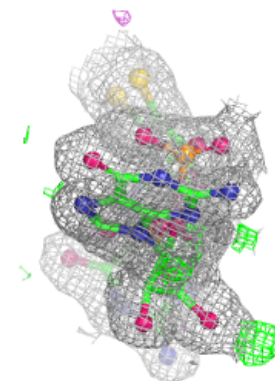
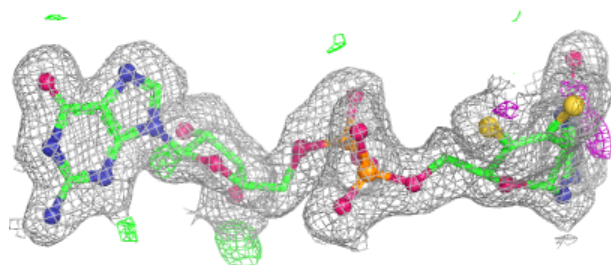
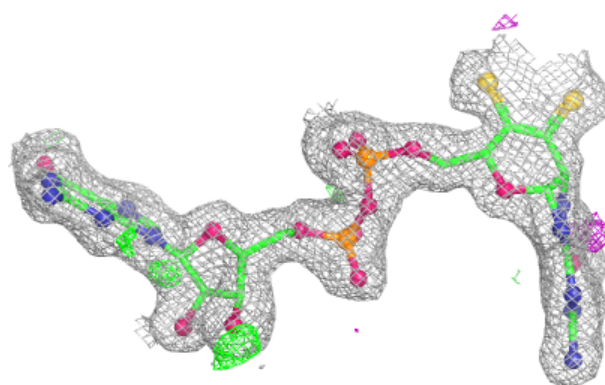


Electron density around PGD A 901:

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

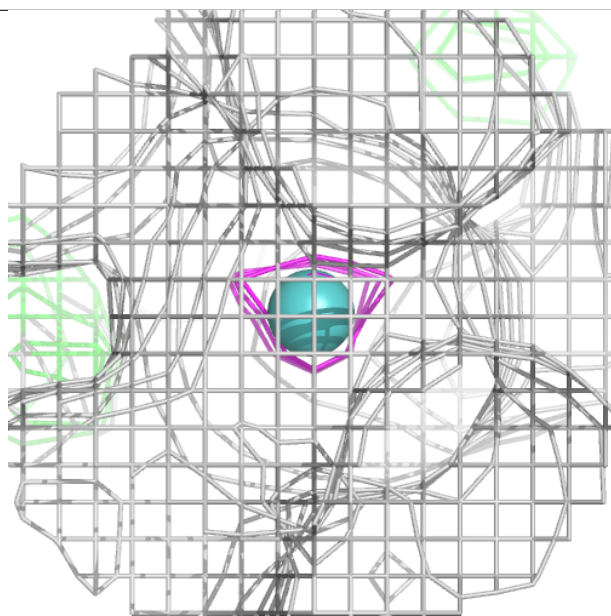
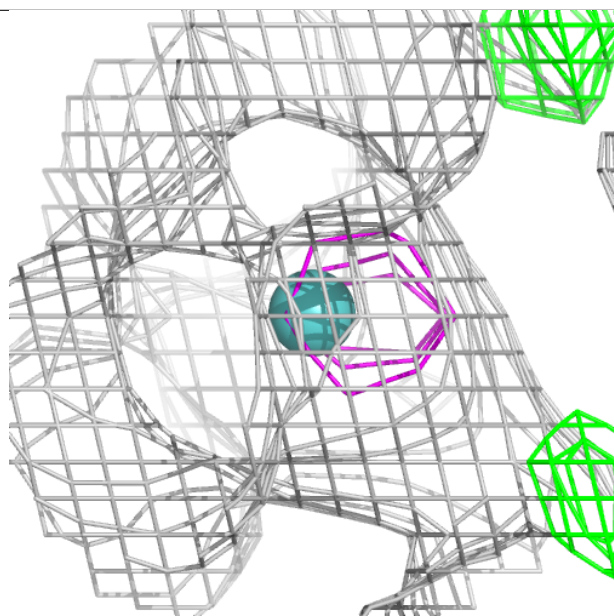
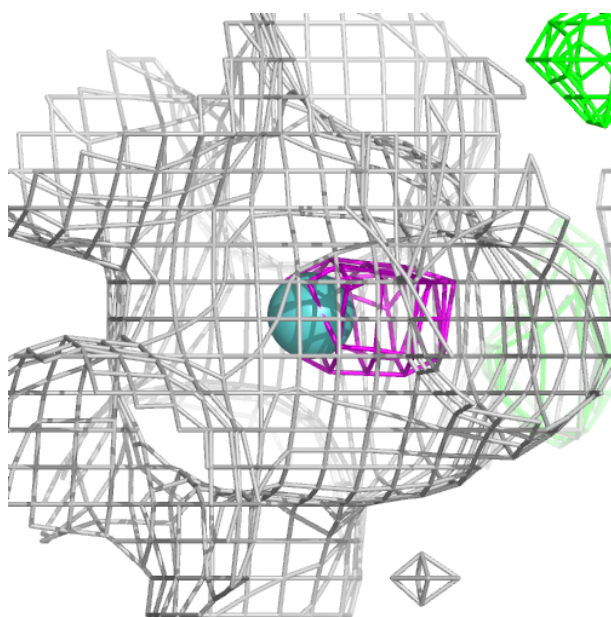
**Electron density around PGD B 902:**

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



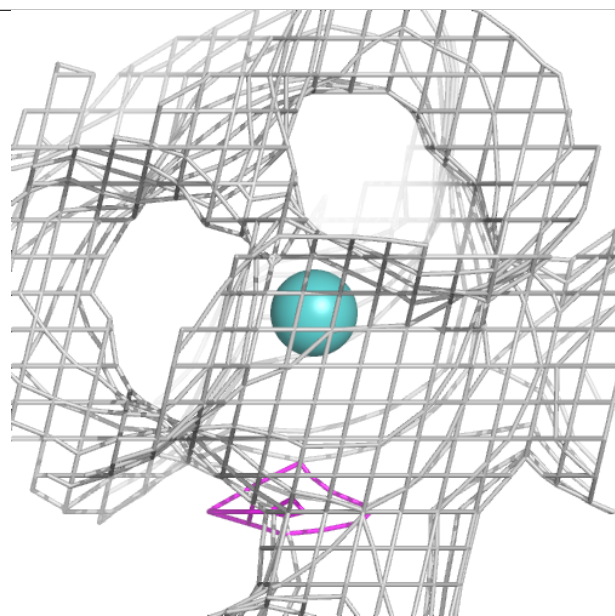
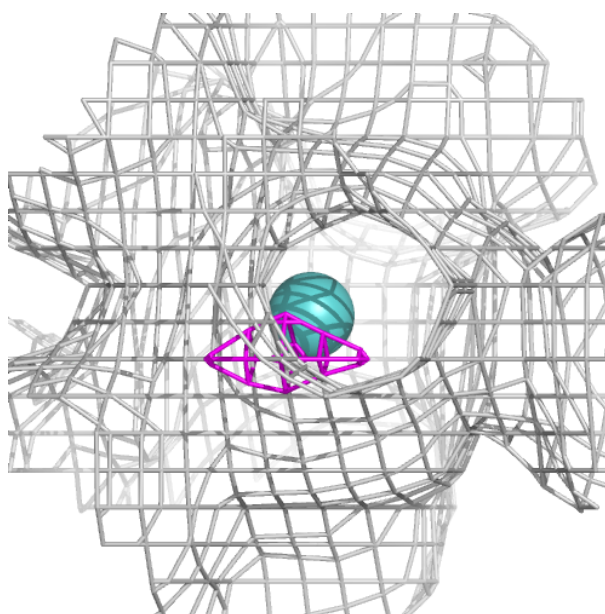
Electron density around 6MO A 903:

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



Electron density around 6MO B 903:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.