



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 07:47 pm BST

PDB ID : 2IHT
Title : Carboxyethylarginine synthase from *Streptomyces clavuligerus*: SeMet structure
Authors : Caines, M.E.; Schofield, C.J.
Deposited on : 2006-09-27
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

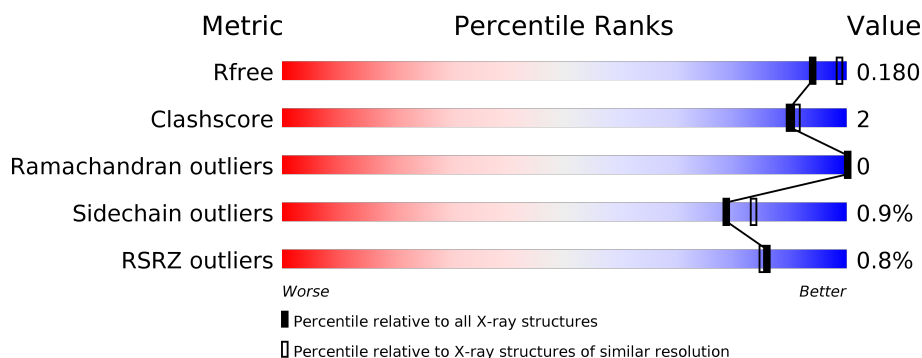
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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	573	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>5%</div> <div>• •</div> </div> </div>
1	B	573	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>5%</div> <div>• •</div> </div> </div>
1	C	573	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>5%</div> <div>•</div> </div> </div>
1	D	573	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>5%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18876 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 Carboxyethylarginine synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	560	Total	C	N	O	S	Se	38	2	0
			4217	2676	727	800	3	11			
1	B	561	Total	C	N	O	S	Se	26	2	0
			4226	2681	730	801	3	11			
1	C	559	Total	C	N	O	S	Se	39	5	0
			4228	2683	731	799	3	12			
1	D	559	Total	C	N	O	S	Se	53	4	0
			4226	2681	732	799	3	11			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
A	85	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
A	132	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
A	157	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
A	272	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
A	284	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
A	306	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
A	382	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
A	391	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
A	395	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
A	450	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
B	85	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
B	132	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
B	157	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
B	272	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
B	284	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
B	306	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
B	382	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
B	391	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
B	395	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	450	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
C	85	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
C	132	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
C	157	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
C	272	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
C	284	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
C	306	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
C	382	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
C	391	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
C	395	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
C	450	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
D	85	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
D	132	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
D	157	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
D	272	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
D	284	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
D	306	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
D	382	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
D	391	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
D	395	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9
D	450	MSE	MET	MODIFIED RESIDUE	UNP Q9LCV9

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

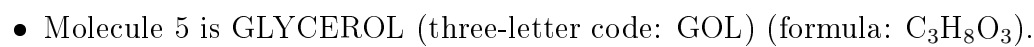
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

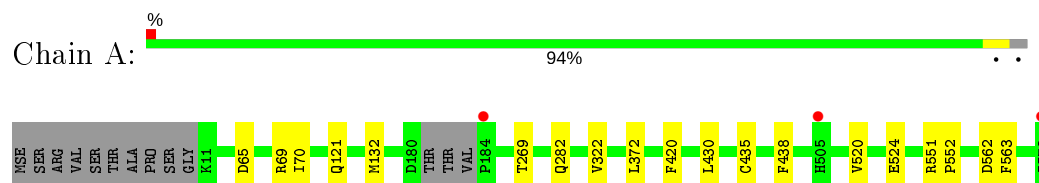
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	462	Total	O	0	0
			462	462		
6	B	502	Total	O	0	0
			502	502		
6	C	429	Total	O	0	0
			429	429		
6	D	414	Total	O	0	0
			414	414		

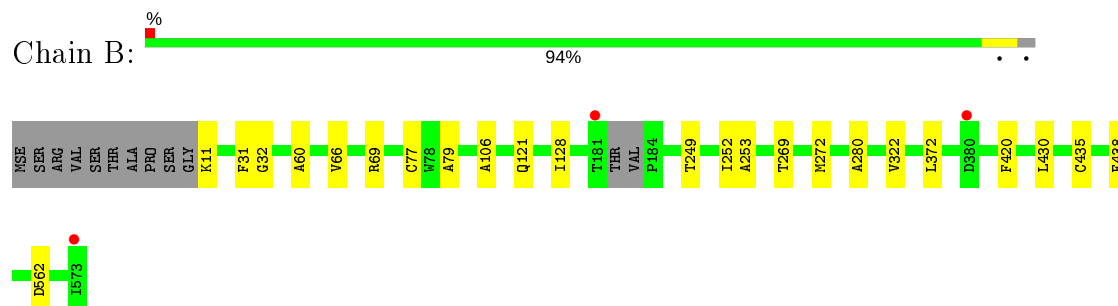
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

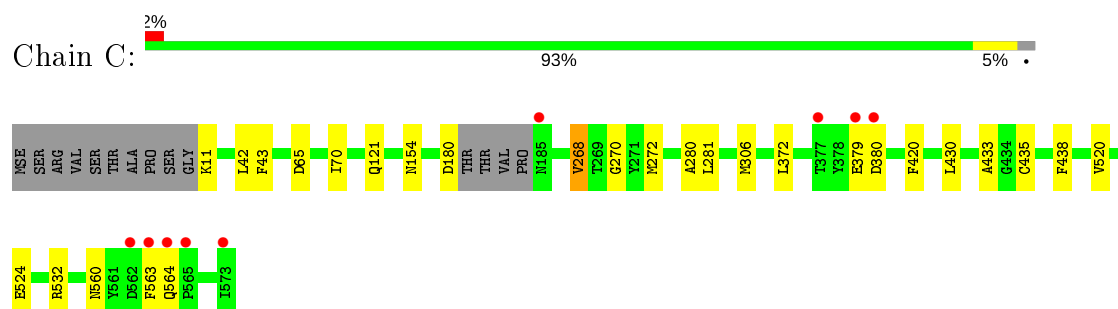
- Molecule 1: Carboxyethylarginine synthase



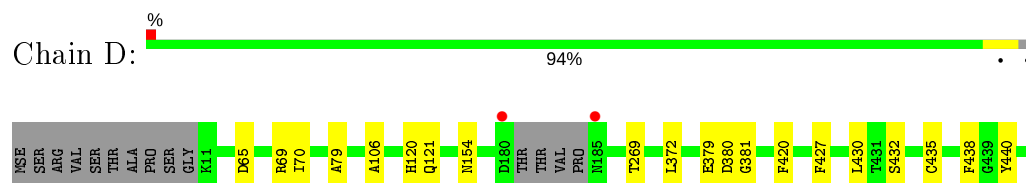
- Molecule 1: Carboxyethylarginine synthase



- Molecule 1: Carboxyethylarginine synthase



- Molecule 1: Carboxyethylarginine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.88Å 127.28Å 197.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.26 – 2.00 42.24 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.2 (42.26-2.00) 96.2 (42.24-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.65 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.154 , 0.178 0.156 , 0.180	Depositor DCC
R_{free} test set	9261 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.4	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	18876	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: GOL, MG, SO4, TPP

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	0.42	0/4308	0.53	1/5861 (0.0%)
1	B	0.43	1/4317 (0.0%)	0.54	2/5874 (0.0%)
1	C	0.46	2/4327 (0.0%)	0.56	4/5885 (0.1%)
1	D	0.46	1/4322 (0.0%)	0.54	1/5878 (0.0%)
All	All	0.44	4/17274 (0.0%)	0.55	8/23498 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	379	GLU	CB-CG	-11.83	1.29	1.52
1	C	379	GLU	CB-CG	9.92	1.71	1.52
1	C	180	ASP	CB-CG	6.20	1.64	1.51
1	B	11	LYS	CB-CG	6.14	1.69	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	180	ASP	CB-CG-OD1	9.45	126.80	118.30
1	C	180	ASP	CB-CG-OD2	-9.11	110.10	118.30
1	B	562	ASP	CB-CG-OD2	5.95	123.66	118.30
1	C	180	ASP	CA-CB-CG	-5.87	100.50	113.40
1	C	11	LYS	CA-CB-CG	-5.81	100.62	113.40
1	A	562	ASP	CB-CG-OD2	5.43	123.18	118.30
1	D	379	GLU	CA-CB-CG	5.21	124.86	113.40
1	B	11	LYS	CA-CB-CG	-5.03	102.33	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4217	0	4173	9	0
1	B	4226	0	4185	13	0
1	C	4228	0	4197	17	0
1	D	4226	0	4191	13	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	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
4	A	26	0	16	4	0
4	B	26	0	16	5	0
4	C	26	0	16	4	0
4	D	26	0	16	4	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
5	D	12	0	16	0	0
6	A	462	0	0	0	0
6	B	502	0	0	1	0
6	C	429	0	0	1	0
6	D	414	0	0	0	0
All	All	18876	0	16842	61	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 2.

All (61) 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)
4:B:600:TPP:C2	4:B:600:TPP:HN42	1.48	1.24
4:A:600:TPP:HN42	4:A:600:TPP:C2	1.48	1.24
4:C:600:TPP:HN42	4:C:600:TPP:C2	1.54	1.21
4:D:600:TPP:HN42	4:D:600:TPP:C2	1.53	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:600:TPP:HN42	4:D:600:TPP:H2	1.08	1.12
4:B:600:TPP:HN42	4:B:600:TPP:H2	1.04	1.10
4:A:600:TPP:H2	4:A:600:TPP:HN42	1.08	1.10
4:C:600:TPP:H2	4:C:600:TPP:HN42	1.09	1.08
4:B:600:TPP:C2	4:B:600:TPP:N4'	2.18	1.04
4:A:600:TPP:N4'	4:A:600:TPP:C2	2.20	1.03
4:D:600:TPP:C2	4:D:600:TPP:N4'	2.22	1.01
4:C:600:TPP:C2	4:C:600:TPP:N4'	2.23	0.99
1:C:281:LEU:HD21	1:C:306[B]:MSE:SE	2.23	0.89
4:B:600:TPP:H2	4:B:600:TPP:N4'	1.88	0.81
4:D:600:TPP:N4'	4:D:600:TPP:H2	1.92	0.81
1:C:281:LEU:CD2	1:C:306[B]:MSE:SE	2.84	0.75
4:C:600:TPP:H2	4:C:600:TPP:N4'	1.93	0.73
4:A:600:TPP:N4'	4:A:600:TPP:H2	1.92	0.71
1:D:381:GLY:H	1:D:560:ASN:HD22	1.41	0.69
1:C:272:MSE:HE2	1:C:280:ALA:HB1	1.81	0.61
1:D:70:ILE:HD11	1:D:430:LEU:HD11	1.84	0.60
1:C:372:LEU:HD21	1:C:420:PHE:HB3	1.85	0.58
1:A:551:ARG:HB2	1:A:552:PRO:HD2	1.86	0.58
1:A:372:LEU:HD21	1:A:420:PHE:HB3	1.87	0.57
1:D:380:ASP:HB2	1:D:560:ASN:ND2	2.19	0.56
1:D:427:PHE:HB3	1:D:430:LEU:HD21	1.87	0.56
1:A:70:ILE:HD11	1:A:430:LEU:HD11	1.89	0.54
1:C:268:VAL:HG12	1:C:272:MSE:SE	2.58	0.54
1:B:372:LEU:HD21	1:B:420:PHE:HB3	1.94	0.50
1:C:281:LEU:HD22	1:C:306[B]:MSE:SE	2.62	0.49
1:C:270:GLY:N	1:C:306[B]:MSE:HE1	2.29	0.48
1:C:435:CYS:O	1:D:121:GLN:HG2	2.13	0.47
1:A:435:CYS:O	1:B:121:GLN:HG2	2.15	0.47
1:D:381:GLY:H	1:D:560:ASN:ND2	2.10	0.47
1:C:520:VAL:O	1:C:524:GLU:HG3	2.15	0.46
1:A:520:VAL:O	1:A:524:GLU:HG3	2.15	0.46
1:C:121:GLN:HG2	1:D:435:CYS:O	2.16	0.45
1:C:380:ASP:HB2	1:C:560:ASN:ND2	2.31	0.45
1:A:121:GLN:HG2	1:B:435:CYS:O	2.17	0.45
1:B:252:ILE:HG12	6:B:1084:HOH:O	2.17	0.45
1:D:372:LEU:HD21	1:D:420:PHE:HB3	1.98	0.44
1:A:69:ARG:HB2	1:A:69:ARG:CZ	2.48	0.44
1:B:322:VAL:HG11	1:D:154:ASN:HB3	1.98	0.43
1:B:272:MSE:HE2	1:B:280:ALA:HB1	2.00	0.43
1:C:70:ILE:HD11	1:C:430:LEU:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLY:HA2	1:B:60:ALA:CB	2.49	0.43
1:B:31:PHE:O	1:B:77:CYS:HA	2.18	0.43
1:C:532:ARG:NH2	6:C:765:HOH:O	2.51	0.42
1:B:79:ALA:O	1:B:106:ALA:HA	2.20	0.42
1:C:42:LEU:O	1:C:43:PHE:HB2	2.19	0.42
1:A:132:MSE:HE2	1:B:128:ILE:HD13	2.00	0.42
4:B:600:TPP:C2	4:B:600:TPP:C4'	2.93	0.42
1:D:69:ARG:CZ	1:D:69:ARG:HB2	2.50	0.41
1:B:249:THR:HB	1:B:253:ALA:HB3	2.03	0.41
1:D:79:ALA:O	1:D:106:ALA:HA	2.21	0.41
1:B:66:VAL:CG1	1:B:430:LEU:HD21	2.50	0.41
1:B:69:ARG:HB2	1:B:69:ARG:CZ	2.50	0.41
1:A:322:VAL:HG11	1:C:154:ASN:HB3	2.03	0.41
1:D:432:SER:HB2	1:D:440:TYR:CE1	2.56	0.41
1:C:433:ALA:O	1:D:120:HIS:ND1	2.55	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	558/573 (97%)	545 (98%)	13 (2%)	0	100	100
1	B	559/573 (98%)	546 (98%)	13 (2%)	0	100	100
1	C	560/573 (98%)	548 (98%)	12 (2%)	0	100	100
1	D	559/573 (98%)	547 (98%)	12 (2%)	0	100	100
All	All	2236/2292 (98%)	2186 (98%)	50 (2%)	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	443/441 (100%)	437 (99%)	6 (1%)	67	72
1	B	444/441 (101%)	442 (100%)	2 (0%)	88	92
1	C	445/441 (101%)	440 (99%)	5 (1%)	73	78
1	D	444/441 (101%)	441 (99%)	3 (1%)	84	88
All	All	1776/1764 (101%)	1760 (99%)	16 (1%)	78	83

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ASP
1	A	269	THR
1	A	282[A]	GLN
1	A	282[B]	GLN
1	A	438	PHE
1	A	563	PHE
1	B	269	THR
1	B	438	PHE
1	C	65	ASP
1	C	268	VAL
1	C	438	PHE
1	C	563	PHE
1	C	564	GLN
1	D	65	ASP
1	D	269	THR
1	D	438	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	308	GLN
1	A	505	HIS

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Mol	Chain	Res	Type
1	C	564	GLN
1	D	121	GLN
1	D	560	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	$\# Z > 2$
3	SO4	B	602	-	4,4,4	0.18	0	6,6,6	0.21	0
4	TPP	B	600	2	22,27,27	1.85	7 (31%)	29,40,40	2.22	7 (24%)
3	SO4	D	602	-	4,4,4	0.17	0	6,6,6	0.21	0
4	TPP	A	600	2	22,27,27	1.88	6 (27%)	29,40,40	2.26	7 (24%)
5	GOL	D	604	-	5,5,5	0.35	0	5,5,5	0.38	0
3	SO4	A	603	-	4,4,4	0.14	0	6,6,6	0.09	0
3	SO4	C	603	-	4,4,4	0.13	0	6,6,6	0.10	0
5	GOL	D	1905	-	5,5,5	0.33	0	5,5,5	0.40	0
4	TPP	D	600	2	22,27,27	1.80	6 (27%)	29,40,40	2.25	7 (24%)
3	SO4	D	603	-	4,4,4	0.15	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	602	-	4,4,4	0.19	0	6,6,6	0.30	0
3	SO4	B	603	-	4,4,4	0.14	0	6,6,6	0.10	0
5	GOL	A	604	-	5,5,5	0.34	0	5,5,5	0.37	0
3	SO4	C	602	-	4,4,4	0.16	0	6,6,6	0.15	0
4	TPP	C	600	2	22,27,27	1.77	6 (27%)	29,40,40	2.23	7 (24%)
5	GOL	B	604	-	5,5,5	0.39	0	5,5,5	0.37	0

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	TPP	B	600	2	-	4/16/17/17	0/2/2/2
4	TPP	D	600	2	-	3/16/17/17	0/2/2/2
5	GOL	D	604	-	-	2/4/4/4	-
5	GOL	D	1905	-	-	4/4/4/4	-
4	TPP	C	600	2	-	4/16/17/17	0/2/2/2
5	GOL	A	604	-	-	0/4/4/4	-
4	TPP	A	600	2	-	4/16/17/17	0/2/2/2
5	GOL	B	604	-	-	2/4/4/4	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	600	TPP	C4-N3	-5.42	1.35	1.39
4	B	600	TPP	C4-N3	-5.40	1.35	1.39
4	A	600	TPP	C4-N3	-5.33	1.35	1.39
4	C	600	TPP	C4-N3	-5.19	1.35	1.39
4	A	600	TPP	C2'-N1'	2.94	1.39	1.34
4	D	600	TPP	C7'-N3	-2.84	1.43	1.48
4	A	600	TPP	C7'-N3	-2.79	1.43	1.48
4	B	600	TPP	C2'-N1'	2.76	1.38	1.34
4	D	600	TPP	C4'-N3'	2.69	1.38	1.35
4	D	600	TPP	C2'-N1'	2.68	1.38	1.34
4	A	600	TPP	C6'-N1'	2.67	1.40	1.34
4	C	600	TPP	C2'-N1'	2.67	1.38	1.34
4	C	600	TPP	C4'-N3'	2.66	1.38	1.35
4	A	600	TPP	C4'-N3'	2.65	1.38	1.35
4	B	600	TPP	C7'-N3	-2.53	1.44	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	TPP	C6-C5	-2.53	1.49	1.50
4	C	600	TPP	C7'-N3	-2.51	1.44	1.48
4	B	600	TPP	C4'-N3'	2.51	1.38	1.35
4	D	600	TPP	C6'-N1'	2.38	1.39	1.34
4	C	600	TPP	C6'-N1'	2.33	1.39	1.34
4	B	600	TPP	C2'-N3'	2.30	1.38	1.34
4	C	600	TPP	C2'-N3'	2.30	1.38	1.34
4	B	600	TPP	C6'-N1'	2.28	1.39	1.34
4	A	600	TPP	C2'-N3'	2.24	1.38	1.34
4	D	600	TPP	C2'-N3'	2.22	1.38	1.34

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	600	TPP	C5'-C7'-N3	-8.18	99.67	113.28
4	B	600	TPP	C5'-C7'-N3	-7.89	100.15	113.28
4	C	600	TPP	C5'-C7'-N3	-7.81	100.28	113.28
4	A	600	TPP	C5'-C7'-N3	-7.51	100.78	113.28
4	A	600	TPP	CM2-C2'-N1'	4.96	122.60	117.14
4	B	600	TPP	CM2-C2'-N1'	4.36	121.93	117.14
4	A	600	TPP	C6-C5-C4	3.90	130.57	127.43
4	D	600	TPP	CM2-C2'-N1'	3.90	121.43	117.14
4	A	600	TPP	N1'-C2'-N3'	-3.82	118.96	125.54
4	C	600	TPP	CM2-C2'-N1'	3.82	121.34	117.14
4	D	600	TPP	C6-C5-C4	3.73	130.43	127.43
4	C	600	TPP	C6-C5-C4	3.69	130.40	127.43
4	B	600	TPP	C6-C5-C4	3.68	130.39	127.43
4	C	600	TPP	N1'-C2'-N3'	-3.68	119.20	125.54
4	D	600	TPP	N1'-C2'-N3'	-3.61	119.33	125.54
4	B	600	TPP	N1'-C2'-N3'	-3.56	119.42	125.54
4	C	600	TPP	C6'-N1'-C2'	3.38	121.71	115.96
4	D	600	TPP	C6'-N1'-C2'	3.18	121.38	115.96
4	A	600	TPP	C6'-N1'-C2'	3.14	121.31	115.96
4	B	600	TPP	C6'-N1'-C2'	2.96	121.00	115.96
4	C	600	TPP	PA-O3A-PB	-2.85	123.03	132.83
4	A	600	TPP	PA-O3A-PB	-2.59	123.94	132.83
4	D	600	TPP	PA-O3A-PB	-2.42	124.51	132.83
4	B	600	TPP	PA-O3A-PB	-2.37	124.69	132.83
4	C	600	TPP	C5'-C6'-N1'	-2.32	119.95	123.82
4	D	600	TPP	C5'-C6'-N1'	-2.20	120.16	123.82
4	A	600	TPP	C5'-C6'-N1'	-2.12	120.28	123.82
4	B	600	TPP	C5'-C6'-N1'	-2.01	120.47	123.82

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	600	TPP	C4'-C5'-C7'-N3
5	D	604	GOL	O1-C1-C2-C3
4	D	600	TPP	C4'-C5'-C7'-N3
5	D	1905	GOL	C1-C2-C3-O3
4	C	600	TPP	C4'-C5'-C7'-N3
4	A	600	TPP	C4'-C5'-C7'-N3
5	B	604	GOL	O1-C1-C2-C3
5	D	604	GOL	O1-C1-C2-O2
5	D	1905	GOL	O1-C1-C2-C3
5	D	1905	GOL	O2-C2-C3-O3
5	D	1905	GOL	O1-C1-C2-O2
5	B	604	GOL	O1-C1-C2-O2
4	B	600	TPP	PB-O3A-PA-O7
4	D	600	TPP	PB-O3A-PA-O7
4	C	600	TPP	PB-O3A-PA-O7
4	A	600	TPP	PB-O3A-PA-O7
4	B	600	TPP	C6'-C5'-C7'-N3
4	D	600	TPP	C6'-C5'-C7'-N3
4	A	600	TPP	C6'-C5'-C7'-N3
4	A	600	TPP	PA-O3A-PB-O1B
4	B	600	TPP	PA-O3A-PB-O1B
4	C	600	TPP	C6'-C5'-C7'-N3
4	C	600	TPP	PA-O3A-PB-O1B

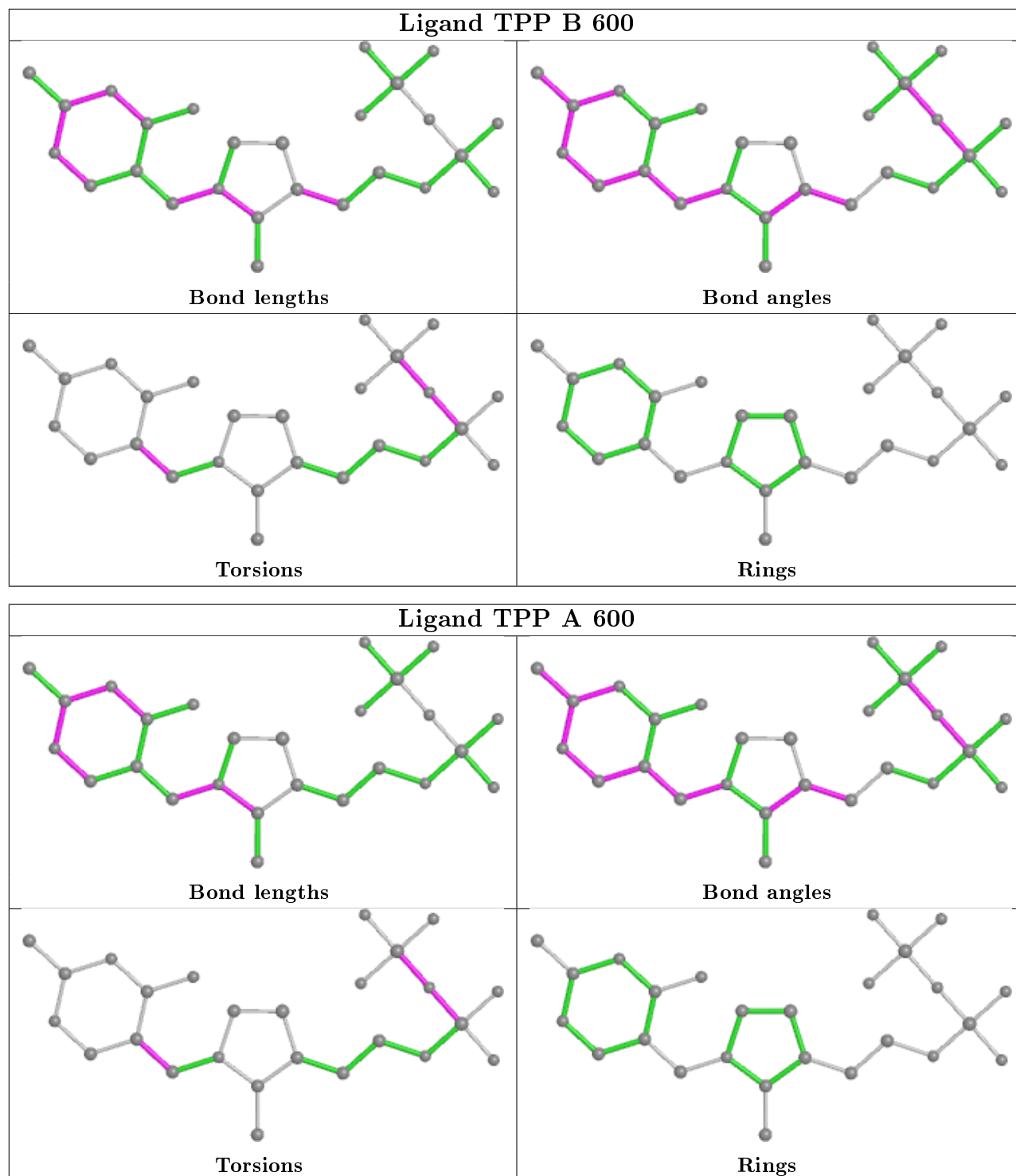
There are no ring outliers.

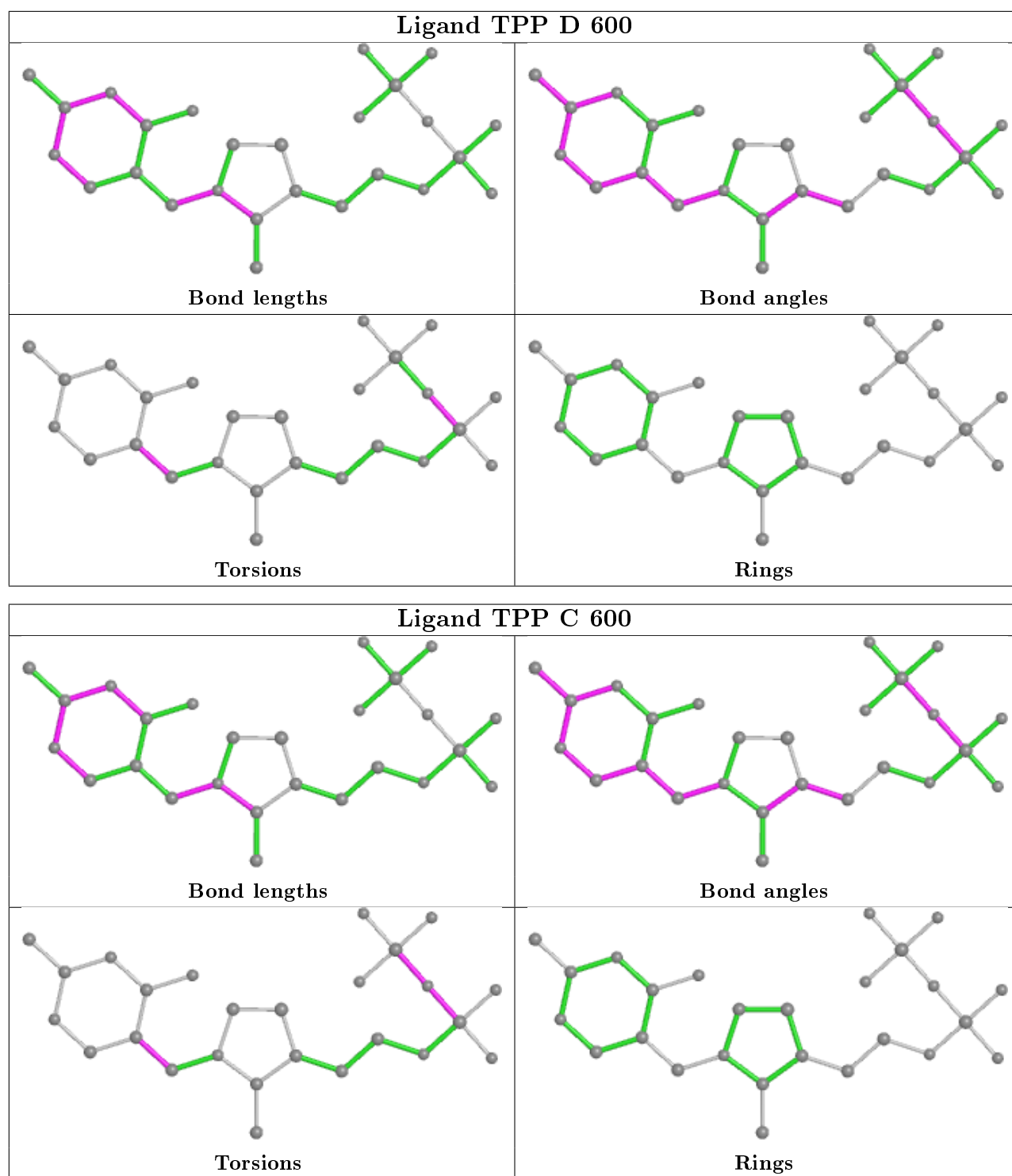
4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	600	TPP	5	0
4	A	600	TPP	4	0
4	D	600	TPP	4	0
4	C	600	TPP	4	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 ⓘ

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	550/573 (95%)	-0.51	3 (0%) 91 90	6, 12, 22, 31	16 (2%)
1	B	551/573 (96%)	-0.63	3 (0%) 91 90	6, 12, 22, 32	14 (2%)
1	C	549/573 (95%)	-0.47	9 (1%) 72 70	6, 12, 22, 32	23 (4%)
1	D	549/573 (95%)	-0.54	3 (0%) 91 90	6, 12, 22, 31	22 (4%)
All	All	2199/2292 (95%)	-0.53	18 (0%) 86 85	6, 12, 22, 32	75 (3%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	380	ASP	4.1
1	A	184	PRO	3.9
1	C	564	GLN	3.4
1	B	181	THR	3.3
1	C	573	ILE	3.3
1	C	562	ASP	3.3
1	A	573	ILE	3.2
1	B	573	ILE	2.8
1	D	573	ILE	2.8
1	D	180	ASP	2.8
1	C	185	ASN	2.7
1	D	185	ASN	2.7
1	C	565	PRO	2.6
1	B	380	ASP	2.4
1	C	377	THR	2.4
1	C	563	PHE	2.3
1	C	379	GLU	2.1
1	A	505	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

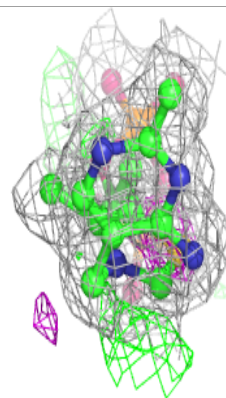
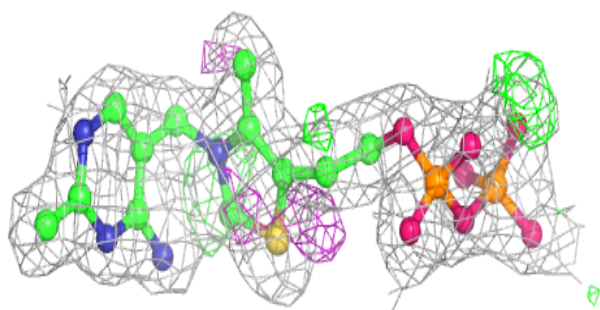
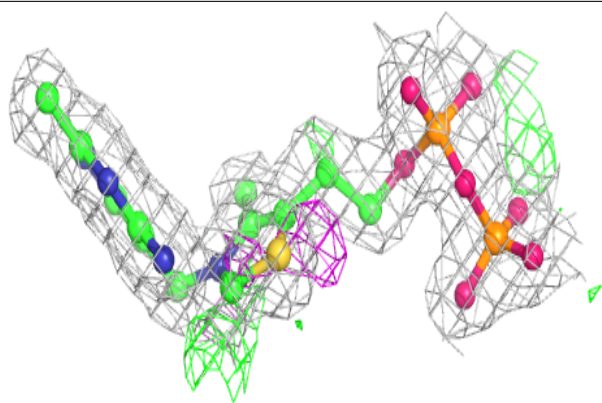
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	D	604	6/6	0.85	0.15	49,49,49,49	0
3	SO4	A	603	5/5	0.86	0.30	61,62,62,62	0
3	SO4	C	603	5/5	0.86	0.32	71,71,71,72	0
5	GOL	A	604	6/6	0.88	0.19	39,40,40,40	0
5	GOL	B	604	6/6	0.92	0.15	42,43,43,43	0
5	GOL	D	1905	6/6	0.93	0.13	36,37,37,37	0
3	SO4	B	603	5/5	0.93	0.15	22,23,23,23	5
4	TPP	D	600	26/26	0.97	0.10	9,11,13,14	0
4	TPP	B	600	26/26	0.97	0.09	8,11,12,14	0
4	TPP	A	600	26/26	0.97	0.10	9,11,12,14	0
4	TPP	C	600	26/26	0.97	0.11	9,12,14,16	0
3	SO4	C	602	5/5	0.98	0.09	31,31,32,32	0
2	MG	D	601	1/1	0.98	0.13	2,2,2,2	0
3	SO4	D	603	5/5	0.98	0.21	41,41,41,42	0
2	MG	C	601	1/1	0.99	0.14	2,2,2,2	0
3	SO4	A	602	5/5	0.99	0.10	17,18,19,20	0
3	SO4	D	602	5/5	0.99	0.08	17,18,19,19	0
3	SO4	B	602	5/5	0.99	0.06	19,20,21,21	0
2	MG	A	601	1/1	1.00	0.12	2,2,2,2	0
2	MG	B	601	1/1	1.00	0.14	2,2,2,2	0

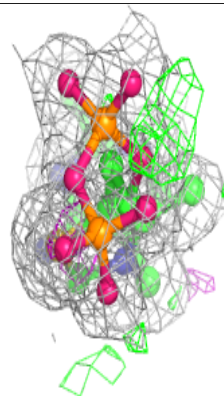
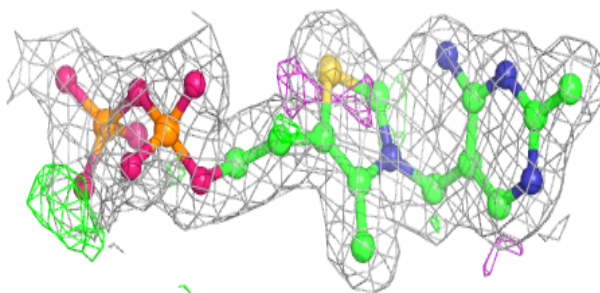
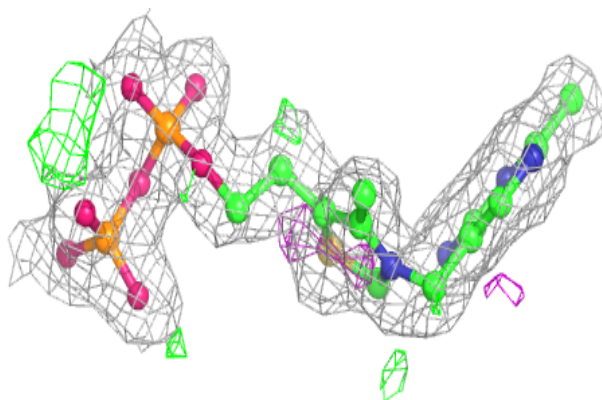
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP D 600:

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

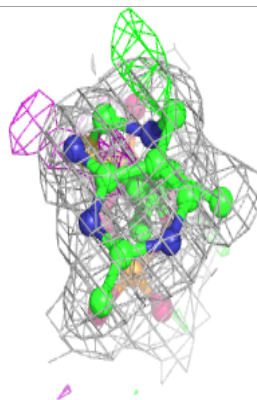
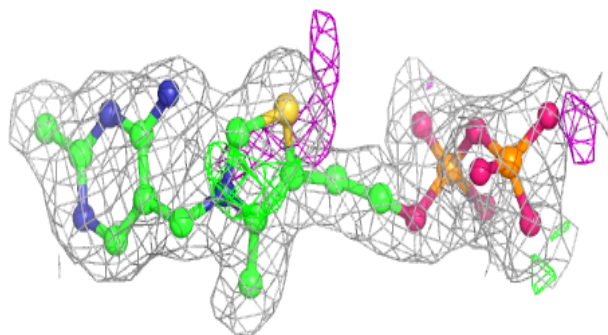
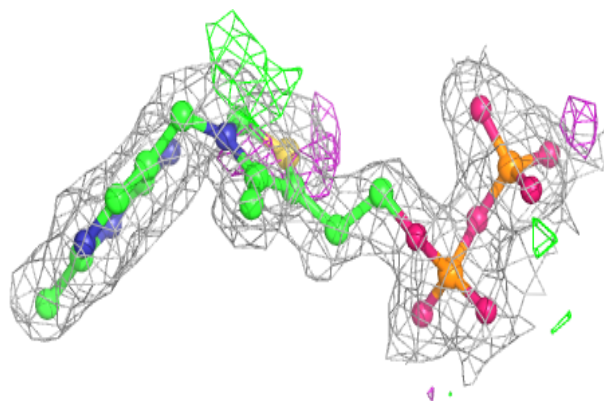
**Electron density around TPP B 600:**

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

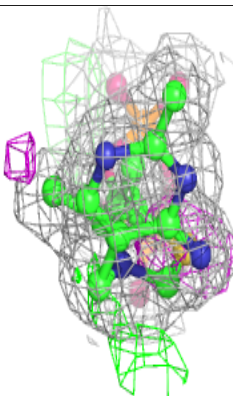
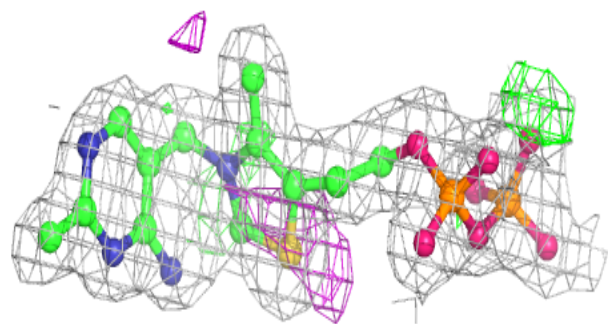
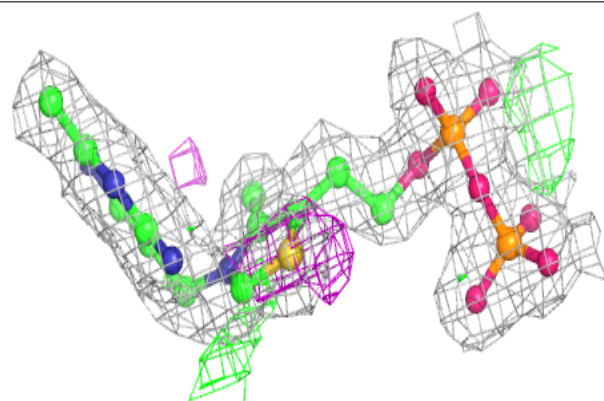


Electron density around TPP A 600:

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

**Electron density around TPP C 600:**

$2mF_o-DF_c$ (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.