Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 08:42 pm BST

PDB ID	:	1UPB
Title	:	Carboxyethylarginine synthase from Streptomyces clavuligerus
Authors	:	Caines, M.E.C.; Elkins, J.M.; Hewitson, K.S.; Schofield, C.J.
Deposited on	:	2003-09-29
Resolution	:	2.35 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 (i) 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 (i)) were used in the production of this report:

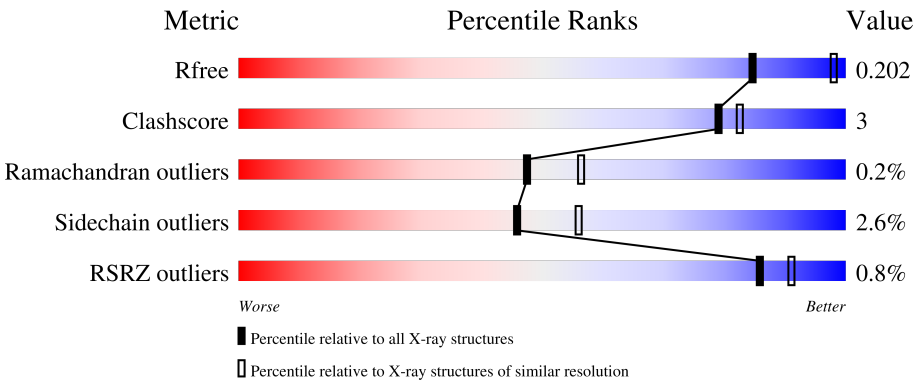
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

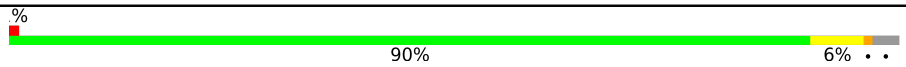
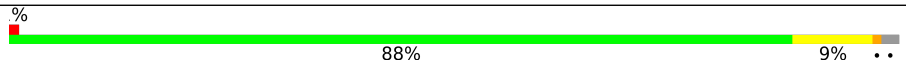
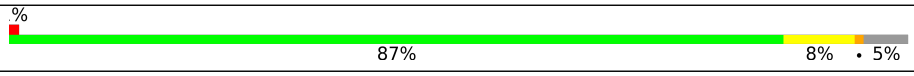
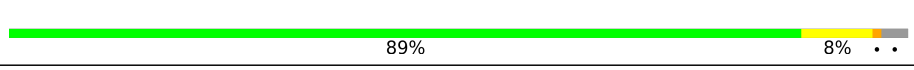
The reported resolution of this entry is 2.35 Å.

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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 <=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	
1	B	573	
1	C	573	
1	D	573	

2 Entry composition (i)

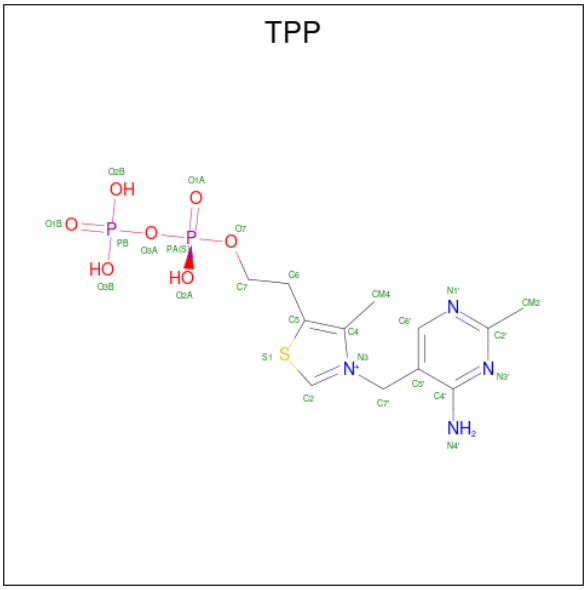
There are 5 unique types of molecules in this entry. The entry contains 17612 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	558	4160	2640	720	787	13	0	0	0
1	B	559	4186	2656	724	793	13	0	0	0
1	C	547	4086	2596	709	768	13	0	0	0
1	D	558	4151	2637	716	785	13	0	0	0

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	A	1	26	12	4	7	2	1	0	0
2	B	1	26	12	4	7	2	1	0	0

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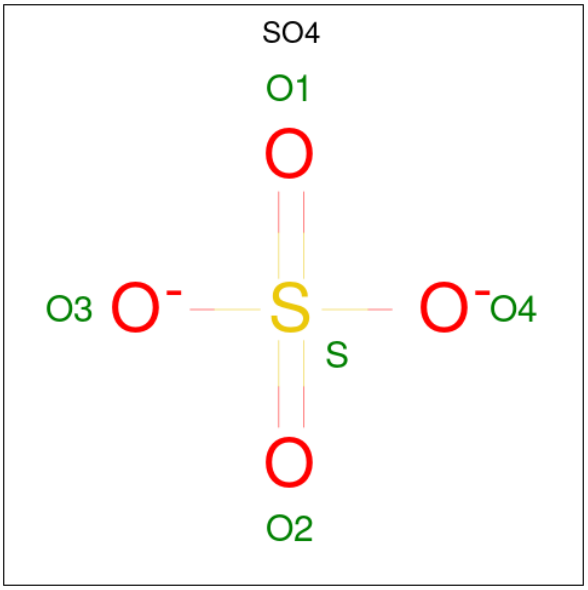
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	C	1	26	12	4	7	2	1	0	0
			Total	C	N	O	P	S		
2	D	1	26	12	4	7	2	1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 5 is water.

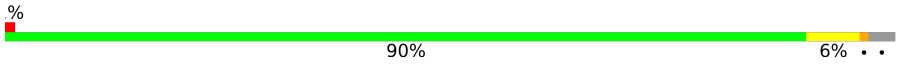
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	227	227	227	0	0
			Total	O		
5	B	236	236	236	0	0
			Total	O		
5	C	192	192	192	0	0
			Total	O		
5	D	226	226	226	0	0

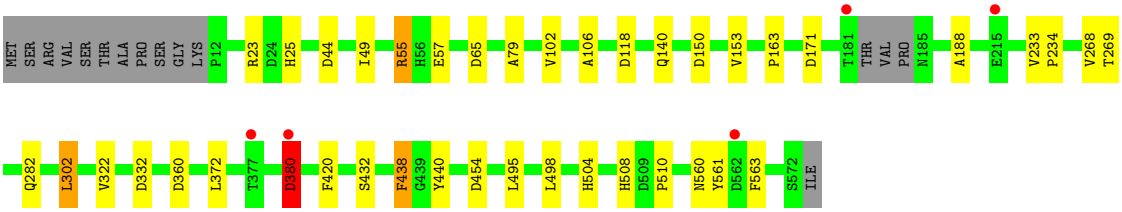
3 Residue-property plots (i)

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: CARBOXYETHYLARGININE SYNTHASE

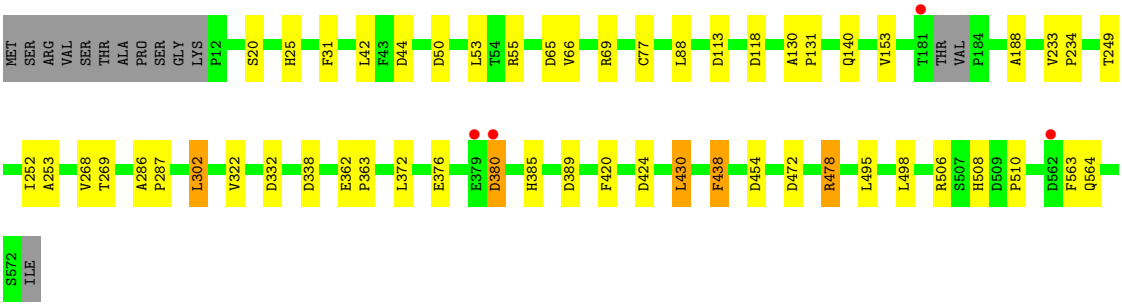
Chain A:





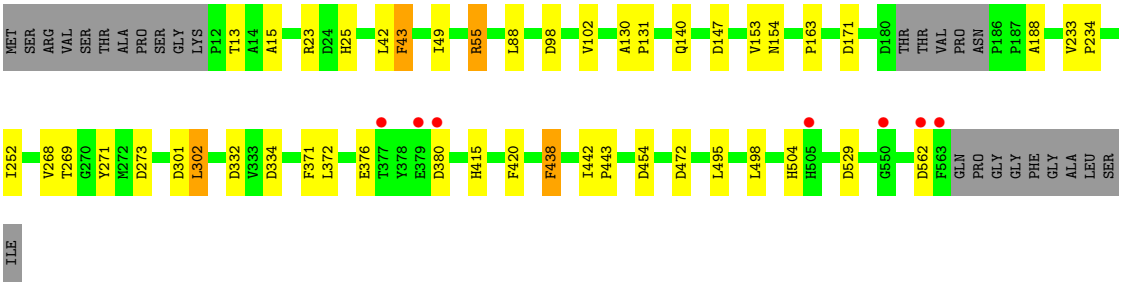
• Molecule 1: CARBOXYETHYLARGININE SYNTHASE

Chain B:



• Molecule 1: CARBOXYETHYLARGININE SYNTHASE

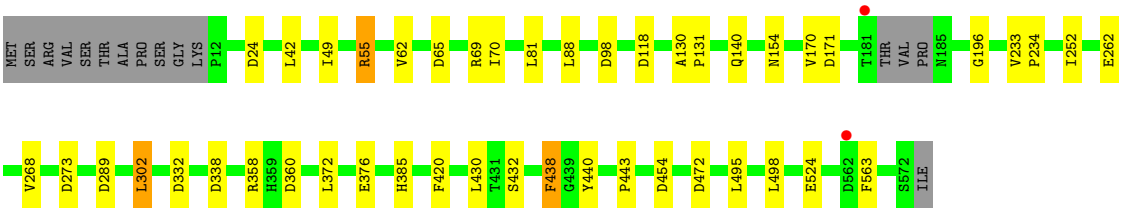
Chain C:



• Molecule 1: CARBOXYETHYLARGININE SYNTHASE

Chain D:

89%
8%


MET SER ARG VAL SER THR ALA PRO SER GLY LYS P12 D24 L42 I49 R55 V62 D65 R69 I70 L81 L88 D98 D118 A130 P131 Q140 N154 V170 D171 T181 THR VAL PRO N185 G196 V233 P234 I252 E262
V268 D273 D289 L302 D332 D338 R358 H359 D360 L372 E376 H385 F420 L430 T431 S432 F438 G439 Y440 P443 D454 D472 L495 L498 E524 D562 F563 S572 ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.70Å 127.28Å 197.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.00 – 2.35 38.48 – 2.35	Depositor EDS
% Data completeness (in resolution range)	92.3 (39.00-2.35) 92.3 (38.48-2.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.66 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.157 , 0.196 0.169 , 0.202	Depositor DCC
R_{free} test set	5581 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	16.3	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 30.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17612	wwPDB-VP
Average B, all atoms (Å^2)	17.0	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, TPP, 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	0.54	0/4254	0.77	10/5811 (0.2%)
1	B	0.56	0/4281	0.82	14/5844 (0.2%)
1	C	0.56	0/4178	0.79	12/5706 (0.2%)
1	D	0.55	0/4245	0.79	13/5799 (0.2%)
All	All	0.55	0/16958	0.79	49/23160 (0.2%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	478	ARG	NE-CZ-NH1	-9.88	115.36	120.30
1	B	478	ARG	NE-CZ-NH2	9.05	124.83	120.30
1	C	55	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	A	55	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	B	55	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	C	301	ASP	CB-CG-OD2	7.17	124.75	118.30
1	D	55	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	55	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	C	273	ASP	CB-CG-OD2	6.79	124.41	118.30
1	A	65	ASP	CB-CG-OD2	6.68	124.31	118.30
1	D	171	ASP	CB-CG-OD2	6.62	124.26	118.30
1	D	273	ASP	CB-CG-OD2	6.19	123.87	118.30
1	D	454	ASP	CB-CG-OD2	6.15	123.83	118.30
1	A	380	ASP	CB-CG-OD2	6.09	123.78	118.30
1	D	332	ASP	CB-CG-OD2	6.06	123.75	118.30
1	B	454	ASP	CB-CG-OD2	6.05	123.74	118.30
1	C	171	ASP	CB-CG-OD2	6.01	123.71	118.30
1	B	472	ASP	CB-CG-OD2	5.90	123.61	118.30
1	C	334	ASP	CB-CG-OD2	5.90	123.61	118.30
1	B	65	ASP	CB-CG-OD2	5.88	123.59	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	360	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	454	ASP	CB-CG-OD2	5.78	123.50	118.30
1	C	98	ASP	CB-CG-OD2	5.77	123.49	118.30
1	C	55	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	332	ASP	CB-CG-OD2	5.72	123.45	118.30
1	C	454	ASP	CB-CG-OD2	5.67	123.41	118.30
1	D	55	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	360	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	118	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	529	ASP	CB-CG-OD2	5.50	123.25	118.30
1	D	472	ASP	CB-CG-OD2	5.48	123.23	118.30
1	D	289	ASP	CB-CG-OD2	5.39	123.15	118.30
1	C	332	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	113	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	424	ASP	CB-CG-OD2	5.35	123.11	118.30
1	C	147	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	472	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	44	ASP	CB-CG-OD1	5.23	123.00	118.30
1	B	389	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	24	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	338	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	118	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	338	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	118	ASP	CB-CG-OD2	5.11	122.89	118.30
1	B	50	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	171	ASP	CB-CG-OD2	5.08	122.88	118.30
1	A	332	ASP	CB-CG-OD2	5.06	122.85	118.30
1	D	98	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	150	ASP	CB-CG-OD2	5.01	122.81	118.30

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	4160	0	4087	20	0
1	B	4186	0	4129	22	0
1	C	4086	0	4033	23	0
1	D	4151	0	4077	16	0
2	A	26	0	16	6	0
2	B	26	0	16	6	0
2	C	26	0	16	5	0
2	D	26	0	16	6	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	10	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	1	0
4	D	10	0	0	0	0
5	A	227	0	0	1	0
5	B	236	0	0	2	0
5	C	192	0	0	2	0
5	D	226	0	0	3	0
All	All	17612	0	16390	91	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 (91) 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)
2:D:600:TPP:HN42	2:D:600:TPP:C2	1.44	1.29
2:C:600:TPP:HN42	2:C:600:TPP:C2	1.51	1.24
2:A:600:TPP:HN42	2:A:600:TPP:C2	1.48	1.24
2:B:600:TPP:HN42	2:B:600:TPP:C2	1.55	1.18
2:D:600:TPP:C2	2:D:600:TPP:N4'	2.11	1.11
2:B:600:TPP:HN42	2:B:600:TPP:H2	1.08	1.11
2:C:600:TPP:HN42	2:C:600:TPP:H2	1.08	1.08
2:A:600:TPP:HN42	2:A:600:TPP:H2	1.13	1.08
2:D:600:TPP:HN42	2:D:600:TPP:H2	1.01	1.04
2:B:600:TPP:C2	2:B:600:TPP:N4'	2.22	1.03
2:A:600:TPP:C2	2:A:600:TPP:N4'	2.20	1.02
2:C:600:TPP:C2	2:C:600:TPP:N4'	2.21	1.02
1:C:271:TYR:CE1	1:C:415:HIS:CE1	2.51	0.98
1:A:25:HIS:CD2	1:A:153:VAL:HG21	2.04	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:THR:HG21	5:C:2010:HOH:O	1.75	0.86
2:D:600:TPP:N4'	2:D:600:TPP:H2	1.84	0.85
2:B:600:TPP:H2	2:B:600:TPP:N4'	1.90	0.83
1:A:504:HIS:CD2	1:B:42:LEU:HG	2.16	0.80
2:C:600:TPP:H2	2:C:600:TPP:N4'	1.92	0.74
1:C:504:HIS:CD2	1:D:42:LEU:HG	2.22	0.73
1:B:252:ILE:HG12	5:B:2139:HOH:O	1.92	0.69
1:B:322:VAL:HG11	1:D:154:ASN:HB3	1.76	0.68
1:C:271:TYR:CD1	1:C:415:HIS:CE1	2.81	0.67
1:B:508:HIS:CD2	1:B:510:PRO:HD2	2.31	0.65
1:D:268:VAL:HB	1:D:302:LEU:HD22	1.79	0.63
1:A:268:VAL:HB	1:A:302:LEU:HD22	1.81	0.61
1:B:25:HIS:ND1	1:B:188:ALA:HB1	2.16	0.60
1:C:13:THR:HG23	1:C:15:ALA:H	1.67	0.60
1:C:438:PHE:CE1	2:C:600:TPP:HM23	2.38	0.59
2:A:600:TPP:H2	2:A:600:TPP:N4'	1.98	0.58
1:C:271:TYR:HE1	1:C:415:HIS:CE1	2.17	0.57
1:B:53:LEU:O	1:B:478:ARG:NH1	2.35	0.56
1:B:25:HIS:CE1	1:B:188:ALA:HB1	2.41	0.56
1:A:380:ASP:HB3	1:A:560:ASN:OD1	2.06	0.56
1:D:372:LEU:HD21	1:D:420:PHE:HB3	1.89	0.55
1:B:372:LEU:HD21	1:B:420:PHE:HB3	1.90	0.54
1:B:25:HIS:CD2	1:B:153:VAL:HG21	2.43	0.53
1:C:372:LEU:HD21	1:C:420:PHE:HB3	1.91	0.53
1:A:25:HIS:ND1	1:A:188:ALA:HB1	2.25	0.52
1:B:66:VAL:HG13	1:B:430:LEU:HD21	1.92	0.51
1:A:322:VAL:HG11	1:C:154:ASN:HB3	1.94	0.50
1:C:268:VAL:CG2	1:C:302:LEU:HD22	2.42	0.48
1:D:438:PHE:CE1	2:D:600:TPP:HM23	2.48	0.48
1:A:25:HIS:CE1	1:A:188:ALA:HB1	2.47	0.48
1:C:233:VAL:HB	1:C:234:PRO:HD3	1.94	0.48
1:C:271:TYR:CD1	1:C:415:HIS:ND1	2.82	0.48
1:A:49:ILE:HG22	5:A:2013:HOH:O	2.14	0.48
1:A:102:VAL:O	1:A:163:PRO:HA	2.13	0.48
1:B:249:THR:HB	1:B:253:ALA:HB3	1.96	0.48
1:A:233:VAL:HB	1:A:234:PRO:HD3	1.96	0.47
1:A:561:TYR:OH	2:A:600:TPP:O1B	2.27	0.47
2:D:600:TPP:C2	2:D:600:TPP:C4'	2.85	0.47
1:B:438:PHE:CE1	2:B:600:TPP:HM23	2.50	0.47
1:A:79:ALA:O	1:A:106:ALA:HA	2.14	0.47
1:A:44:ASP:HB3	1:B:508:HIS:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:GLU:N	1:B:363:PRO:CD	2.79	0.46
1:C:442:ILE:N	1:C:443:PRO:HD2	2.29	0.46
1:B:130:ALA:N	1:B:131:PRO:CD	2.79	0.45
1:B:31:PHE:O	1:B:77:CYS:HA	2.17	0.45
1:D:196:GLY:HA3	5:D:2090:HOH:O	2.16	0.45
1:B:268:VAL:HB	1:B:302:LEU:HD22	1.98	0.45
1:D:69:ARG:CZ	1:D:69:ARG:HB2	2.47	0.45
1:D:252:ILE:HG12	5:D:2127:HOH:O	2.16	0.44
1:D:233:VAL:HB	1:D:234:PRO:HD3	1.98	0.44
1:C:42:LEU:O	1:C:43:PHE:HB2	2.18	0.44
1:D:62:VAL:HB	1:D:443:PRO:HB2	1.99	0.44
1:D:70:ILE:HD11	1:D:430:LEU:HD11	2.00	0.44
1:B:233:VAL:HB	1:B:234:PRO:HD3	2.00	0.44
1:A:438:PHE:CE1	2:A:600:TPP:HM23	2.53	0.44
1:A:508:HIS:CD2	1:A:510:PRO:HD2	2.53	0.44
1:B:140:GLN:OE1	1:C:140:GLN:NE2	2.52	0.43
1:A:432:SER:HB2	1:A:440:TYR:CE1	2.54	0.43
1:B:69:ARG:CZ	1:B:69:ARG:HB2	2.48	0.43
1:A:372:LEU:HD21	1:A:420:PHE:HB3	2.01	0.43
1:B:286:ALA:HB3	1:B:287:PRO:HD3	2.01	0.43
1:C:271:TYR:OH	4:C:602:SO4:O3	2.28	0.42
1:D:385:HIS:CD2	1:D:385:HIS:H	2.37	0.42
1:C:55:ARG:HD2	5:D:2178:HOH:O	2.19	0.42
1:C:102:VAL:O	1:C:163:PRO:HA	2.20	0.42
1:C:25:HIS:CD2	1:C:153:VAL:HG21	2.55	0.42
1:A:57:GLU:OE2	2:B:600:TPP:N1'	2.53	0.42
1:D:432:SER:HB2	1:D:440:TYR:CE1	2.54	0.41
1:C:130:ALA:N	1:C:131:PRO:CD	2.83	0.41
1:D:130:ALA:N	1:D:131:PRO:CD	2.83	0.41
1:A:140:GLN:OE1	1:D:140:GLN:NE2	2.50	0.41
5:C:2161:HOH:O	1:D:55:ARG:HD2	2.21	0.41
1:C:13:THR:HG23	1:C:15:ALA:N	2.33	0.41
1:C:252:ILE:H	1:C:252:ILE:HD12	1.86	0.41
1:A:55:ARG:HD2	5:B:2203:HOH:O	2.20	0.40
1:C:25:HIS:CE1	1:C:188:ALA:HB1	2.55	0.40
1:B:385:HIS:H	1:B:385:HIS:CD2	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	554/573 (97%)	538 (97%)	15 (3%)	1 (0%)	47	56
1	B	555/573 (97%)	539 (97%)	15 (3%)	1 (0%)	47	56
1	C	543/573 (95%)	528 (97%)	12 (2%)	3 (1%)	25	27
1	D	554/573 (97%)	540 (98%)	14 (2%)	0	100	100
All	All	2206/2292 (96%)	2145 (97%)	56 (2%)	5 (0%)	47	56

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	ASP
1	C	380	ASP
1	B	380	ASP
1	C	562	ASP
1	C	43	PHE

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	431/452 (95%)	423 (98%)	8 (2%)	57	68
1	B	437/452 (97%)	424 (97%)	13 (3%)	41	50
1	C	424/452 (94%)	414 (98%)	10 (2%)	49	59
1	D	429/452 (95%)	415 (97%)	14 (3%)	38	46
All	All	1721/1808 (95%)	1676 (97%)	45 (3%)	46	56

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	269	THR
1	A	282	GLN
1	A	302	LEU
1	A	438	PHE
1	A	495	LEU
1	A	498	LEU
1	A	563	PHE
1	B	20	SER
1	B	88	LEU
1	B	269	THR
1	B	302	LEU
1	B	376	GLU
1	B	380	ASP
1	B	430	LEU
1	B	438	PHE
1	B	495	LEU
1	B	498	LEU
1	B	506	ARG
1	B	563	PHE
1	B	564	GLN
1	C	23	ARG
1	C	49	ILE
1	C	88	LEU
1	C	269	THR
1	C	302	LEU
1	C	371	PHE
1	C	376	GLU
1	C	438	PHE
1	C	495	LEU
1	C	498	LEU
1	D	49	ILE
1	D	65	ASP
1	D	81	LEU
1	D	88	LEU
1	D	170	VAL
1	D	262	GLU
1	D	302	LEU
1	D	358	ARG
1	D	376	GLU
1	D	438	PHE
1	D	495	LEU

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Mol	Chain	Res	Type
1	D	498	LEU
1	D	524	GLU
1	D	563	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	GLN
1	B	308	GLN
1	B	357	GLN
1	B	504	HIS
1	C	189	ASN
1	C	282	GLN
1	C	308	GLN
1	C	385	HIS
1	D	16	HIS
1	D	505	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	TPP	B	600	3	22,27,27	2.04	7 (31%)	29,40,40	2.08	5 (17%)
4	SO4	C	602	-	4,4,4	0.23	0	6,6,6	0.81	0
2	TPP	A	600	3	22,27,27	2.00	7 (31%)	29,40,40	2.27	5 (17%)
4	SO4	D	602	-	4,4,4	0.26	0	6,6,6	0.36	0
4	SO4	A	602	-	4,4,4	0.19	0	6,6,6	0.23	0
2	TPP	C	600	3	22,27,27	1.89	6 (27%)	29,40,40	2.14	6 (20%)
2	TPP	D	600	3	22,27,27	2.02	7 (31%)	29,40,40	2.36	6 (20%)
4	SO4	D	603	-	4,4,4	0.15	0	6,6,6	0.14	0
4	SO4	C	603	-	4,4,4	0.16	0	6,6,6	0.24	0
4	SO4	A	603	-	4,4,4	0.17	0	6,6,6	0.30	0
4	SO4	B	602	-	4,4,4	0.23	0	6,6,6	0.31	0
4	SO4	B	603	-	4,4,4	0.16	0	6,6,6	0.19	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
2	TPP	D	600	3	-	3/16/17/17	0/2/2/2
2	TPP	B	600	3	-	3/16/17/17	0/2/2/2
2	TPP	A	600	3	-	3/16/17/17	0/2/2/2
2	TPP	C	600	3	-	3/16/17/17	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	TPP	C4-N3	-6.51	1.34	1.39
2	A	600	TPP	C4-N3	-6.33	1.34	1.39
2	D	600	TPP	C4-N3	-5.33	1.35	1.39
2	C	600	TPP	C4-N3	-5.29	1.35	1.39
2	D	600	TPP	C6-C5	3.67	1.52	1.50
2	C	600	TPP	C7'-N3	-3.47	1.42	1.48
2	D	600	TPP	C7'-N3	-3.23	1.42	1.48
2	A	600	TPP	C7'-N3	-3.04	1.43	1.48
2	B	600	TPP	C7'-N3	-2.88	1.43	1.48
2	D	600	TPP	C2'-N1'	2.60	1.38	1.34
2	B	600	TPP	C2'-N1'	2.57	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	TPP	C2'-N1'	2.54	1.38	1.34
2	A	600	TPP	C2'-N1'	2.53	1.38	1.34
2	B	600	TPP	C2'-N3'	2.51	1.38	1.34
2	C	600	TPP	C2'-N3'	2.48	1.38	1.34
2	A	600	TPP	C2'-N3'	2.47	1.38	1.34
2	D	600	TPP	C2'-N3'	2.45	1.38	1.34
2	A	600	TPP	C4'-N3'	2.43	1.38	1.35
2	B	600	TPP	C4'-N3'	2.42	1.38	1.35
2	C	600	TPP	C4'-N3'	2.39	1.38	1.35
2	D	600	TPP	C4'-N3'	2.39	1.38	1.35
2	A	600	TPP	C6'-N1'	2.37	1.39	1.34
2	B	600	TPP	C6'-N1'	2.27	1.39	1.34
2	C	600	TPP	C6'-N1'	2.18	1.39	1.34
2	D	600	TPP	C5'-C4'	-2.03	1.39	1.42
2	A	600	TPP	C5'-C4'	-2.01	1.39	1.42
2	B	600	TPP	C5'-C4'	-2.01	1.39	1.42

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	600	TPP	C5'-C7'-N3	-8.97	98.35	113.28
2	B	600	TPP	C5'-C7'-N3	-8.15	99.70	113.28
2	A	600	TPP	C5'-C7'-N3	-7.94	100.06	113.28
2	C	600	TPP	C5'-C7'-N3	-7.91	100.12	113.28
2	A	600	TPP	CM2-C2'-N1'	5.28	122.94	117.14
2	D	600	TPP	CM2-C2'-N1'	4.36	121.93	117.14
2	A	600	TPP	N1'-C2'-N3'	-4.08	118.52	125.54
2	D	600	TPP	PA-O3A-PB	-3.92	119.37	132.83
2	B	600	TPP	PA-O3A-PB	-3.64	120.33	132.83
2	C	600	TPP	CM2-C2'-N1'	3.61	121.11	117.14
2	C	600	TPP	N1'-C2'-N3'	-3.56	119.41	125.54
2	B	600	TPP	CM2-C2'-N1'	3.45	120.93	117.14
2	D	600	TPP	N1'-C2'-N3'	-3.42	119.66	125.54
2	A	600	TPP	C6'-N1'-C2'	3.37	121.70	115.96
2	B	600	TPP	N1'-C2'-N3'	-3.07	120.26	125.54
2	C	600	TPP	PA-O3A-PB	-2.99	122.57	132.83
2	C	600	TPP	C6'-N1'-C2'	2.97	121.01	115.96
2	A	600	TPP	PA-O3A-PB	-2.85	123.03	132.83
2	D	600	TPP	C6'-N1'-C2'	2.64	120.46	115.96
2	D	600	TPP	C6-C5-C4	2.54	129.47	127.43
2	B	600	TPP	C6-C5-C4	2.33	129.31	127.43
2	C	600	TPP	C5'-C6'-N1'	-2.16	120.23	123.82

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	TPP	C4'-C5'-C7'-N3
2	B	600	TPP	C4'-C5'-C7'-N3
2	C	600	TPP	C4'-C5'-C7'-N3
2	C	600	TPP	PB-O3A-PA-O7
2	D	600	TPP	C4'-C5'-C7'-N3
2	A	600	TPP	PB-O3A-PA-O7
2	D	600	TPP	PB-O3A-PA-O7
2	A	600	TPP	C6'-C5'-C7'-N3
2	B	600	TPP	PB-O3A-PA-O7
2	B	600	TPP	C6'-C5'-C7'-N3
2	C	600	TPP	C6'-C5'-C7'-N3
2	D	600	TPP	C6'-C5'-C7'-N3

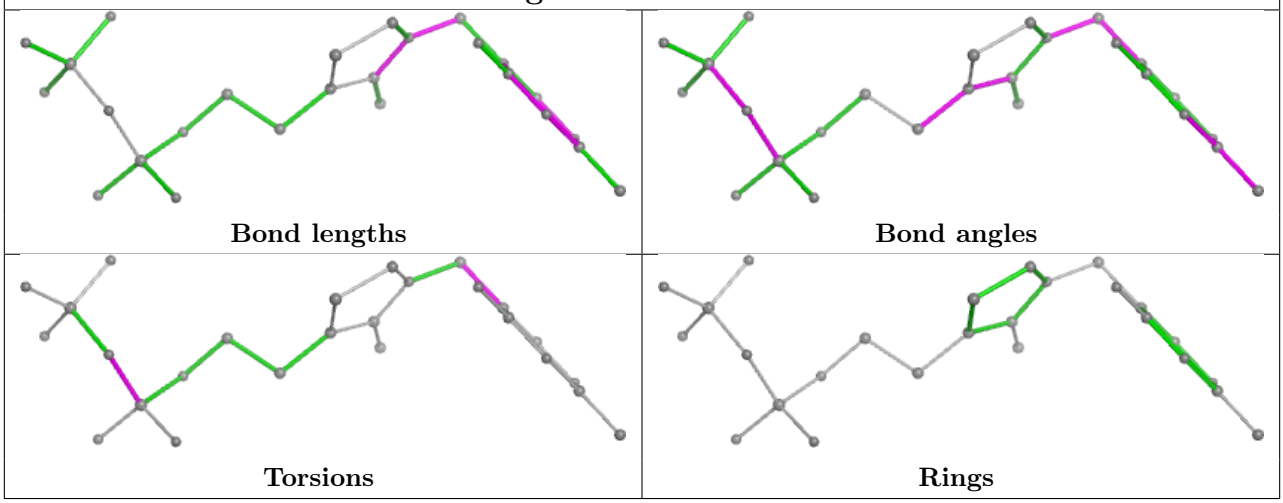
There are no ring outliers.

5 monomers are involved in 24 short contacts:

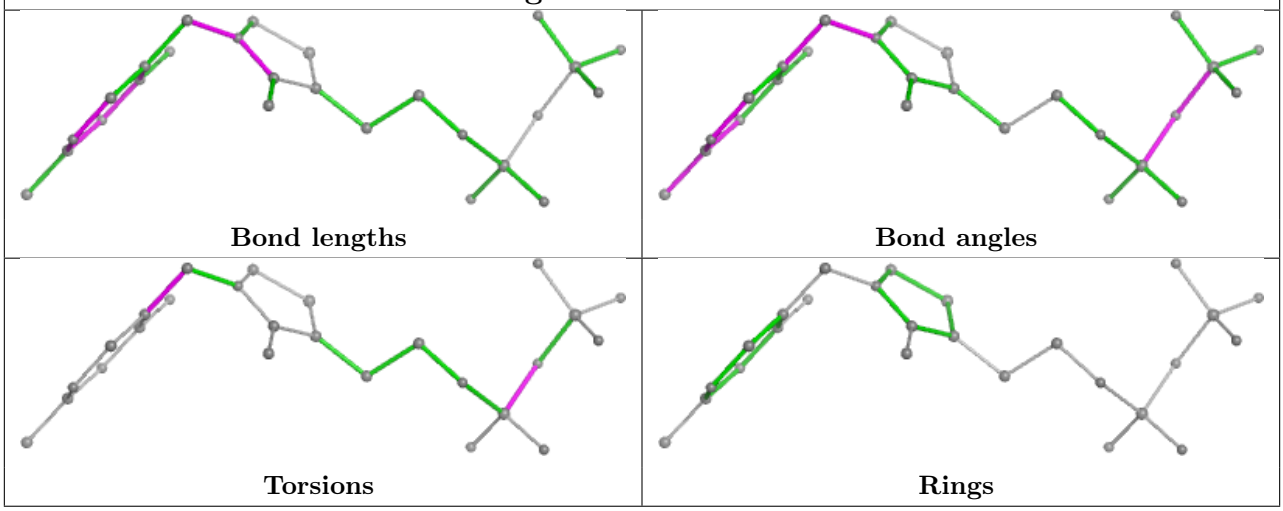
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	TPP	6	0
4	C	602	SO4	1	0
2	A	600	TPP	6	0
2	C	600	TPP	5	0
2	D	600	TPP	6	0

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 then 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.

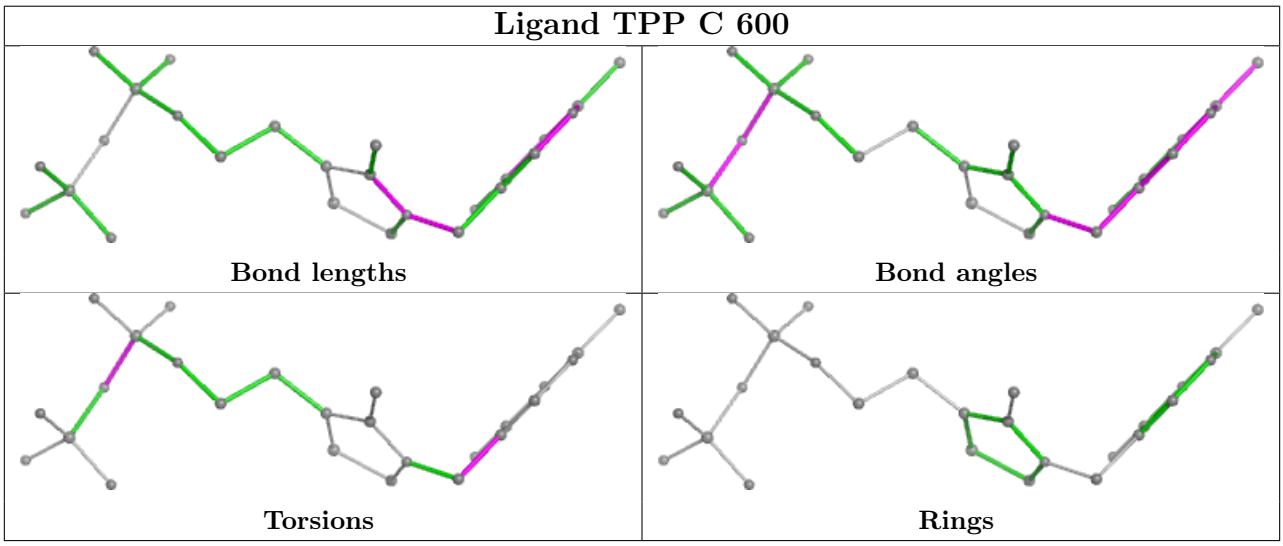
Ligand TPP B 600

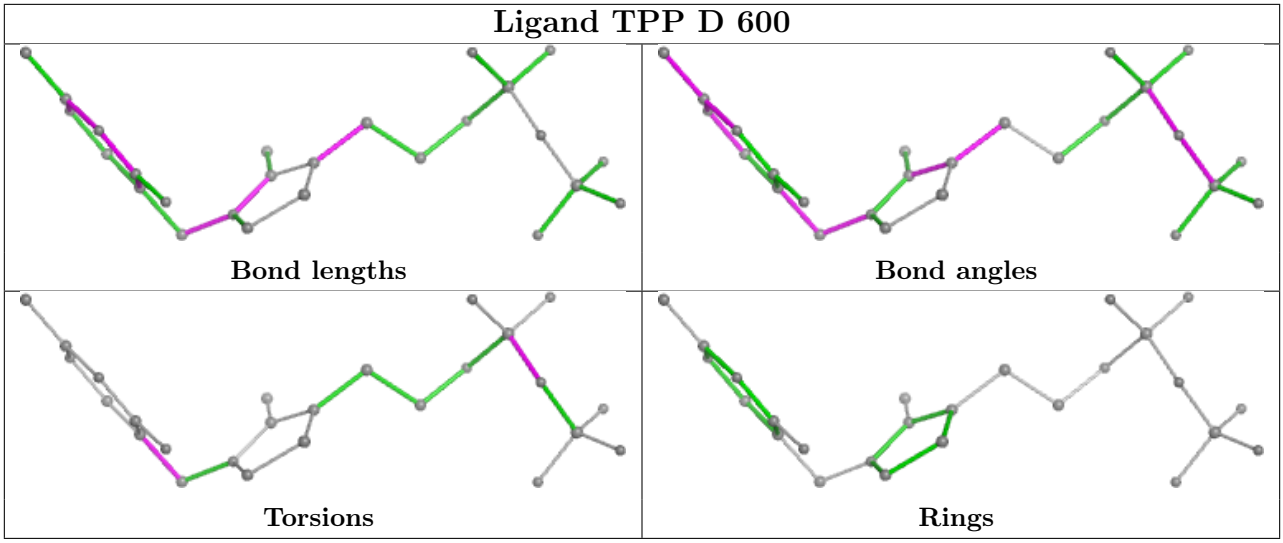


Ligand TPP A 600



Ligand TPP C 600





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	558/573 (97%)	-0.39	5 (0%)	84	90	9, 16, 28, 44	0
1	B	559/573 (97%)	-0.48	4 (0%)	87	92	9, 16, 29, 43	0
1	C	547/573 (95%)	-0.35	7 (1%)	77	84	9, 17, 27, 40	0
1	D	558/573 (97%)	-0.36	2 (0%)	92	96	10, 17, 28, 45	0
All	All	2222/2292 (96%)	-0.39	18 (0%)	86	91	9, 16, 28, 45	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	380	ASP	4.5
1	D	181	THR	4.2
1	C	379	GLU	3.9
1	A	562	ASP	3.7
1	C	563	PHE	3.4
1	A	181	THR	3.3
1	B	562	ASP	3.1
1	A	380	ASP	3.1
1	C	562	ASP	2.9
1	B	380	ASP	2.6
1	C	505	HIS	2.6
1	C	377	THR	2.5
1	B	379	GLU	2.4
1	D	562	ASP	2.3
1	A	377	THR	2.3
1	B	181	THR	2.2
1	C	550	GLY	2.2
1	A	215	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

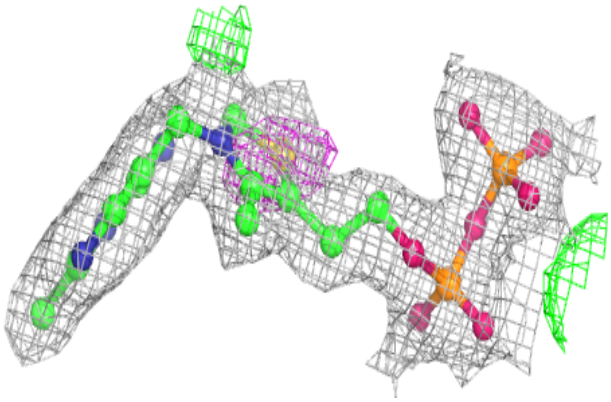
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

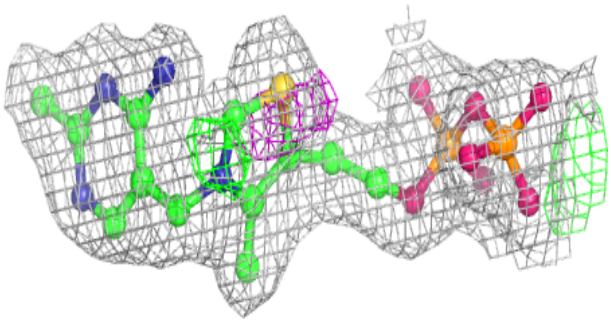
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	A	603	5/5	0.90	0.32	66,67,67,67	0
4	SO4	C	603	5/5	0.90	0.49	67,67,69,69	0
4	SO4	B	603	5/5	0.93	0.33	67,67,68,69	0
3	MG	B	601	1/1	0.94	0.20	6,6,6,6	0
3	MG	A	601	1/1	0.94	0.17	5,5,5,5	0
3	MG	D	601	1/1	0.96	0.17	4,4,4,4	0
3	MG	C	601	1/1	0.96	0.13	5,5,5,5	0
2	TPP	C	600	26/26	0.97	0.11	12,14,19,22	0
2	TPP	D	600	26/26	0.97	0.10	12,14,18,19	0
2	TPP	A	600	26/26	0.97	0.12	11,14,18,19	0
4	SO4	D	603	5/5	0.97	0.20	64,64,65,65	0
2	TPP	B	600	26/26	0.98	0.10	11,14,18,20	0
4	SO4	C	602	5/5	0.98	0.10	29,29,31,31	0
4	SO4	A	602	5/5	0.99	0.11	21,22,23,24	0
4	SO4	D	602	5/5	0.99	0.11	21,23,23,24	0
4	SO4	B	602	5/5	0.99	0.08	22,22,24,25	0

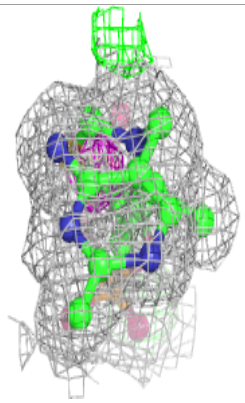
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP 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)

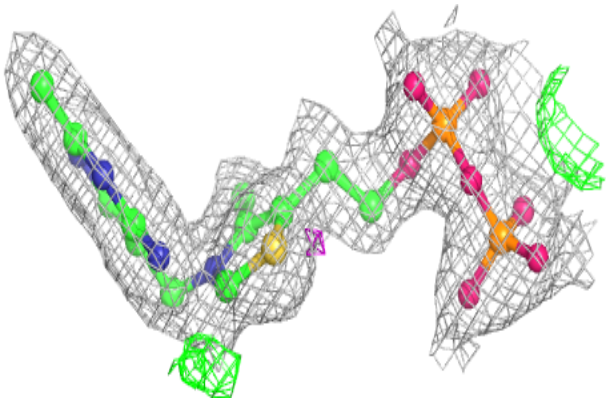


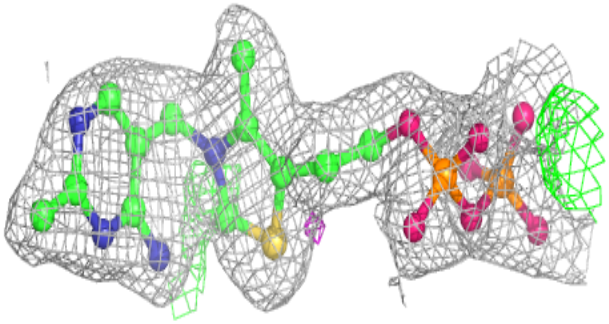


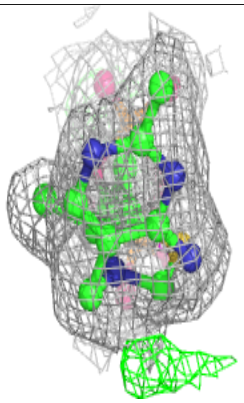


Electron density around TPP D 600:

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

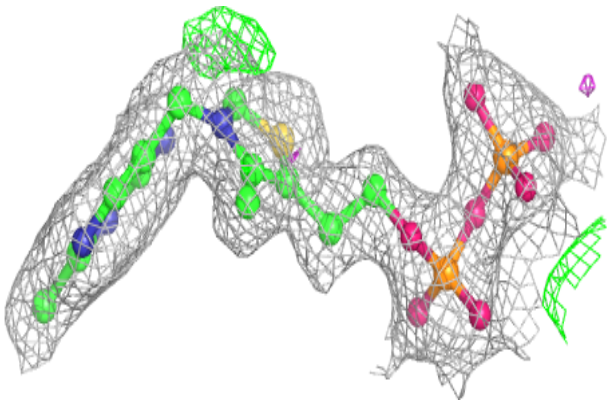


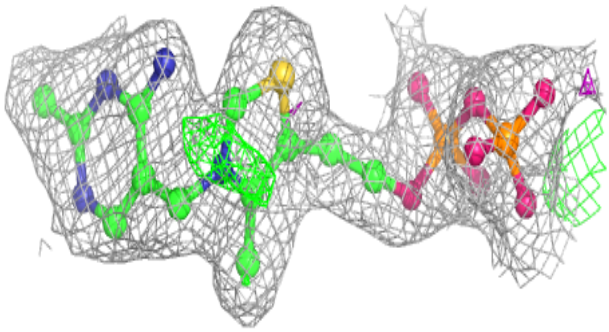


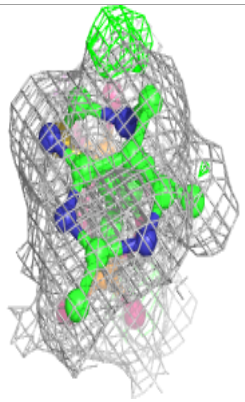


Electron density around TPP A 600:

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

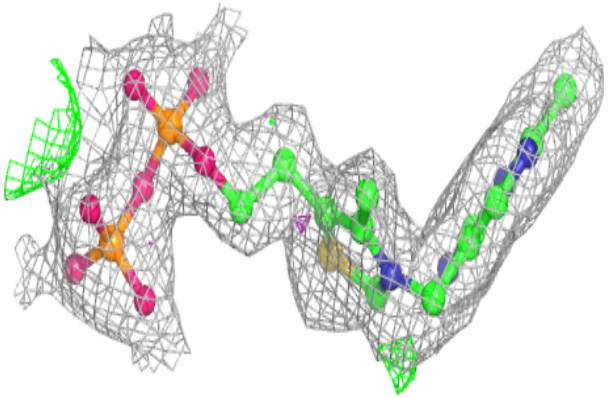


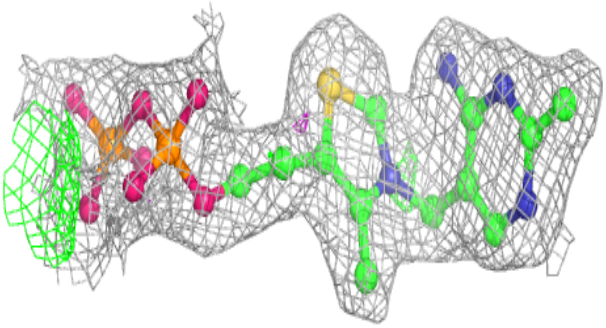


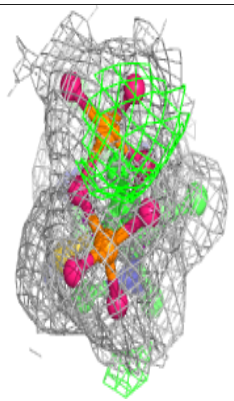


Electron density around TPP B 600:

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







6.5 Other polymers (i)

There are no such residues in this entry.