



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2020 – 02:52 PM BST

PDB ID : 6VGS
Title : Alpha-ketoisovalerate decarboxylase (KivD) from *Lactococcus lactis*, thermostable mutant
Authors : Chan, S.; Korman, T.P.; Sawaya, M.R.; Bowie, J.U.
Deposited on : 2020-01-08
Resolution : 1.80 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 : 2.14.2
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) : 2.14.2

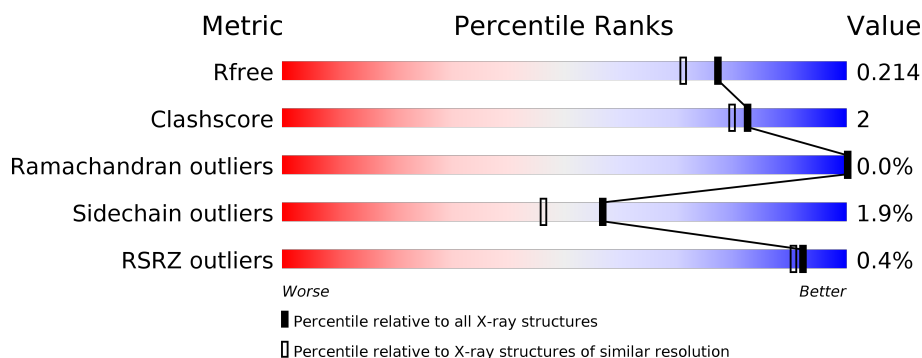
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	AAA	568	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 88% 7% 5% </div> </div>
1	BBB	568	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 90% 5% . </div> </div>
1	CCC	568	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 88% 7% 5% </div> </div>
1	DDD	568	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 89% 6% • 5% </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17973 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 Alpha-keto acid decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	539	Total	C	N	O	S	0	3	0
			4170	2668	685	805	12			
1	BBB	543	Total	C	N	O	S	0	0	0
			4177	2675	682	808	12			
1	CCC	540	Total	C	N	O	S	0	3	0
			4165	2665	680	808	12			
1	DDD	542	Total	C	N	O	S	0	1	0
			4170	2674	683	801	12			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-19	MET	-	initiating methionine	UNP A0A0B8QZ66
AAA	-18	GLY	-	expression tag	UNP A0A0B8QZ66
AAA	-17	SER	-	expression tag	UNP A0A0B8QZ66
AAA	-16	SER	-	expression tag	UNP A0A0B8QZ66
AAA	-15	HIS	-	expression tag	UNP A0A0B8QZ66
AAA	-14	HIS	-	expression tag	UNP A0A0B8QZ66
AAA	-13	HIS	-	expression tag	UNP A0A0B8QZ66
AAA	-12	HIS	-	expression tag	UNP A0A0B8QZ66
AAA	-11	HIS	-	expression tag	UNP A0A0B8QZ66
AAA	-10	HIS	-	expression tag	UNP A0A0B8QZ66
AAA	-9	SER	-	expression tag	UNP A0A0B8QZ66
AAA	-8	SER	-	expression tag	UNP A0A0B8QZ66
AAA	-7	GLY	-	expression tag	UNP A0A0B8QZ66
AAA	-6	LEU	-	expression tag	UNP A0A0B8QZ66
AAA	-5	VAL	-	expression tag	UNP A0A0B8QZ66
AAA	-4	PRO	-	expression tag	UNP A0A0B8QZ66
AAA	-3	ARG	-	expression tag	UNP A0A0B8QZ66
AAA	-2	GLY	-	expression tag	UNP A0A0B8QZ66
AAA	-1	SER	-	expression tag	UNP A0A0B8QZ66
AAA	0	HIS	-	expression tag	UNP A0A0B8QZ66
AAA	34	HIS	GLN	engineered mutation	UNP A0A0B8QZ66

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	290	VAL	ALA	engineered mutation	UNP A0A0B8QZ66
AAA	386	PRO	SER	engineered mutation	UNP A0A0B8QZ66
BBB	-19	MET	-	initiating methionine	UNP A0A0B8QZ66
BBB	-18	GLY	-	expression tag	UNP A0A0B8QZ66
BBB	-17	SER	-	expression tag	UNP A0A0B8QZ66
BBB	-16	SER	-	expression tag	UNP A0A0B8QZ66
BBB	-15	HIS	-	expression tag	UNP A0A0B8QZ66
BBB	-14	HIS	-	expression tag	UNP A0A0B8QZ66
BBB	-13	HIS	-	expression tag	UNP A0A0B8QZ66
BBB	-12	HIS	-	expression tag	UNP A0A0B8QZ66
BBB	-11	HIS	-	expression tag	UNP A0A0B8QZ66
BBB	-10	HIS	-	expression tag	UNP A0A0B8QZ66
BBB	-9	SER	-	expression tag	UNP A0A0B8QZ66
BBB	-8	SER	-	expression tag	UNP A0A0B8QZ66
BBB	-7	GLY	-	expression tag	UNP A0A0B8QZ66
BBB	-6	LEU	-	expression tag	UNP A0A0B8QZ66
BBB	-5	VAL	-	expression tag	UNP A0A0B8QZ66
BBB	-4	PRO	-	expression tag	UNP A0A0B8QZ66
BBB	-3	ARG	-	expression tag	UNP A0A0B8QZ66
BBB	-2	GLY	-	expression tag	UNP A0A0B8QZ66
BBB	-1	SER	-	expression tag	UNP A0A0B8QZ66
BBB	0	HIS	-	expression tag	UNP A0A0B8QZ66
BBB	34	HIS	GLN	engineered mutation	UNP A0A0B8QZ66
BBB	290	VAL	ALA	engineered mutation	UNP A0A0B8QZ66
BBB	386	PRO	SER	engineered mutation	UNP A0A0B8QZ66
CCC	-19	MET	-	initiating methionine	UNP A0A0B8QZ66
CCC	-18	GLY	-	expression tag	UNP A0A0B8QZ66
CCC	-17	SER	-	expression tag	UNP A0A0B8QZ66
CCC	-16	SER	-	expression tag	UNP A0A0B8QZ66
CCC	-15	HIS	-	expression tag	UNP A0A0B8QZ66
CCC	-14	HIS	-	expression tag	UNP A0A0B8QZ66
CCC	-13	HIS	-	expression tag	UNP A0A0B8QZ66
CCC	-12	HIS	-	expression tag	UNP A0A0B8QZ66
CCC	-11	HIS	-	expression tag	UNP A0A0B8QZ66
CCC	-10	HIS	-	expression tag	UNP A0A0B8QZ66
CCC	-9	SER	-	expression tag	UNP A0A0B8QZ66
CCC	-8	SER	-	expression tag	UNP A0A0B8QZ66
CCC	-7	GLY	-	expression tag	UNP A0A0B8QZ66
CCC	-6	LEU	-	expression tag	UNP A0A0B8QZ66
CCC	-5	VAL	-	expression tag	UNP A0A0B8QZ66
CCC	-4	PRO	-	expression tag	UNP A0A0B8QZ66
CCC	-3	ARG	-	expression tag	UNP A0A0B8QZ66

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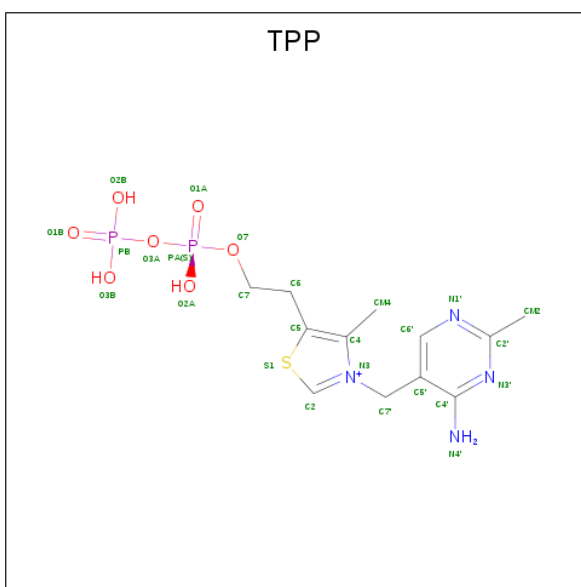
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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	-2	GLY	-	expression tag	UNP A0A0B8QZ66
CCC	-1	SER	-	expression tag	UNP A0A0B8QZ66
CCC	0	HIS	-	expression tag	UNP A0A0B8QZ66
CCC	34	HIS	GLN	engineered mutation	UNP A0A0B8QZ66
CCC	290	VAL	ALA	engineered mutation	UNP A0A0B8QZ66
CCC	386	PRO	SER	engineered mutation	UNP A0A0B8QZ66
DDD	-19	MET	-	initiating methionine	UNP A0A0B8QZ66
DDD	-18	GLY	-	expression tag	UNP A0A0B8QZ66
DDD	-17	SER	-	expression tag	UNP A0A0B8QZ66
DDD	-16	SER	-	expression tag	UNP A0A0B8QZ66
DDD	-15	HIS	-	expression tag	UNP A0A0B8QZ66
DDD	-14	HIS	-	expression tag	UNP A0A0B8QZ66
DDD	-13	HIS	-	expression tag	UNP A0A0B8QZ66
DDD	-12	HIS	-	expression tag	UNP A0A0B8QZ66
DDD	-11	HIS	-	expression tag	UNP A0A0B8QZ66
DDD	-10	HIS	-	expression tag	UNP A0A0B8QZ66
DDD	-9	SER	-	expression tag	UNP A0A0B8QZ66
DDD	-8	SER	-	expression tag	UNP A0A0B8QZ66
DDD	-7	GLY	-	expression tag	UNP A0A0B8QZ66
DDD	-6	LEU	-	expression tag	UNP A0A0B8QZ66
DDD	-5	VAL	-	expression tag	UNP A0A0B8QZ66
DDD	-4	PRO	-	expression tag	UNP A0A0B8QZ66
DDD	-3	ARG	-	expression tag	UNP A0A0B8QZ66
DDD	-2	GLY	-	expression tag	UNP A0A0B8QZ66
DDD	-1	SER	-	expression tag	UNP A0A0B8QZ66
DDD	0	HIS	-	expression tag	UNP A0A0B8QZ66
DDD	34	HIS	GLN	engineered mutation	UNP A0A0B8QZ66
DDD	290	VAL	ALA	engineered mutation	UNP A0A0B8QZ66
DDD	386	PRO	SER	engineered mutation	UNP A0A0B8QZ66

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	CCC	1	Total Mg 1 1	0	0
2	BBB	1	Total Mg 1 1	0	0
2	DDD	1	Total Mg 1 1	0	0
2	AAA	1	Total Mg 1 1	0	0

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	AAA	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	BBB	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	CCC	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	DDD	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

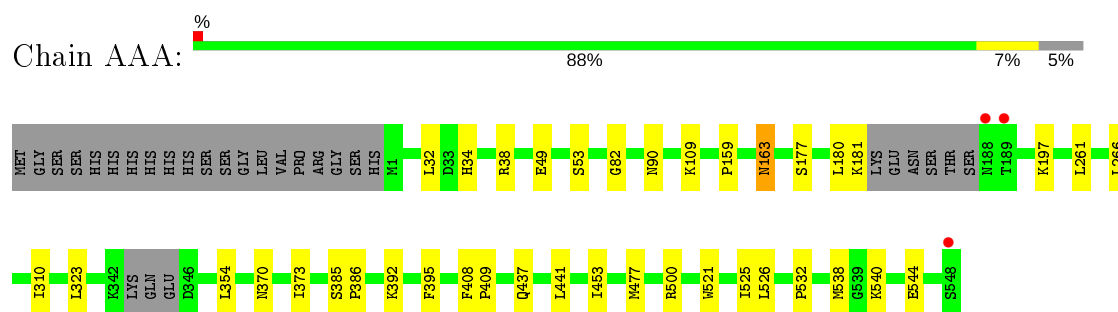
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	301	Total O 302 302	0	2
4	BBB	277	Total O 277 277	0	0
4	CCC	300	Total O 301 301	0	2
4	DDD	303	Total O 303 303	0	0

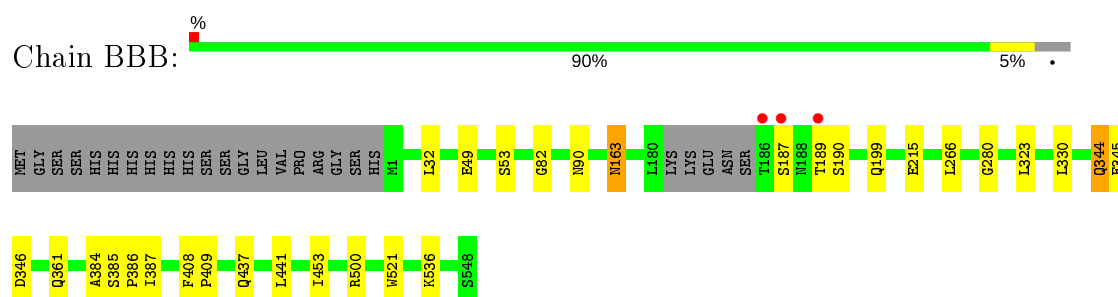
3 Residue-property plots [i](#)

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.

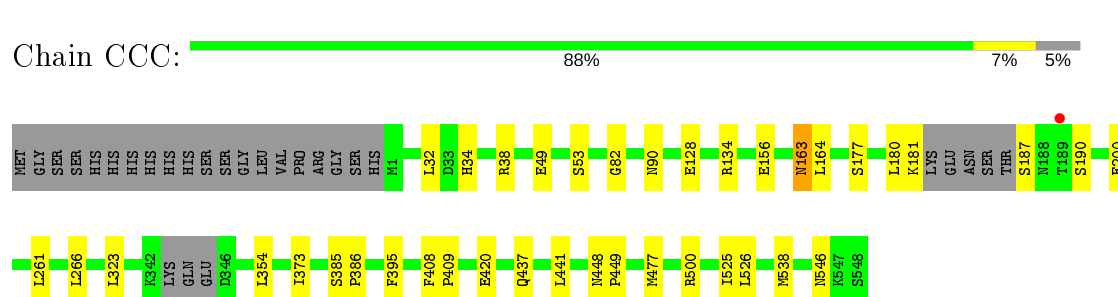
- Molecule 1: Alpha-keto acid decarboxylase



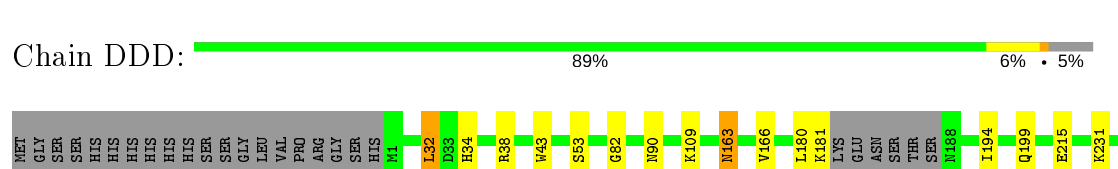
- Molecule 1: Alpha-keto acid decarboxylase



- Molecule 1: Alpha-keto acid decarboxylase



- Molecule 1: Alpha-keto acid decarboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	128.19Å 128.27Å 147.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.86 – 1.80 96.86 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (96.86-1.80) 99.3 (96.86-1.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.183 , 0.210 0.190 , 0.214	Depositor DCC
R_{free} test set	11416 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.176 for k,h,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	17973	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	AAA	0.72	0/4264	0.76	1/5785 (0.0%)
1	BBB	0.73	0/4263	0.75	0/5789
1	CCC	0.73	0/4259	0.76	3/5783 (0.1%)
1	DDD	0.72	0/4259	0.75	0/5780
All	All	0.72	0/17045	0.76	4/23137 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	500	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	AAA	477	MET	N-CA-CB	6.13	121.63	110.60
1	CCC	477	MET	N-CA-CB	5.18	119.92	110.60
1	CCC	500	ARG	NE-CZ-NH1	5.17	122.88	120.30

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	AAA	4170	0	4071	20	0
1	BBB	4177	0	4066	18	0
1	CCC	4165	0	4040	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DDD	4170	0	4067	20	0
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
2	CCC	1	0	0	0	0
2	DDD	1	0	0	0	0
3	AAA	26	0	16	3	0
3	BBB	26	0	16	1	0
3	CCC	26	0	16	2	0
3	DDD	26	0	16	2	0
4	AAA	302	0	0	2	0
4	BBB	277	0	0	2	0
4	CCC	301	0	0	1	0
4	DDD	303	0	0	3	0
All	All	17973	0	16308	82	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 (82) 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:CCC:128:GLU:HG2	1:CCC:134[B]:ARG:CZ	2.12	0.79
1:CCC:163:ASN:C	1:CCC:163:ASN:HD22	1.89	0.74
1:BBB:163:ASN:C	1:BBB:163:ASN:HD22	1.91	0.73
1:DDD:163:ASN:HD22	1:DDD:163:ASN:C	1.95	0.69
1:BBB:361:GLN:NE2	4:BBB:702:HOH:O	2.27	0.68
1:AAA:163:ASN:HD22	1:AAA:163:ASN:C	1.99	0.67
3:AAA:602:TPP:H2	3:AAA:602:TPP:HN42	1.62	0.64
1:CCC:128:GLU:HG2	1:CCC:134[B]:ARG:NE	2.16	0.61
1:DDD:342:LYS:NZ	4:DDD:701:HOH:O	2.21	0.58
1:BBB:266:LEU:HD23	1:BBB:266:LEU:C	2.25	0.58
1:BBB:345:GLU:HG2	1:BBB:346:ASP:O	2.05	0.56
3:AAA:602:TPP:C2	3:AAA:602:TPP:HN42	2.19	0.56
1:CCC:266:LEU:C	1:CCC:266:LEU:HD23	2.26	0.56
1:DDD:534:VAL:HG11	4:DDD:905:HOH:O	2.05	0.55
1:DDD:109:LYS:NZ	4:DDD:706:HOH:O	2.39	0.55
1:DDD:266:LEU:C	1:DDD:266:LEU:HD23	2.27	0.55
1:AAA:266:LEU:HD23	1:AAA:266:LEU:C	2.27	0.54
3:CCC:602:TPP:HN42	3:CCC:602:TPP:H2	1.73	0.54
1:AAA:500:ARG:NH2	4:AAA:705:HOH:O	2.39	0.54
1:AAA:197:LYS:HD3	1:AAA:310:ILE:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:163:ASN:C	1:CCC:163:ASN:ND2	2.62	0.51
1:CCC:546:ASN:O	1:DDD:166:VAL:HG11	2.10	0.51
3:CCC:602:TPP:HN42	3:CCC:602:TPP:C2	2.23	0.51
1:AAA:109:LYS:NZ	4:AAA:711:HOH:O	2.41	0.50
1:DDD:194:ILE:HG12	1:DDD:310:ILE:HD11	1.92	0.50
1:BBB:163:ASN:C	1:BBB:163:ASN:ND2	2.63	0.50
1:AAA:370:ASN:HA	1:AAA:392:LYS:O	2.12	0.49
1:AAA:163:ASN:C	1:AAA:163:ASN:ND2	2.66	0.48
1:AAA:408:PHE:HB3	1:AAA:409:PRO:HD3	1.95	0.48
1:BBB:453:ILE:HD11	1:BBB:521:TRP:CE2	2.49	0.48
1:DDD:180:LEU:O	1:DDD:181:LYS:C	2.52	0.48
1:CCC:408:PHE:HB3	1:CCC:409:PRO:HD3	1.96	0.47
1:CCC:180:LEU:O	1:CCC:181:LYS:C	2.52	0.47
1:BBB:187:SER:O	1:BBB:190:SER:HB3	2.15	0.47
3:DDD:602:TPP:C2	3:DDD:602:TPP:HN42	2.27	0.47
1:BBB:53:SER:OG	1:BBB:82:GLY:HA3	2.15	0.46
1:BBB:215:GLU:HB2	1:BBB:280:GLY:CA	2.46	0.46
1:BBB:408:PHE:HB3	1:BBB:409:PRO:HD3	1.97	0.46
1:BBB:500:ARG:NH2	4:BBB:704:HOH:O	2.32	0.46
1:CCC:53:SER:OG	1:CCC:82:GLY:HA3	2.15	0.46
1:AAA:180:LEU:O	1:AAA:181:LYS:C	2.54	0.45
1:DDD:53:SER:OG	1:DDD:82:GLY:HA3	2.16	0.45
1:DDD:342:LYS:O	1:DDD:343:LYS:C	2.55	0.45
1:DDD:408:PHE:HB3	1:DDD:409:PRO:HD3	1.97	0.45
1:DDD:231:LYS:NZ	1:DDD:328:LEU:O	2.49	0.45
1:AAA:540:LYS:HG3	1:CCC:420:GLU:OE1	2.17	0.45
1:AAA:53:SER:OG	1:AAA:82:GLY:HA3	2.17	0.45
1:BBB:344:GLN:HG2	1:BBB:344:GLN:O	2.17	0.45
1:DDD:163:ASN:ND2	1:DDD:163:ASN:C	2.67	0.44
1:CCC:385:SER:N	1:CCC:386:PRO:CD	2.80	0.44
1:AAA:385:SER:N	1:AAA:386:PRO:CD	2.81	0.44
1:CCC:34:HIS:O	1:CCC:38:ARG:HG3	2.18	0.43
1:DDD:215:GLU:HB2	1:DDD:280:GLY:CA	2.49	0.43
1:AAA:34:HIS:O	1:AAA:38:ARG:HG3	2.19	0.43
1:BBB:441:LEU:C	1:BBB:441:LEU:HD23	2.39	0.43
1:DDD:34:HIS:O	1:DDD:38:ARG:HG3	2.18	0.43
1:AAA:544:GLU:HG2	4:CCC:811:HOH:O	2.19	0.43
1:DDD:385:SER:N	1:DDD:386:PRO:CD	2.82	0.43
1:DDD:441:LEU:C	1:DDD:441:LEU:HD23	2.39	0.43
1:CCC:441:LEU:C	1:CCC:441:LEU:HD23	2.39	0.43
1:AAA:261:LEU:HD12	1:AAA:538:MET:SD	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:163:ASN:HD22	1:CCC:164:LEU:N	2.17	0.42
1:AAA:525:ILE:C	1:AAA:526:LEU:HD22	2.39	0.42
1:BBB:385:SER:N	1:BBB:386:PRO:CD	2.83	0.42
1:AAA:441:LEU:C	1:AAA:441:LEU:HD23	2.40	0.42
1:DDD:199:GLN:HB2	1:DDD:330:LEU:HD22	2.02	0.42
1:CCC:187:SER:O	1:CCC:190:SER:HB3	2.18	0.42
1:AAA:49:GLU:OE2	3:BBB:602:TPP:N1'	2.52	0.42
1:CCC:128:GLU:HG2	1:CCC:134[B]:ARG:NH2	2.35	0.42
3:AAA:602:TPP:N1'	1:BBB:49:GLU:OE2	2.53	0.42
1:DDD:32:LEU:HD21	1:DDD:43:TRP:CD2	2.55	0.41
1:AAA:373:ILE:O	1:AAA:395:PHE:HA	2.21	0.41
1:AAA:453:ILE:HD11	1:AAA:521:TRP:CE2	2.55	0.41
1:CCC:261:LEU:HD12	1:CCC:538:MET:SD	2.60	0.41
1:BBB:199:GLN:HB2	1:BBB:330:LEU:HD22	2.03	0.41
1:BBB:345:GLU:HG3	1:BBB:346:ASP:N	2.35	0.41
1:BBB:384:ALA:HA	1:BBB:387:ILE:HD12	2.03	0.41
1:CCC:49:GLU:OE2	3:DDD:602:TPP:N1'	2.54	0.41
1:DDD:525:ILE:C	1:DDD:526:LEU:HD22	2.42	0.41
1:CCC:373:ILE:O	1:CCC:395:PHE:HA	2.21	0.41
1:CCC:448:ASN:N	1:CCC:449:PRO:CD	2.84	0.40
1:CCC:525:ILE:C	1:CCC:526:LEU:HD22	2.41	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	AAA	536/568 (94%)	524 (98%)	12 (2%)	0	100	100
1	BBB	539/568 (95%)	527 (98%)	12 (2%)	0	100	100
1	CCC	537/568 (94%)	526 (98%)	11 (2%)	0	100	100
1	DDD	539/568 (95%)	527 (98%)	11 (2%)	1 (0%)	47	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2151/2272 (95%)	2104 (98%)	46 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	DDD	343	LYS

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	AAA	447/493 (91%)	438 (98%)	9 (2%)	55	44
1	BBB	445/493 (90%)	437 (98%)	8 (2%)	59	48
1	CCC	444/493 (90%)	435 (98%)	9 (2%)	55	44
1	DDD	442/493 (90%)	435 (98%)	7 (2%)	62	54
All	All	1778/1972 (90%)	1745 (98%)	33 (2%)	57	46

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	32	LEU
1	AAA	90	ASN
1	AAA	159	PRO
1	AAA	163	ASN
1	AAA	177	SER
1	AAA	323	LEU
1	AAA	354	LEU
1	AAA	437	GLN
1	AAA	532	PRO
1	BBB	32	LEU
1	BBB	90	ASN
1	BBB	163	ASN
1	BBB	189	THR
1	BBB	323	LEU

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Mol	Chain	Res	Type
1	BBB	344	GLN
1	BBB	437	GLN
1	BBB	536	LYS
1	CCC	32	LEU
1	CCC	90	ASN
1	CCC	156	GLU
1	CCC	163	ASN
1	CCC	177	SER
1	CCC	200	GLU
1	CCC	323	LEU
1	CCC	354	LEU
1	CCC	437	GLN
1	DDD	32	LEU
1	DDD	90	ASN
1	DDD	163	ASN
1	DDD	323	LEU
1	DDD	353	LEU
1	DDD	437	GLN
1	DDD	528	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TPP	AAA	602	2	22,27,27	0.66	0	29,40,40	0.93	1 (3%)
3	TPP	DDD	602	2	22,27,27	0.68	0	29,40,40	0.87	0
3	TPP	CCC	602	2	22,27,27	0.70	0	29,40,40	0.82	1 (3%)
3	TPP	BBB	602	2	22,27,27	0.57	0	29,40,40	0.95	1 (3%)

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
3	TPP	AAA	602	2	-	4/16/17/17	0/2/2/2
3	TPP	DDD	602	2	-	4/16/17/17	0/2/2/2
3	TPP	CCC	602	2	-	4/16/17/17	0/2/2/2
3	TPP	BBB	602	2	-	5/16/17/17	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BBB	602	TPP	C5-C4-N3	2.57	112.71	107.57
3	CCC	602	TPP	C5-C4-N3	2.28	112.13	107.57
3	AAA	602	TPP	C5-C4-N3	2.27	112.11	107.57

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	602	TPP	C4-C5-C6-C7
3	AAA	602	TPP	PA-O3A-PB-O3B
3	DDD	602	TPP	C4-C5-C6-C7
3	CCC	602	TPP	C4-C5-C6-C7
3	CCC	602	TPP	PA-O3A-PB-O3B
3	BBB	602	TPP	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	BBB	602	TPP	PA-O3A-PB-O3B
3	DDD	602	TPP	PA-O3A-PB-O1B
3	BBB	602	TPP	PB-O3A-PA-O2A
3	AAA	602	TPP	C4'-C5'-C7'-N3
3	BBB	602	TPP	PA-O3A-PB-O1B
3	AAA	602	TPP	PA-O3A-PB-O2B
3	DDD	602	TPP	PA-O3A-PB-O2B
3	DDD	602	TPP	PA-O3A-PB-O3B
3	CCC	602	TPP	PA-O3A-PB-O2B
3	BBB	602	TPP	PA-O3A-PB-O2B
3	CCC	602	TPP	PA-O3A-PB-O1B

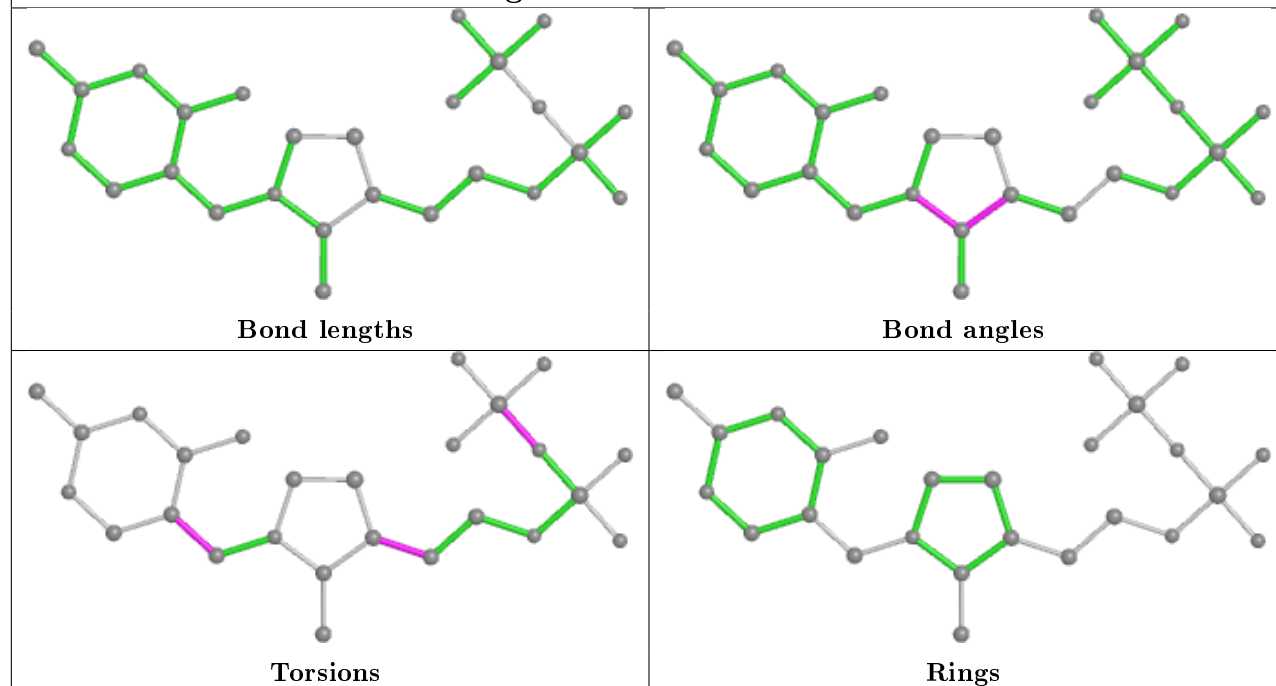
There are no ring outliers.

4 monomers are involved in 8 short contacts:

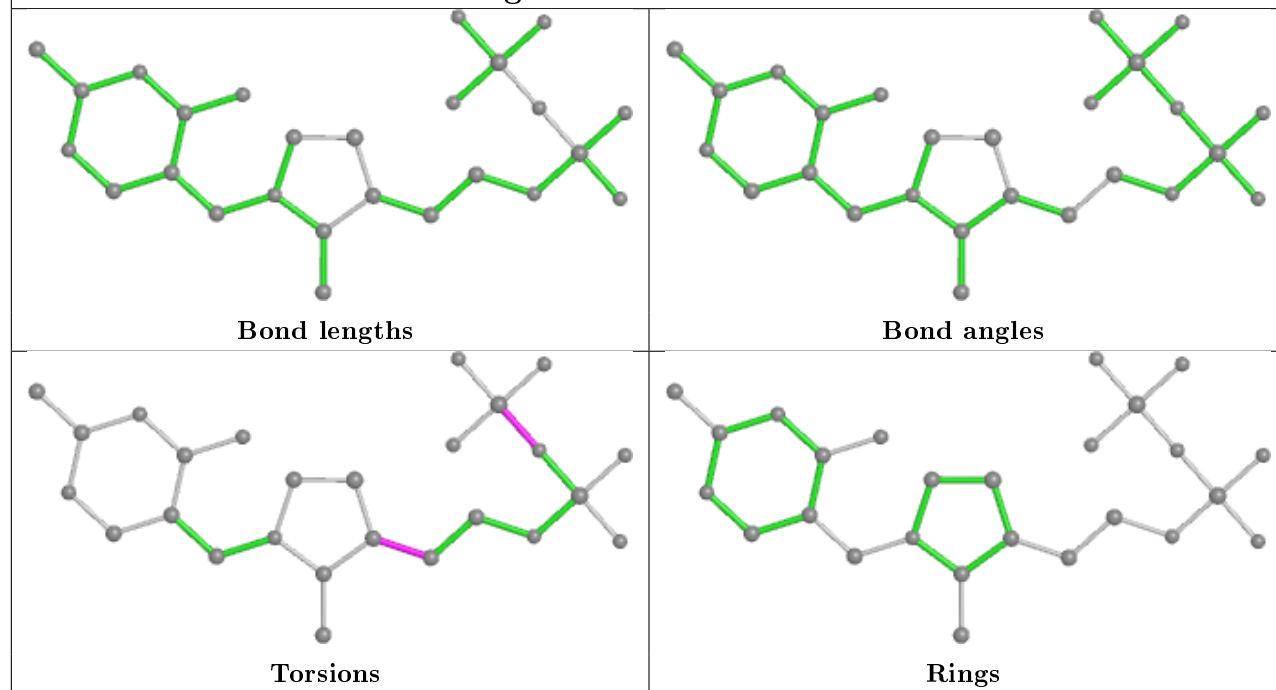
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	602	TPP	3	0
3	DDD	602	TPP	2	0
3	CCC	602	TPP	2	0
3	BBB	602	TPP	1	0

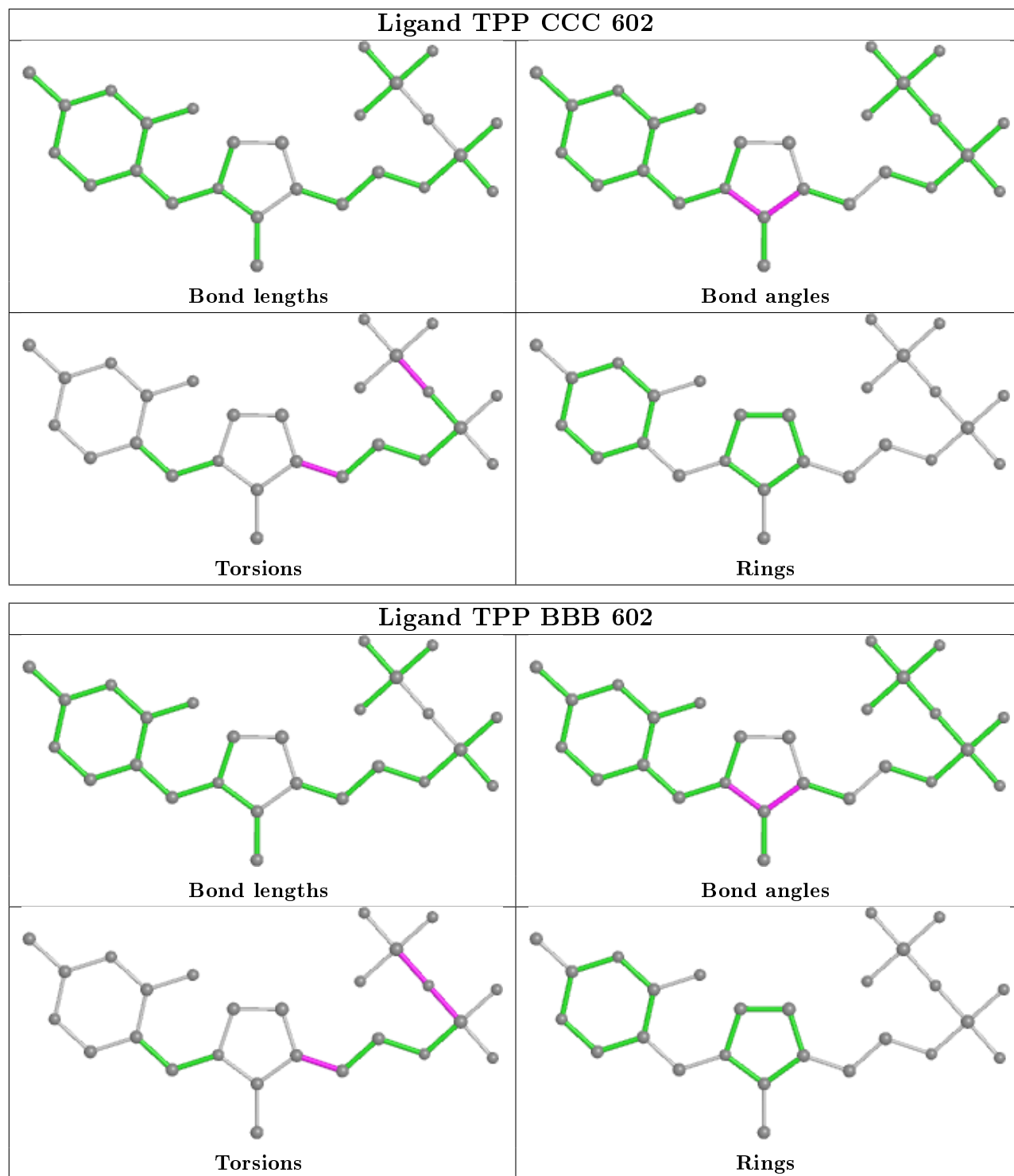
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand TPP AAA 602



Ligand TPP DDD 602





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 [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	AAA	539/568 (94%)	-0.48	3 (0%) 89 87	27, 36, 56, 79	0
1	BBB	543/568 (95%)	-0.44	3 (0%) 89 87	28, 38, 62, 114	0
1	CCC	540/568 (95%)	-0.44	1 (0%) 95 93	27, 36, 60, 107	0
1	DDD	542/568 (95%)	-0.44	2 (0%) 92 90	27, 37, 59, 90	0
All	All	2164/2272 (95%)	-0.45	9 (0%) 92 90	27, 37, 59, 114	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	189	THR	8.3
1	BBB	186	THR	6.6
1	BBB	189	THR	4.3
1	DDD	343	LYS	3.7
1	DDD	344	GLN	3.7
1	CCC	189	THR	3.3
1	AAA	188	ASN	3.1
1	AAA	548	SER	2.9
1	BBB	187	SER	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 ⓘ

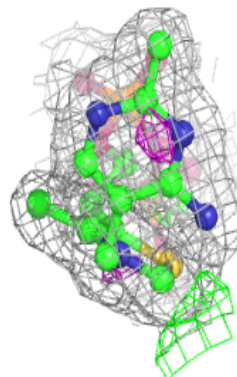
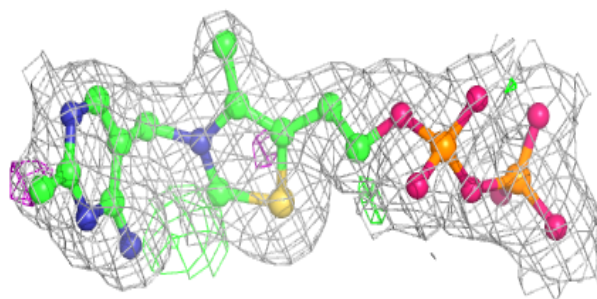
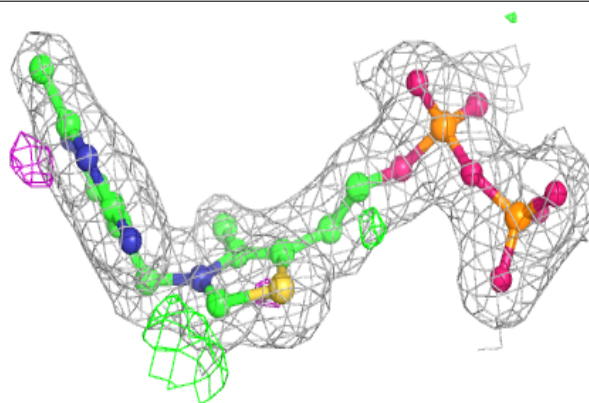
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TPP	DDD	602	26/26	0.98	0.08	26,29,33,36	0
3	TPP	CCC	602	26/26	0.98	0.09	28,31,36,42	0
2	MG	CCC	601	1/1	0.98	0.08	30,30,30,30	0
2	MG	BBB	601	1/1	0.98	0.08	28,28,28,28	0
3	TPP	BBB	602	26/26	0.99	0.09	26,30,33,41	0
3	TPP	AAA	602	26/26	0.99	0.07	27,32,36,41	0
2	MG	AAA	601	1/1	0.99	0.08	30,30,30,30	0
2	MG	DDD	601	1/1	1.00	0.06	27,27,27,27	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.

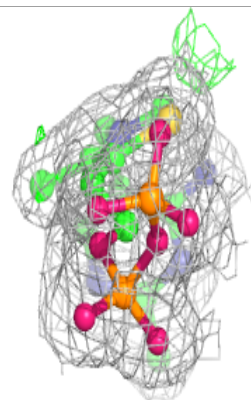
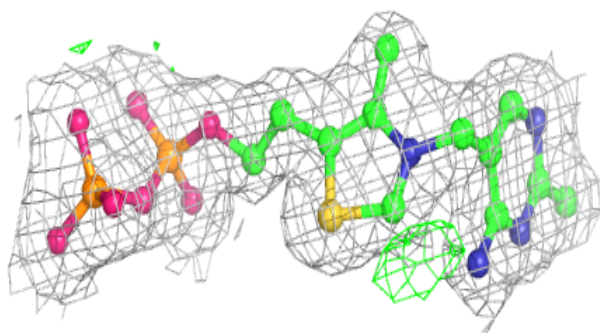
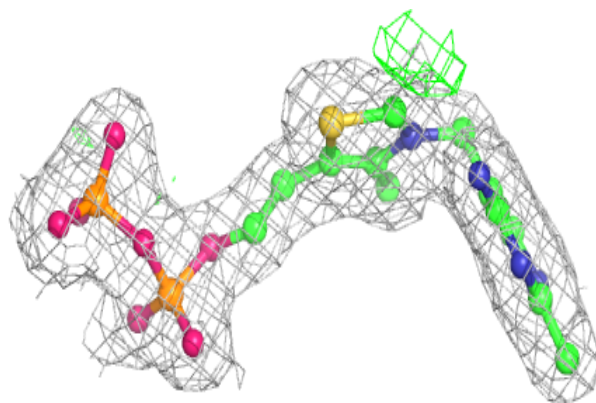
Electron density around TPP DDD 602:

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

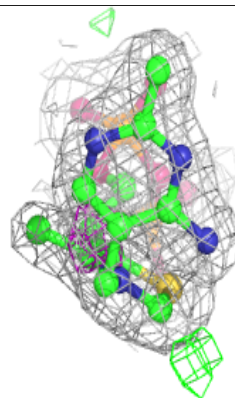
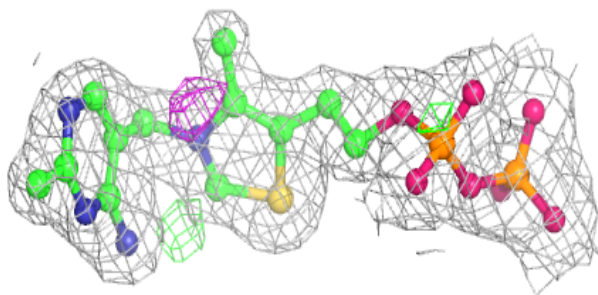
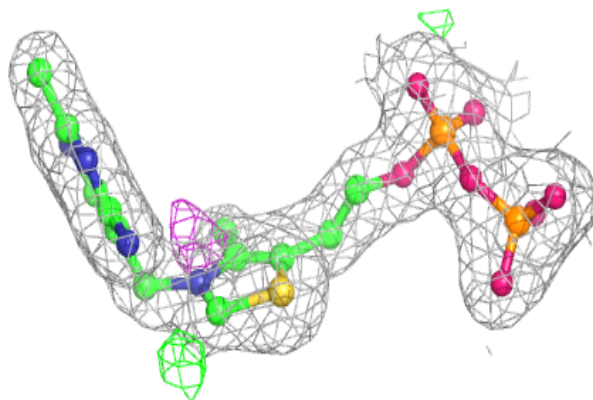


Electron density around TPP CCC 602:

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

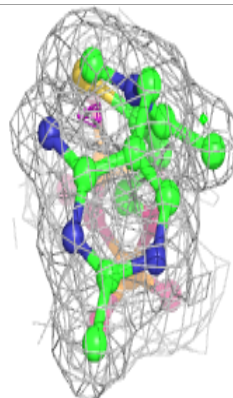
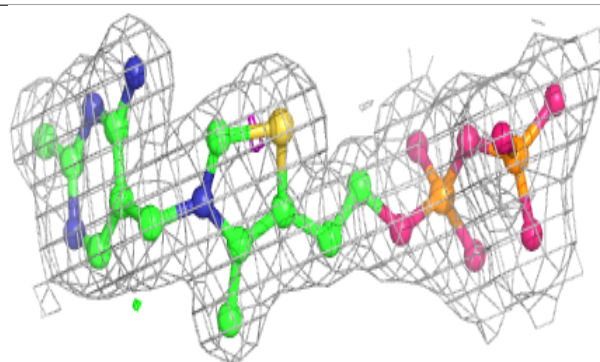
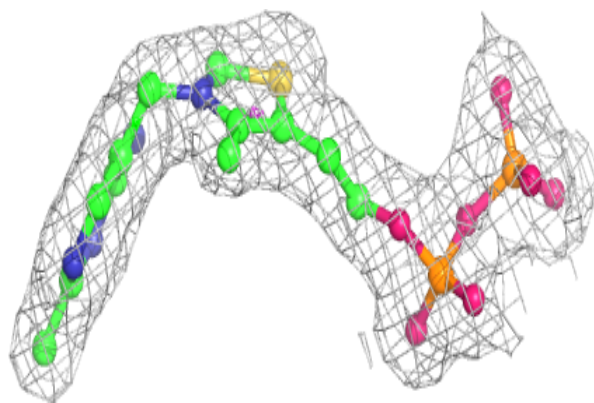
**Electron density around TPP BBB 602:**

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



Electron density around TPP AAA 602:

$2mF_o-DF_c$ (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.