



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2024 – 06:31 pm GMT

PDB ID : 7ORX
Title : Rhodococcus jostii RHA1 thiamine diphosphate-dependent 4-hydroxybenzoyl formate decarboxylase
Authors : Wilkinson, R.C.; Fulop, V.
Deposited on : 2021-06-06
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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

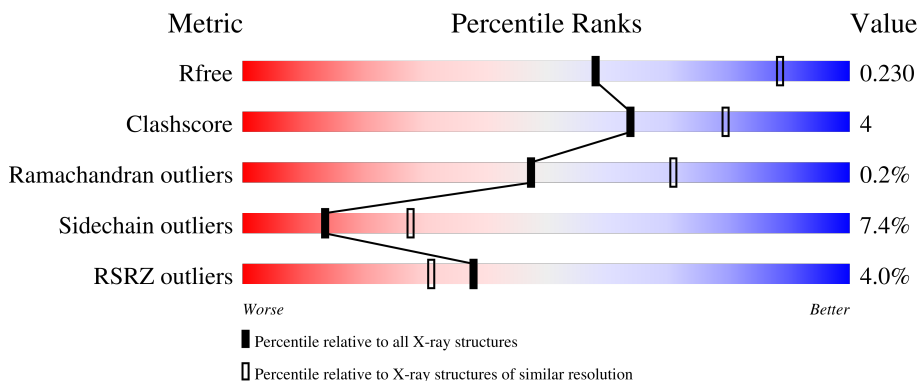
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	531	 6% 85% 13% ..
1	BBB	531	 5% 85% 13% ..
1	CCC	531	 2% 87% 12% .
1	DDD	531	 2% 86% 12% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15727 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 Probable benzoylformate decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	AAA	527	3881	2456	653	762	1	9	0	0	0
1	BBB	527	3881	2456	653	762	1	9	0	0	0
1	CCC	531	3913	2477	658	767	1	10	0	0	0
1	DDD	527	3881	2456	653	762	1	9	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-2	PHE	-	expression tag	UNP Q0SCE8
AAA	-1	GLN	-	expression tag	UNP Q0SCE8
AAA	0	GLY	-	expression tag	UNP Q0SCE8
BBB	-2	PHE	-	expression tag	UNP Q0SCE8
BBB	-1	GLN	-	expression tag	UNP Q0SCE8
BBB	0	GLY	-	expression tag	UNP Q0SCE8
CCC	-2	PHE	-	expression tag	UNP Q0SCE8
CCC	-1	GLN	-	expression tag	UNP Q0SCE8
CCC	0	GLY	-	expression tag	UNP Q0SCE8
DDD	-2	PHE	-	expression tag	UNP Q0SCE8
DDD	-1	GLN	-	expression tag	UNP Q0SCE8
DDD	0	GLY	-	expression tag	UNP Q0SCE8

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	AAA	1	Total	Na	0	0
			1	1		
3	BBB	1	Total	Na	0	0
			1	1		
3	CCC	1	Total	Na	0	0
			1	1		
3	DDD	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	AAA	12	Total	O	0	0
			12	12		

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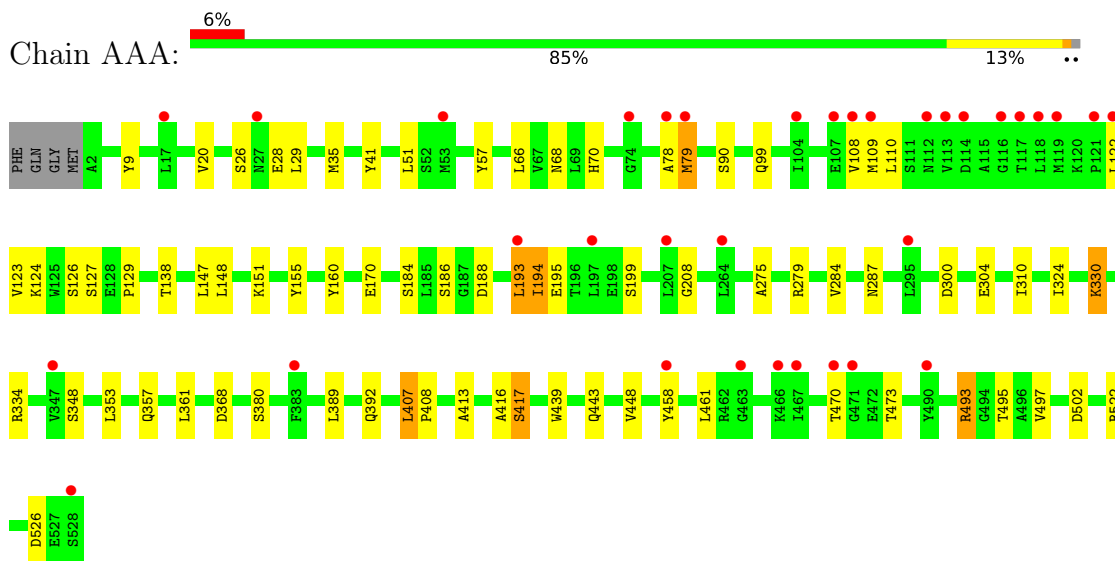
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	BBB	17	Total 17	O 17	0	0
4	CCC	15	Total 15	O 15	0	0
4	DDD	19	Total 19	O 19	0	0

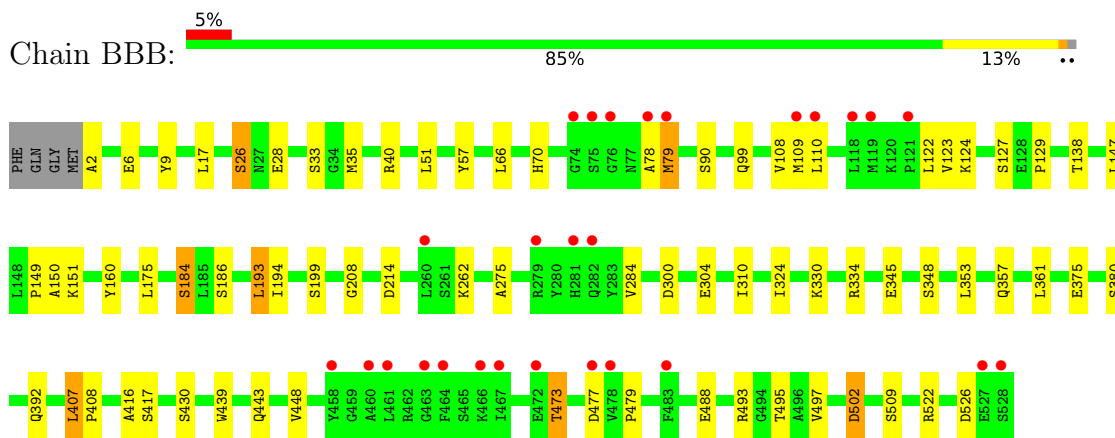
3 Residue-property plots

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.

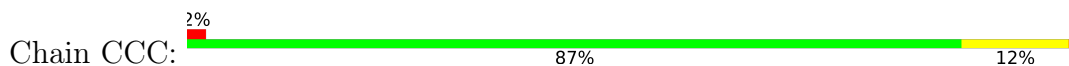
- Molecule 1: Probable benzoylformate decarboxylase

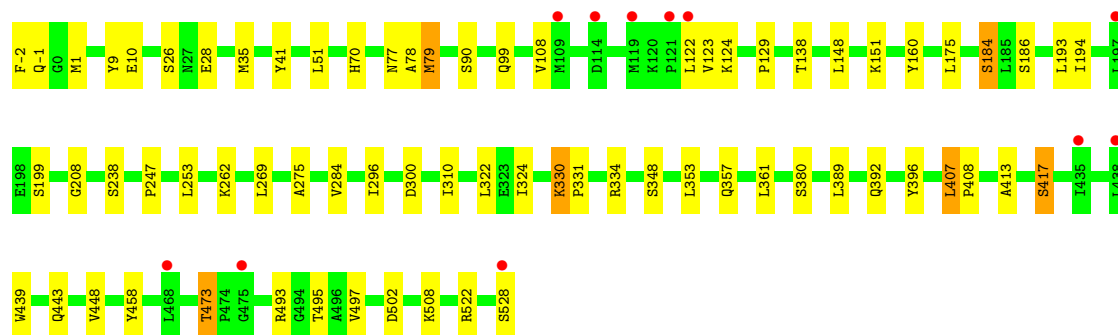


- Molecule 1: Probable benzoylformate decarboxylase

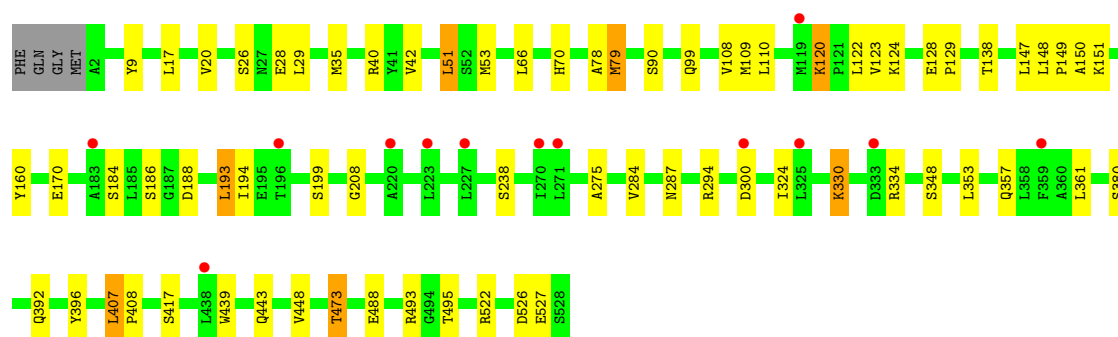
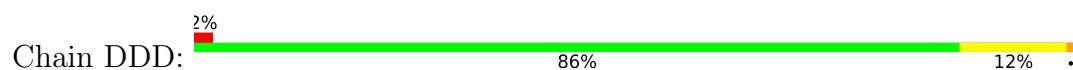


- Molecule 1: Probable benzoylformate decarboxylase





- Molecule 1: Probable benzoylformate decarboxylase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	123.50Å 132.24Å 138.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.42 – 2.60 90.26 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (90.42-2.60) 100.0 (90.26-2.60)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.62Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.195 , 0.233 0.192 , 0.230	Depositor DCC
R_{free} test set	2975 reflections (4.22%)	wwPDB-VP
Wilson B-factor (Å ²)	67.8	Xtrriage
Anisotropy	0.680	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.008 for -h,l,k	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15727	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: NA, TPP, SEP

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	0.77	1/3962 (0.0%)	0.92	2/5425 (0.0%)
1	BBB	0.84	3/3962 (0.1%)	0.97	4/5425 (0.1%)
1	CCC	0.82	0/3995	0.96	1/5468 (0.0%)
1	DDD	0.80	2/3962 (0.1%)	0.94	2/5425 (0.0%)
All	All	0.81	6/15881 (0.0%)	0.95	9/21743 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AAA	0	1
1	BBB	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DDD	128	GLU	CD-OE2	7.77	1.34	1.25
1	BBB	304	GLU	CD-OE1	6.30	1.32	1.25
1	AAA	304	GLU	CD-OE2	5.83	1.32	1.25
1	BBB	345	GLU	CD-OE2	5.72	1.31	1.25
1	BBB	488	GLU	CD-OE1	5.65	1.31	1.25
1	DDD	128	GLU	CD-OE1	5.21	1.31	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	40	ARG	CG-CD-NE	7.47	127.48	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	124	LYS	CB-CA-C	-7.06	96.28	110.40
1	BBB	124	LYS	CB-CA-C	-6.83	96.75	110.40
1	CCC	124	LYS	CB-CA-C	-6.74	96.91	110.40
1	BBB	40	ARG	CG-CD-NE	6.73	125.93	111.80
1	AAA	124	LYS	CB-CA-C	-6.58	97.23	110.40
1	AAA	279	ARG	CG-CD-NE	-5.53	100.19	111.80
1	BBB	502	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	BBB	502	ASP	CB-CA-C	-5.07	100.26	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	127	SER	Peptide
1	BBB	127	SER	Peptide

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	AAA	3881	0	3802	39	0
1	BBB	3881	0	3802	31	0
1	CCC	3913	0	3834	32	0
1	DDD	3881	0	3802	32	0
2	AAA	26	0	16	4	0
2	BBB	26	0	16	0	0
2	CCC	26	0	16	1	0
2	DDD	26	0	16	1	0
3	AAA	1	0	0	0	0
3	BBB	1	0	0	0	0
3	CCC	1	0	0	0	0
3	DDD	1	0	0	0	0
4	AAA	12	0	0	1	0
4	BBB	17	0	0	0	0
4	CCC	15	0	0	1	0
4	DDD	19	0	0	1	0
All	All	15727	0	15304	130	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 4.

All (130) 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:DDD:79:MET:HE2	1:DDD:122:LEU:HD12	1.60	0.83
1:BBB:79:MET:HE2	1:BBB:122:LEU:HD12	1.64	0.78
1:CCC:79:MET:HE2	1:CCC:122:LEU:HD12	1.68	0.75
1:AAA:79:MET:HE2	1:AAA:122:LEU:HD12	1.69	0.73
2:AAA:601:TPP:HN42	2:AAA:601:TPP:H2	1.54	0.71
1:AAA:29:LEU:HD22	1:BBB:473:THR:HG21	1.75	0.67
2:AAA:601:TPP:HN42	2:AAA:601:TPP:C2	2.11	0.63
1:DDD:473:THR:HB	4:DDD:716:HOH:O	1.97	0.63
2:DDD:601:TPP:HN42	2:DDD:601:TPP:H2	1.65	0.61
1:AAA:493:ARG:HG2	1:AAA:493:ARG:HH11	1.65	0.59
1:BBB:79:MET:CE	1:BBB:122:LEU:HD12	2.33	0.59
1:BBB:184:SER:O	1:CCC:184:SER:O	2.21	0.59
1:BBB:348:SER:OG	1:BBB:357:GLN:NE2	2.36	0.58
1:BBB:51:LEU:HD13	1:BBB:78:ALA:HB1	1.85	0.58
1:CCC:51:LEU:HD13	1:CCC:78:ALA:HB1	1.85	0.58
1:CCC:79:MET:CE	1:CCC:122:LEU:HD12	2.33	0.57
1:AAA:51:LEU:HD13	1:AAA:78:ALA:HB1	1.86	0.57
1:CCC:348:SER:OG	1:CCC:357:GLN:NE2	2.38	0.57
1:DDD:348:SER:OG	1:DDD:357:GLN:NE2	2.38	0.56
1:DDD:79:MET:CE	1:DDD:122:LEU:HD12	2.33	0.56
1:AAA:348:SER:OG	1:AAA:357:GLN:NE2	2.39	0.55
1:AAA:458:TYR:CD1	2:AAA:601:TPP:H61	2.42	0.54
1:CCC:473:THR:HG21	1:DDD:29:LEU:HD22	1.90	0.54
1:AAA:208:GLY:HA3	1:AAA:275:ALA:HB2	1.91	0.52
1:CCC:129:PRO:HG3	1:CCC:138:THR:HG21	1.92	0.52
1:BBB:497:VAL:HG22	1:BBB:502:ASP:HB3	1.92	0.51
1:CCC:208:GLY:HA3	1:CCC:275:ALA:HB2	1.92	0.51
1:DDD:109:MET:HG3	1:DDD:110:LEU:HD22	1.93	0.50
1:CCC:458:TYR:CD1	2:CCC:601:TPP:H61	2.45	0.50
1:DDD:208:GLY:HA3	1:DDD:275:ALA:HB2	1.93	0.50
1:BBB:208:GLY:HA3	1:BBB:275:ALA:HB2	1.94	0.50
1:DDD:488:GLU:OE1	1:DDD:493:ARG:NH1	2.45	0.49
1:BBB:439:TRP:CZ2	1:BBB:443:GLN:HG3	2.48	0.48
1:CCC:330:LYS:HE2	1:CCC:331:PRO:HD2	1.94	0.48
1:CCC:407:LEU:HB3	1:CCC:408:PRO:HD3	1.96	0.48
1:DDD:9:TYR:CZ	1:DDD:35:MET:HA	2.49	0.48
1:AAA:29:LEU:CD2	1:BBB:473:THR:HG21	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:407:LEU:HB3	1:DDD:408:PRO:HD3	1.95	0.47
1:BBB:439:TRP:CH2	1:BBB:443:GLN:HG3	2.50	0.47
1:AAA:79:MET:CE	1:AAA:122:LEU:HD12	2.41	0.47
1:AAA:170:GLU:OE1	1:DDD:287:ASN:HA	2.15	0.47
1:AAA:470:THR:HB	1:BBB:33:SER:HB3	1.95	0.47
1:CCC:35:MET:HE1	1:CCC:41:TYR:HB2	1.96	0.47
1:DDD:330:LYS:HA	1:DDD:330:LYS:HE2	1.95	0.47
1:BBB:99:GLN:HG2	1:BBB:108:VAL:CG2	2.45	0.46
1:DDD:51:LEU:HD13	1:DDD:78:ALA:HB1	1.96	0.46
1:DDD:20:VAL:HG22	1:DDD:66:LEU:HD23	1.98	0.45
1:AAA:287:ASN:HA	1:DDD:170:GLU:OE1	2.16	0.45
1:AAA:439:TRP:CH2	1:AAA:443:GLN:HG3	2.51	0.45
1:DDD:147:LEU:HA	1:DDD:151:LYS:HG2	1.98	0.45
1:AAA:348:SER:HB2	1:AAA:357:GLN:HE22	1.82	0.45
1:AAA:407:LEU:HB3	1:AAA:408:PRO:HD3	1.99	0.45
1:DDD:28:GLU:OE2	1:DDD:70:HIS:HA	2.17	0.45
1:AAA:439:TRP:CZ2	1:AAA:443:GLN:HG3	2.52	0.45
1:BBB:28:GLU:OE2	1:BBB:70:HIS:HA	2.17	0.45
1:CCC:322:LEU:HD12	1:CCC:322:LEU:HA	1.85	0.45
1:DDD:439:TRP:CZ2	1:DDD:443:GLN:HG3	2.52	0.44
1:CCC:28:GLU:OE2	1:CCC:70:HIS:HA	2.17	0.44
1:DDD:42:VAL:HG12	1:DDD:53:MET:HE1	2.00	0.44
1:CCC:497:VAL:HG22	1:CCC:502:ASP:HB3	1.98	0.44
1:CCC:77:ASN:OD1	4:CCC:701:HOH:O	2.21	0.44
1:DDD:99:GLN:HG2	1:DDD:108:VAL:CG2	2.48	0.44
1:AAA:109:MET:HG3	1:AAA:110:LEU:HD22	2.00	0.44
1:BBB:149:PRO:HA	1:BBB:150:ALA:HA	1.84	0.44
1:DDD:129:PRO:HG3	1:DDD:138:THR:HG21	1.99	0.44
1:DDD:348:SER:HB2	1:DDD:357:GLN:HE22	1.82	0.43
1:AAA:28:GLU:OE2	1:AAA:70:HIS:HA	2.18	0.43
1:AAA:330:LYS:HA	1:AAA:330:LYS:HE2	2.00	0.43
1:CCC:269:LEU:HD11	1:CCC:296:ILE:HG12	2.00	0.43
1:DDD:149:PRO:HA	1:DDD:150:ALA:HA	1.86	0.43
1:BBB:9:TYR:CZ	1:BBB:35:MET:HA	2.53	0.43
1:DDD:439:TRP:CH2	1:DDD:443:GLN:HG3	2.53	0.43
1:AAA:35:MET:HE1	1:AAA:41:TYR:HB2	2.00	0.43
1:DDD:193:LEU:HD13	1:DDD:193:LEU:HA	1.87	0.43
1:BBB:147:LEU:HA	1:BBB:151:LYS:HG2	2.00	0.43
1:BBB:99:GLN:HG2	1:BBB:108:VAL:HG23	2.01	0.43
1:BBB:407:LEU:HB3	1:BBB:408:PRO:HD3	1.99	0.43
1:AAA:330:LYS:HA	1:AAA:330:LYS:CE	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:348:SER:HB2	1:CCC:357:GLN:HE22	1.84	0.43
1:CCC:148:LEU:HD12	1:CCC:148:LEU:HA	1.83	0.43
1:CCC:99:GLN:HG2	1:CCC:108:VAL:CG2	2.49	0.42
1:CCC:348:SER:CB	1:CCC:357:GLN:NE2	2.82	0.42
1:AAA:413:ALA:O	1:AAA:417:SER:HB2	2.19	0.42
1:BBB:193:LEU:HD13	1:BBB:193:LEU:HA	1.85	0.42
1:DDD:330:LYS:HA	1:DDD:330:LYS:CE	2.48	0.42
1:DDD:348:SER:CB	1:DDD:357:GLN:NE2	2.82	0.42
1:AAA:9:TYR:CZ	1:AAA:35:MET:HA	2.55	0.42
1:AAA:497:VAL:HG22	1:AAA:502:ASP:HB3	2.02	0.42
1:CCC:439:TRP:CZ2	1:CCC:443:GLN:HG3	2.54	0.42
1:AAA:129:PRO:HG3	1:AAA:138:THR:HG21	2.01	0.42
1:AAA:147:LEU:HA	1:AAA:151:LYS:HG2	2.02	0.42
1:AAA:310:ILE:HD12	1:AAA:310:ILE:C	2.40	0.42
1:AAA:348:SER:CB	1:AAA:357:GLN:NE2	2.83	0.42
1:AAA:148:LEU:HD12	1:AAA:148:LEU:HA	1.91	0.42
1:BBB:2:ALA:HA	1:BBB:6:GLU:OE1	2.20	0.42
1:AAA:57:TYR:CD1	1:AAA:416:ALA:HB2	2.55	0.41
2:AAA:601:TPP:C2	2:AAA:601:TPP:N4'	2.82	0.41
1:AAA:99:GLN:HG2	1:AAA:108:VAL:CG2	2.49	0.41
1:DDD:148:LEU:HD12	1:DDD:148:LEU:HA	1.92	0.41
1:BBB:17:LEU:HD23	1:BBB:66:LEU:HB2	2.03	0.41
1:BBB:109:MET:HG3	1:BBB:110:LEU:HD22	2.02	0.41
1:CCC:407:LEU:CB	1:CCC:408:PRO:HD3	2.51	0.41
1:CCC:439:TRP:CH2	1:CCC:443:GLN:HG3	2.54	0.41
1:BBB:129:PRO:HG3	1:BBB:138:THR:HG21	2.01	0.41
1:BBB:375:GLU:OE2	1:BBB:430:SER:HB3	2.20	0.41
1:CCC:330:LYS:HE2	1:CCC:330:LYS:HA	2.02	0.41
1:DDD:120:LYS:HA	1:DDD:120:LYS:HD2	1.62	0.41
1:BBB:407:LEU:CB	1:BBB:408:PRO:HD3	2.50	0.41
1:AAA:310:ILE:HD12	1:AAA:310:ILE:O	2.20	0.41
1:AAA:348:SER:HB2	1:AAA:357:GLN:NE2	2.36	0.41
1:BBB:348:SER:CB	1:BBB:357:GLN:NE2	2.84	0.41
1:CCC:9:TYR:CZ	1:CCC:35:MET:HA	2.56	0.41
1:AAA:20:VAL:HG22	1:AAA:66:LEU:HD23	2.02	0.41
1:AAA:68:ASN:ND2	4:AAA:703:HOH:O	2.53	0.41
1:CCC:1:MET:O	1:CCC:1:MET:CG	2.69	0.41
1:CCC:253:LEU:HD23	1:CCC:253:LEU:HA	1.95	0.41
1:AAA:193:LEU:HD13	1:AAA:193:LEU:HA	1.86	0.41
1:AAA:461:LEU:HD21	1:BBB:26:SEP:O1P	2.21	0.41
1:BBB:57:TYR:CD2	1:BBB:416:ALA:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:310:ILE:HD12	1:BBB:310:ILE:O	2.21	0.41
1:BBB:477:ASP:HB3	1:BBB:479:PRO:HD3	2.03	0.41
1:AAA:194:ILE:HG13	1:AAA:195:GLU:N	2.35	0.40
1:CCC:413:ALA:O	1:CCC:417:SER:HB2	2.21	0.40
1:DDD:238:SER:O	1:DDD:396:TYR:HA	2.22	0.40
1:AAA:126:SER:HA	1:AAA:155:TYR:O	2.21	0.40
1:CCC:238:SER:O	1:CCC:396:TYR:HA	2.22	0.40
1:CCC:310:ILE:O	1:CCC:310:ILE:HD12	2.21	0.40
1:CCC:348:SER:HB2	1:CCC:357:GLN:NE2	2.37	0.40
1:DDD:17:LEU:HD23	1:DDD:66:LEU:HB2	2.04	0.40
1:DDD:348:SER:HB2	1:DDD:357:GLN:NE2	2.36	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	AAA	524/531 (99%)	502 (96%)	21 (4%)	1 (0%)	47 71
1	BBB	524/531 (99%)	501 (96%)	22 (4%)	1 (0%)	47 71
1	CCC	528/531 (99%)	505 (96%)	22 (4%)	1 (0%)	47 71
1	DDD	524/531 (99%)	502 (96%)	21 (4%)	1 (0%)	47 71
All	All	2100/2124 (99%)	2010 (96%)	86 (4%)	4 (0%)	47 71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	123	VAL
1	AAA	123	VAL
1	DDD	123	VAL
1	CCC	123	VAL

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	AAA	406/409 (99%)	378 (93%)	28 (7%)	15	31
1	BBB	406/409 (99%)	377 (93%)	29 (7%)	14	29
1	CCC	409/409 (100%)	375 (92%)	34 (8%)	11	22
1	DDD	406/409 (99%)	377 (93%)	29 (7%)	14	29
All	All	1627/1636 (99%)	1507 (93%)	120 (7%)	13	28

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	79	MET
1	AAA	90	SER
1	AAA	160	TYR
1	AAA	184	SER
1	AAA	186	SER
1	AAA	188	ASP
1	AAA	193	LEU
1	AAA	194	ILE
1	AAA	199	SER
1	AAA	284	VAL
1	AAA	300	ASP
1	AAA	324	ILE
1	AAA	330	LYS
1	AAA	334	ARG
1	AAA	353	LEU
1	AAA	361	LEU
1	AAA	368	ASP
1	AAA	380	SER
1	AAA	389	LEU
1	AAA	392	GLN
1	AAA	407	LEU
1	AAA	417	SER
1	AAA	448	VAL
1	AAA	473	THR

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Mol	Chain	Res	Type
1	AAA	493	ARG
1	AAA	495	THR
1	AAA	522	ARG
1	AAA	526	ASP
1	BBB	79	MET
1	BBB	90	SER
1	BBB	160	TYR
1	BBB	175	LEU
1	BBB	184	SER
1	BBB	186	SER
1	BBB	193	LEU
1	BBB	194	ILE
1	BBB	199	SER
1	BBB	214	ASP
1	BBB	262	LYS
1	BBB	284	VAL
1	BBB	300	ASP
1	BBB	324	ILE
1	BBB	330	LYS
1	BBB	334	ARG
1	BBB	353	LEU
1	BBB	361	LEU
1	BBB	380	SER
1	BBB	392	GLN
1	BBB	407	LEU
1	BBB	417	SER
1	BBB	448	VAL
1	BBB	473	THR
1	BBB	493	ARG
1	BBB	495	THR
1	BBB	509	SER
1	BBB	522	ARG
1	BBB	526	ASP
1	CCC	-2	PHE
1	CCC	-1	GLN
1	CCC	10	GLU
1	CCC	79	MET
1	CCC	90	SER
1	CCC	151	LYS
1	CCC	160	TYR
1	CCC	175	LEU
1	CCC	184	SER

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Mol	Chain	Res	Type
1	CCC	186	SER
1	CCC	193	LEU
1	CCC	194	ILE
1	CCC	199	SER
1	CCC	247	PRO
1	CCC	262	LYS
1	CCC	284	VAL
1	CCC	300	ASP
1	CCC	324	ILE
1	CCC	330	LYS
1	CCC	334	ARG
1	CCC	353	LEU
1	CCC	361	LEU
1	CCC	380	SER
1	CCC	389	LEU
1	CCC	392	GLN
1	CCC	407	LEU
1	CCC	417	SER
1	CCC	448	VAL
1	CCC	473	THR
1	CCC	493	ARG
1	CCC	495	THR
1	CCC	508	LYS
1	CCC	522	ARG
1	CCC	528	SER
1	DDD	51	LEU
1	DDD	79	MET
1	DDD	90	SER
1	DDD	120	LYS
1	DDD	160	TYR
1	DDD	184	SER
1	DDD	186	SER
1	DDD	188	ASP
1	DDD	193	LEU
1	DDD	194	ILE
1	DDD	199	SER
1	DDD	284	VAL
1	DDD	294	ARG
1	DDD	300	ASP
1	DDD	324	ILE
1	DDD	330	LYS
1	DDD	334	ARG

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Mol	Chain	Res	Type
1	DDD	353	LEU
1	DDD	361	LEU
1	DDD	380	SER
1	DDD	392	GLN
1	DDD	407	LEU
1	DDD	417	SER
1	DDD	448	VAL
1	DDD	473	THR
1	DDD	495	THR
1	DDD	522	ARG
1	DDD	526	ASP
1	DDD	527	GLU

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
1	SEP	DDD	26	1	8,9,10	2.22	3 (37%)	8,12,14	3.19	3 (37%)
1	SEP	CCC	26	1	8,9,10	2.39	3 (37%)	8,12,14	3.18	2 (25%)
1	SEP	BBB	26	1	8,9,10	2.42	3 (37%)	8,12,14	3.18	3 (37%)
1	SEP	AAA	26	1	8,9,10	2.07	3 (37%)	8,12,14	3.07	2 (25%)

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
1	SEP	DDD	26	1	-	2/5/8/10	-
1	SEP	CCC	26	1	-	2/5/8/10	-
1	SEP	BBB	26	1	-	2/5/8/10	-
1	SEP	AAA	26	1	-	2/5/8/10	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	26	SEP	P-OG	5.57	1.78	1.60
1	CCC	26	SEP	P-OG	5.33	1.77	1.60
1	DDD	26	SEP	P-OG	4.49	1.74	1.60
1	AAA	26	SEP	P-OG	4.39	1.74	1.60
1	BBB	26	SEP	CB-CA	2.91	1.60	1.52
1	DDD	26	SEP	OG-CB	2.87	1.55	1.44
1	CCC	26	SEP	OG-CB	2.81	1.55	1.44
1	DDD	26	SEP	CB-CA	2.78	1.60	1.52
1	BBB	26	SEP	OG-CB	2.60	1.54	1.44
1	AAA	26	SEP	CB-CA	2.52	1.59	1.52
1	CCC	26	SEP	CB-CA	2.48	1.59	1.52
1	AAA	26	SEP	OG-CB	2.44	1.54	1.44

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	26	SEP	OG-CB-CA	8.18	116.10	108.14
1	CCC	26	SEP	OG-CB-CA	8.18	116.10	108.14
1	AAA	26	SEP	OG-CB-CA	7.93	115.86	108.14
1	BBB	26	SEP	OG-CB-CA	7.75	115.69	108.14
1	CCC	26	SEP	P-OG-CB	3.38	127.60	118.30
1	BBB	26	SEP	P-OG-CB	3.21	127.14	118.30
1	DDD	26	SEP	P-OG-CB	3.05	126.69	118.30
1	AAA	26	SEP	P-OG-CB	3.04	126.67	118.30
1	BBB	26	SEP	O3P-P-OG	2.80	114.19	106.73
1	DDD	26	SEP	OG-P-O1P	2.15	112.51	106.47

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AAA	26	SEP	N-CA-CB-OG
1	AAA	26	SEP	CA-CB-OG-P
1	BBB	26	SEP	N-CA-CB-OG
1	BBB	26	SEP	CA-CB-OG-P
1	CCC	26	SEP	N-CA-CB-OG
1	CCC	26	SEP	CA-CB-OG-P
1	DDD	26	SEP	N-CA-CB-OG
1	DDD	26	SEP	CA-CB-OG-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	BBB	26	SEP	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	TPP	BBB	601	3	22,27,27	0.57	0	29,40,40	0.85	1 (3%)
2	TPP	DDD	601	3	22,27,27	0.63	0	29,40,40	0.79	1 (3%)
2	TPP	CCC	601	3	22,27,27	0.49	0	29,40,40	0.89	1 (3%)
2	TPP	AAA	601	3	22,27,27	0.66	0	29,40,40	1.08	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
2	TPP	BBB	601	3	-	2/16/17/17	0/2/2/2
2	TPP	DDD	601	3	-	2/16/17/17	0/2/2/2
2	TPP	CCC	601	3	-	4/16/17/17	0/2/2/2
2	TPP	AAA	601	3	-	6/16/17/17	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	601	TPP	C7'-N3-C2	-2.72	120.44	125.35
2	CCC	601	TPP	O7-PA-O1A	2.31	118.11	109.07
2	DDD	601	TPP	O2A-PA-O1A	2.20	123.11	112.24
2	BBB	601	TPP	C7'-N3-C2	-2.07	121.61	125.35

There are no chirality outliers.

All (14) torsion outliers are listed below:

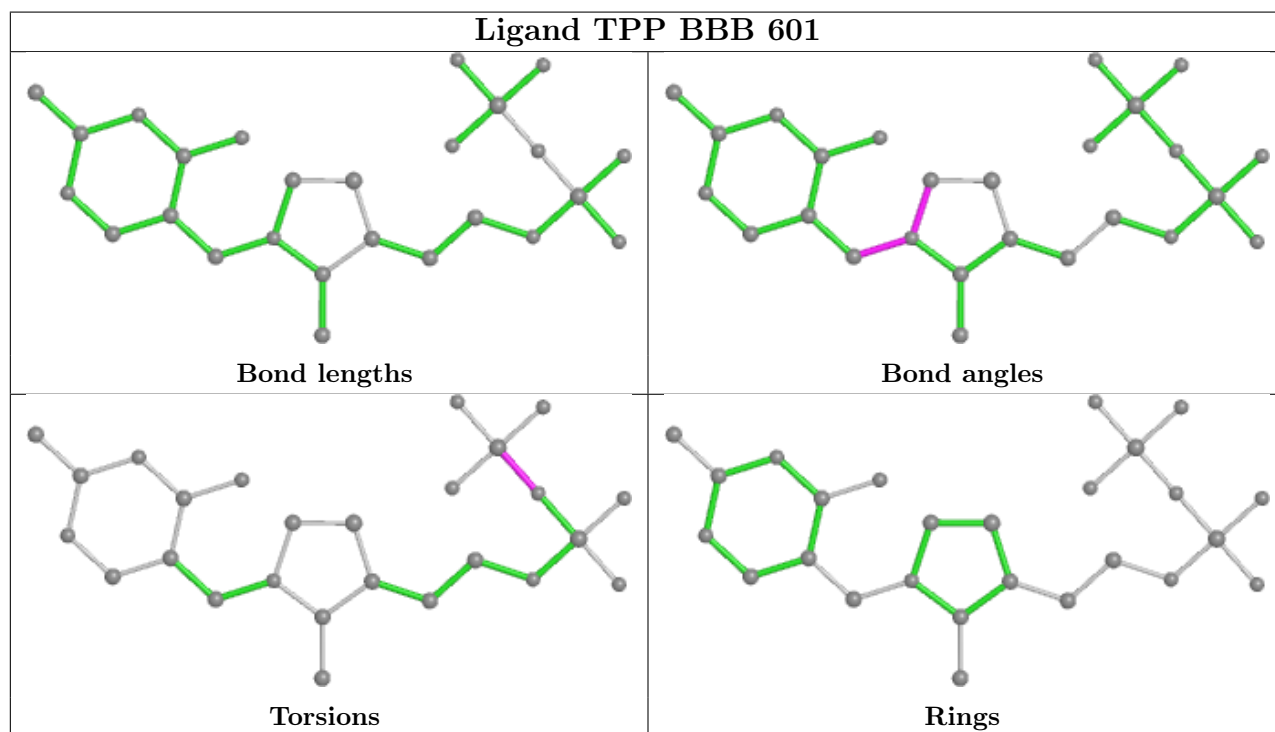
Mol	Chain	Res	Type	Atoms
2	AAA	601	TPP	C4'-C5'-C7'-N3
2	AAA	601	TPP	C5-C6-C7-O7
2	AAA	601	TPP	C7-O7-PA-O1A
2	AAA	601	TPP	C7-O7-PA-O2A
2	AAA	601	TPP	PB-O3A-PA-O7
2	BBB	601	TPP	PA-O3A-PB-O3B
2	CCC	601	TPP	C5-C6-C7-O7
2	CCC	601	TPP	C7-O7-PA-O3A
2	DDD	601	TPP	PA-O3A-PB-O3B
2	CCC	601	TPP	PB-O3A-PA-O7
2	CCC	601	TPP	C7-O7-PA-O2A
2	DDD	601	TPP	PA-O3A-PB-O1B
2	BBB	601	TPP	PA-O3A-PB-O2B
2	AAA	601	TPP	C7-O7-PA-O3A

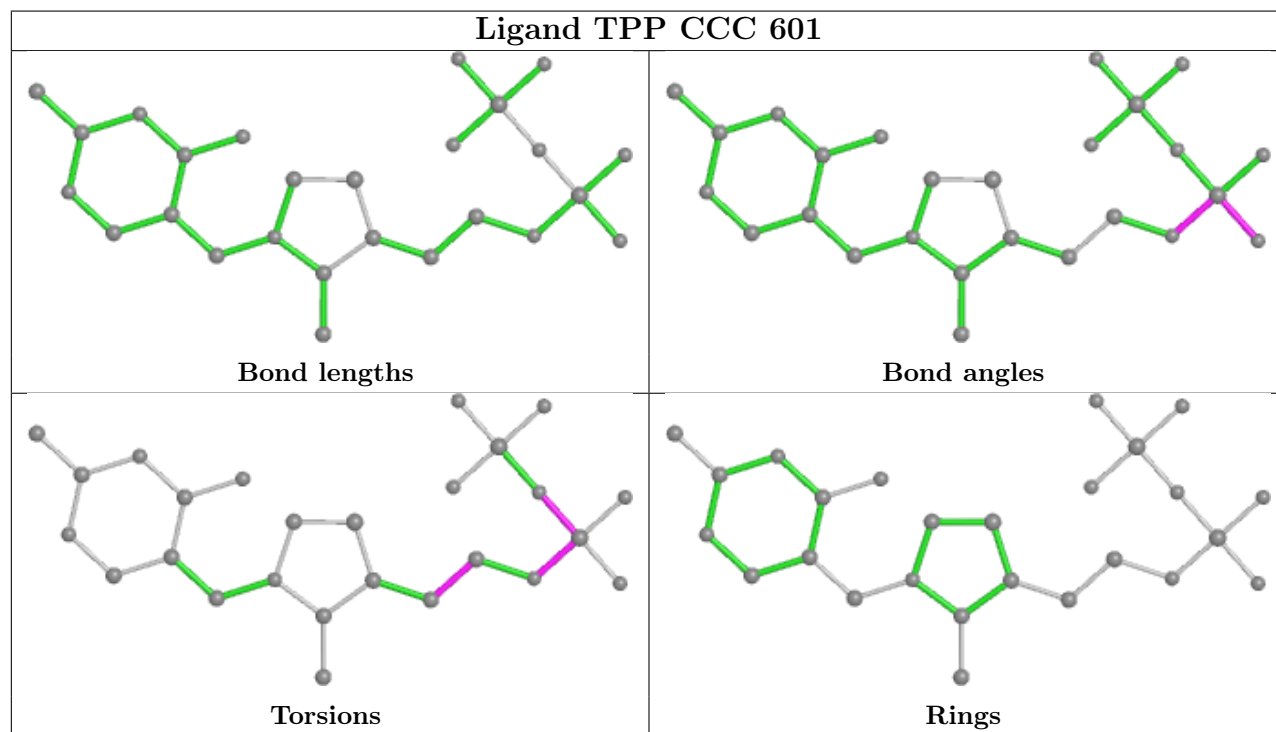
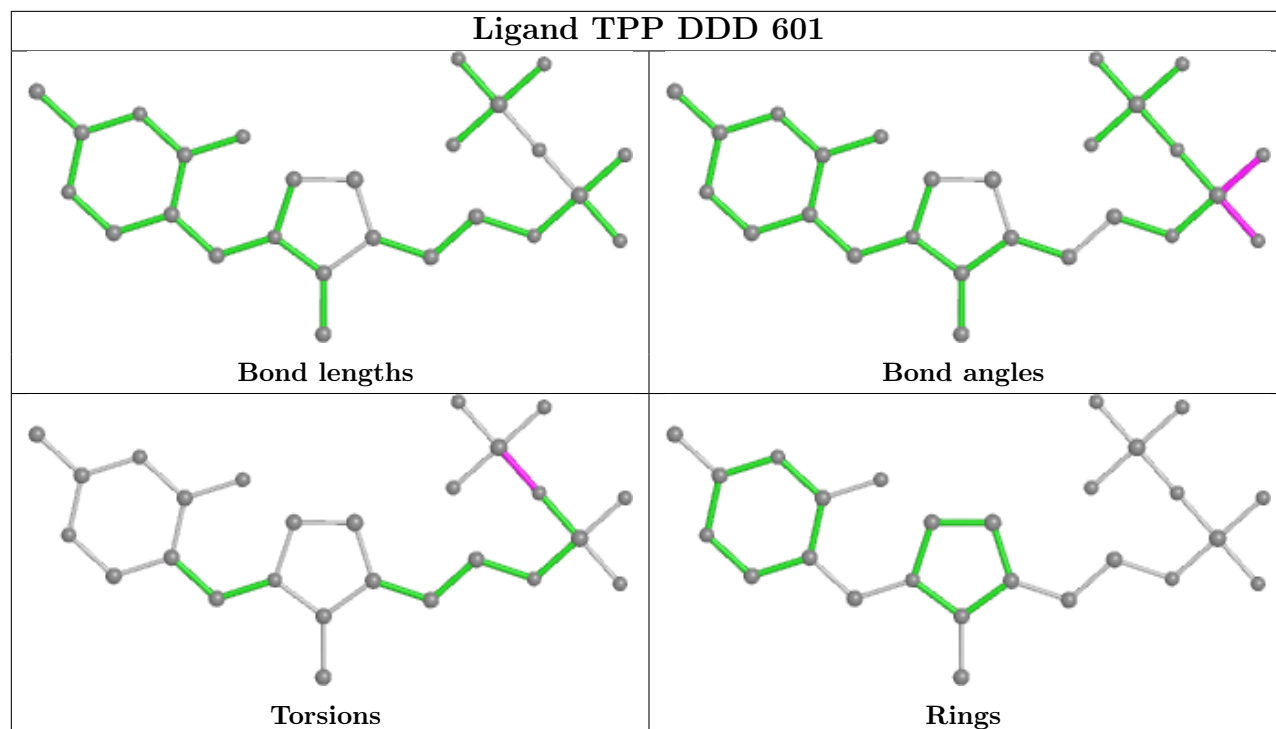
There are no ring outliers.

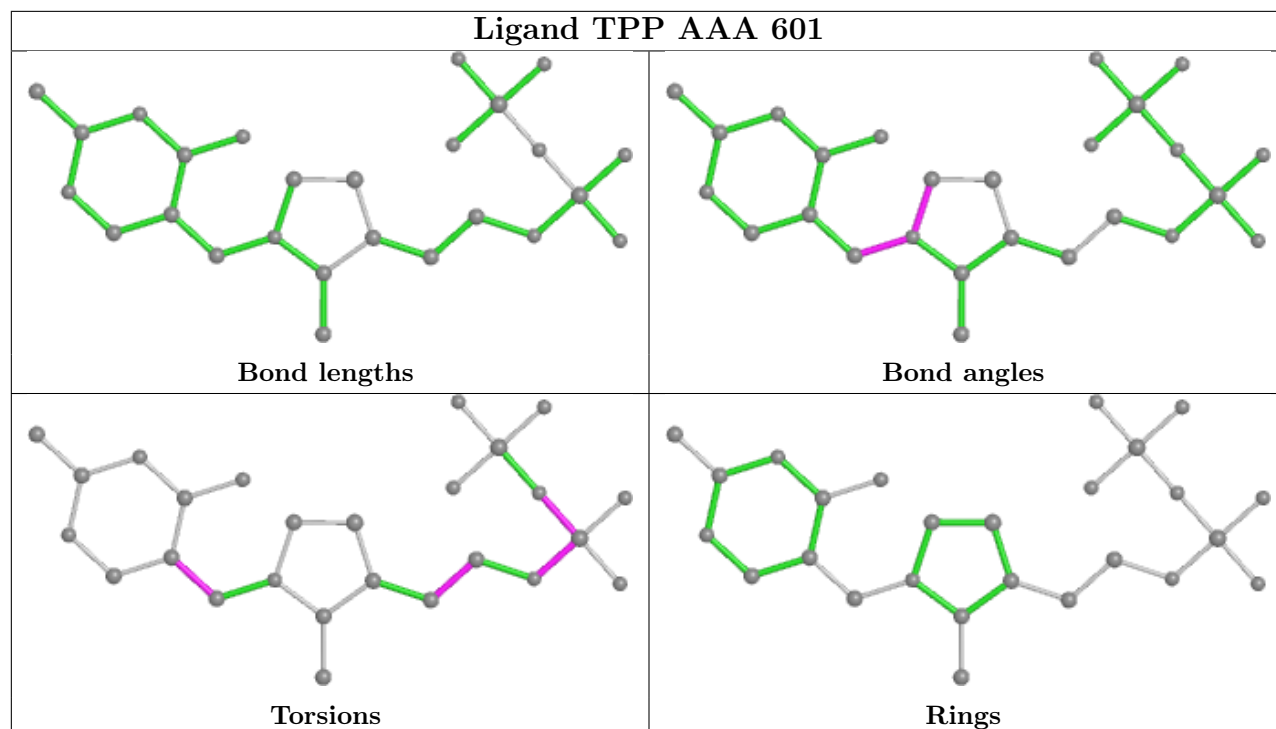
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	DDD	601	TPP	1	0
2	CCC	601	TPP	1	0
2	AAA	601	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 [i](#)

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	AAA	526/531 (99%)	0.26	34 (6%) 18 14	70, 93, 133, 159	0
1	BBB	526/531 (99%)	0.23	27 (5%) 28 22	57, 80, 122, 174	0
1	CCC	530/531 (99%)	0.07	11 (2%) 63 58	59, 79, 108, 150	0
1	DDD	526/531 (99%)	0.15	13 (2%) 57 51	63, 87, 131, 160	0
All	All	2108/2124 (99%)	0.18	85 (4%) 38 31	57, 85, 127, 174	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	528	SER	9.9
1	AAA	119	MET	5.7
1	CCC	528	SER	5.6
1	BBB	75	SER	5.5
1	BBB	467	ILE	4.9
1	BBB	527	GLU	4.7
1	AAA	467	ILE	4.6
1	BBB	466	LYS	4.5
1	AAA	121	PRO	4.5
1	DDD	333	ASP	4.5
1	DDD	270	ILE	4.4
1	BBB	109	MET	4.1
1	DDD	227	LEU	4.0
1	BBB	78	ALA	4.0
1	BBB	121	PRO	3.9
1	BBB	260	LEU	3.8
1	BBB	79	MET	3.7
1	BBB	74	GLY	3.6
1	AAA	193	LEU	3.6
1	AAA	79	MET	3.5
1	AAA	116	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	BBB	458	TYR	3.4
1	AAA	114	ASP	3.3
1	AAA	109	MET	3.2
1	BBB	119	MET	3.2
1	AAA	122	LEU	3.1
1	BBB	461	LEU	3.1
1	BBB	282	GLN	3.1
1	AAA	74	GLY	3.1
1	DDD	183	ALA	3.0
1	AAA	470	THR	3.0
1	AAA	471	GLY	3.0
1	AAA	107	GLU	3.0
1	AAA	197	LEU	3.0
1	DDD	119	MET	2.9
1	BBB	463	GLY	2.9
1	CCC	122	LEU	2.9
1	AAA	113	VAL	2.8
1	BBB	118	LEU	2.8
1	AAA	118	LEU	2.8
1	CCC	475	GLY	2.7
1	DDD	359	PHE	2.7
1	AAA	347	VAL	2.7
1	BBB	464	PHE	2.7
1	AAA	458	TYR	2.6
1	DDD	325	LEU	2.6
1	CCC	121	PRO	2.6
1	AAA	112	ASN	2.5
1	BBB	76	GLY	2.5
1	DDD	220	ALA	2.5
1	DDD	438	LEU	2.5
1	BBB	460	ALA	2.5
1	DDD	196	THR	2.5
1	CCC	119	MET	2.4
1	DDD	271	LEU	2.4
1	BBB	281	HIS	2.3
1	AAA	466	LYS	2.3
1	AAA	53	MET	2.3
1	CCC	468	LEU	2.3
1	AAA	463	GLY	2.3
1	BBB	110	LEU	2.3
1	AAA	17	LEU	2.3
1	BBB	478	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	DDD	300	ASP	2.2
1	CCC	435	ILE	2.2
1	BBB	472	GLU	2.2
1	CCC	438	LEU	2.2
1	AAA	383	PHE	2.2
1	BBB	279	ARG	2.2
1	AAA	117	THR	2.2
1	AAA	108	VAL	2.2
1	AAA	295	LEU	2.2
1	DDD	223	LEU	2.2
1	AAA	27	ASN	2.1
1	BBB	483	PHE	2.1
1	AAA	207	LEU	2.1
1	AAA	78	ALA	2.1
1	AAA	104	ILE	2.1
1	AAA	528	SER	2.1
1	BBB	477	ASP	2.0
1	CCC	197	LEU	2.0
1	CCC	109	MET	2.0
1	AAA	264	LEU	2.0
1	AAA	490	TYR	2.0
1	CCC	114	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	CCC	26	10/11	0.88	0.17	88,90,95,100	0
1	SEP	BBB	26	10/11	0.91	0.21	87,95,102,104	0
1	SEP	AAA	26	10/11	0.93	0.20	116,123,132,135	0
1	SEP	DDD	26	10/11	0.93	0.17	85,95,106,109	0

6.3 Carbohydrates [i](#)

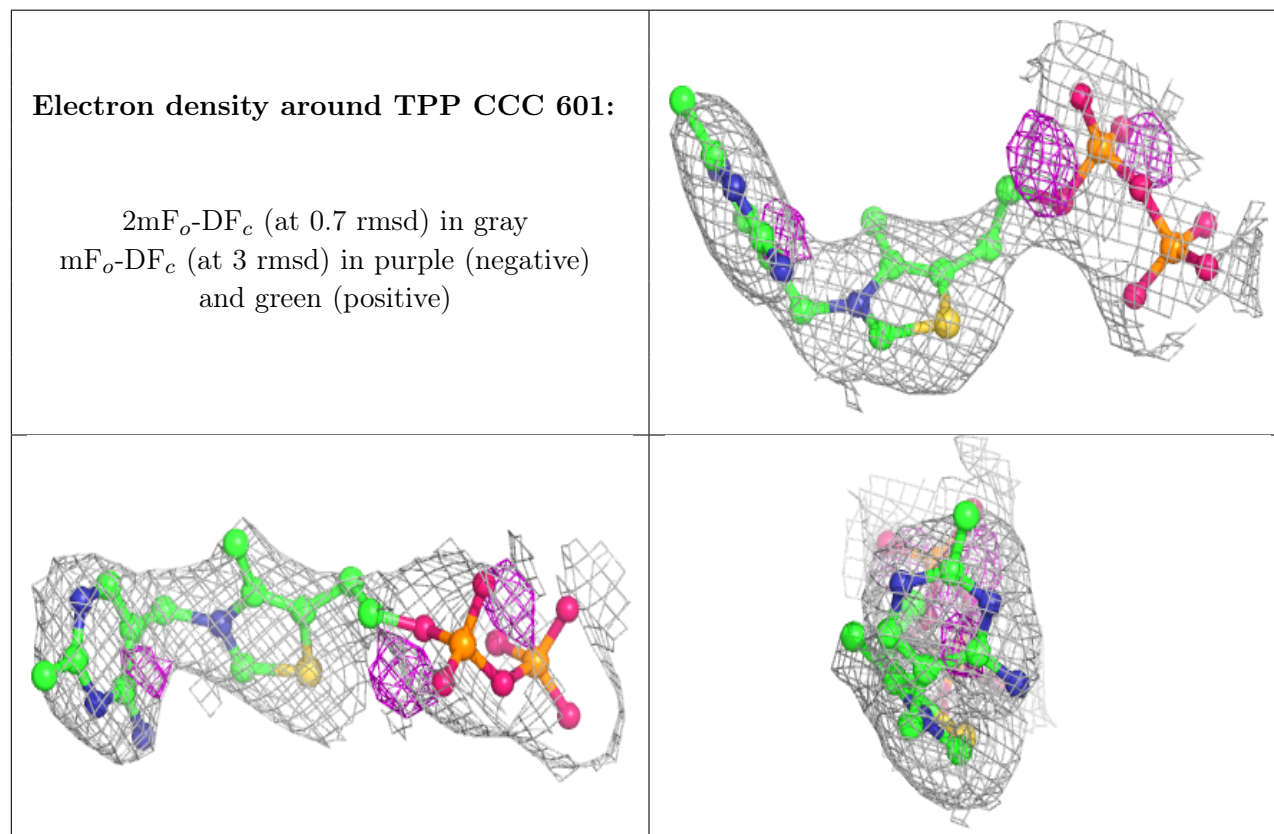
There are no monosaccharides in this entry.

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.

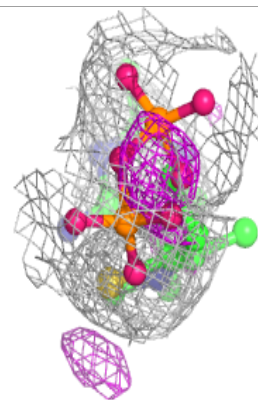
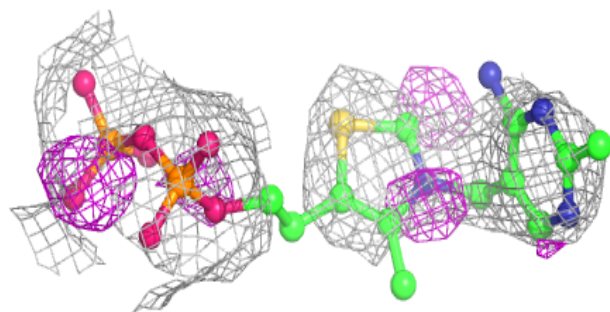
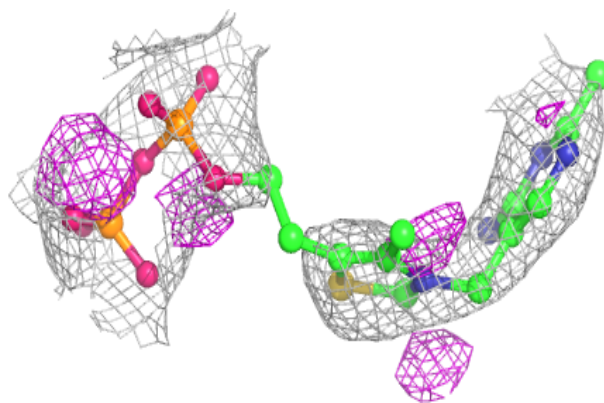
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NA	BBB	602	1/1	0.90	0.04	83,83,83,83	0
3	NA	DDD	602	1/1	0.95	0.10	67,67,67,67	0
2	TPP	CCC	601	26/26	0.96	0.19	64,83,90,109	0
3	NA	AAA	602	1/1	0.96	0.06	84,84,84,84	0
2	TPP	AAA	601	26/26	0.96	0.25	76,96,106,108	0
3	NA	CCC	602	1/1	0.96	0.10	66,66,66,66	0
2	TPP	BBB	601	26/26	0.96	0.27	90,112,126,132	0
2	TPP	DDD	601	26/26	0.97	0.18	69,80,99,104	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.

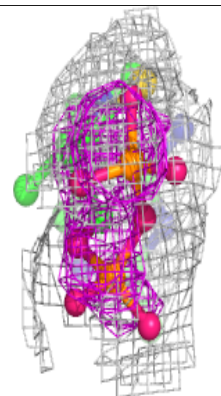
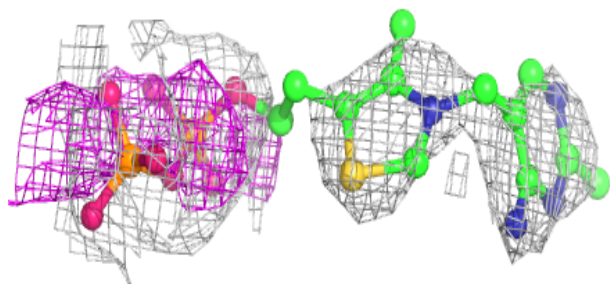
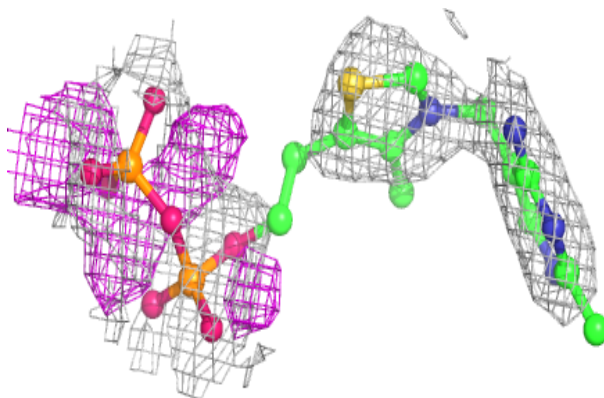


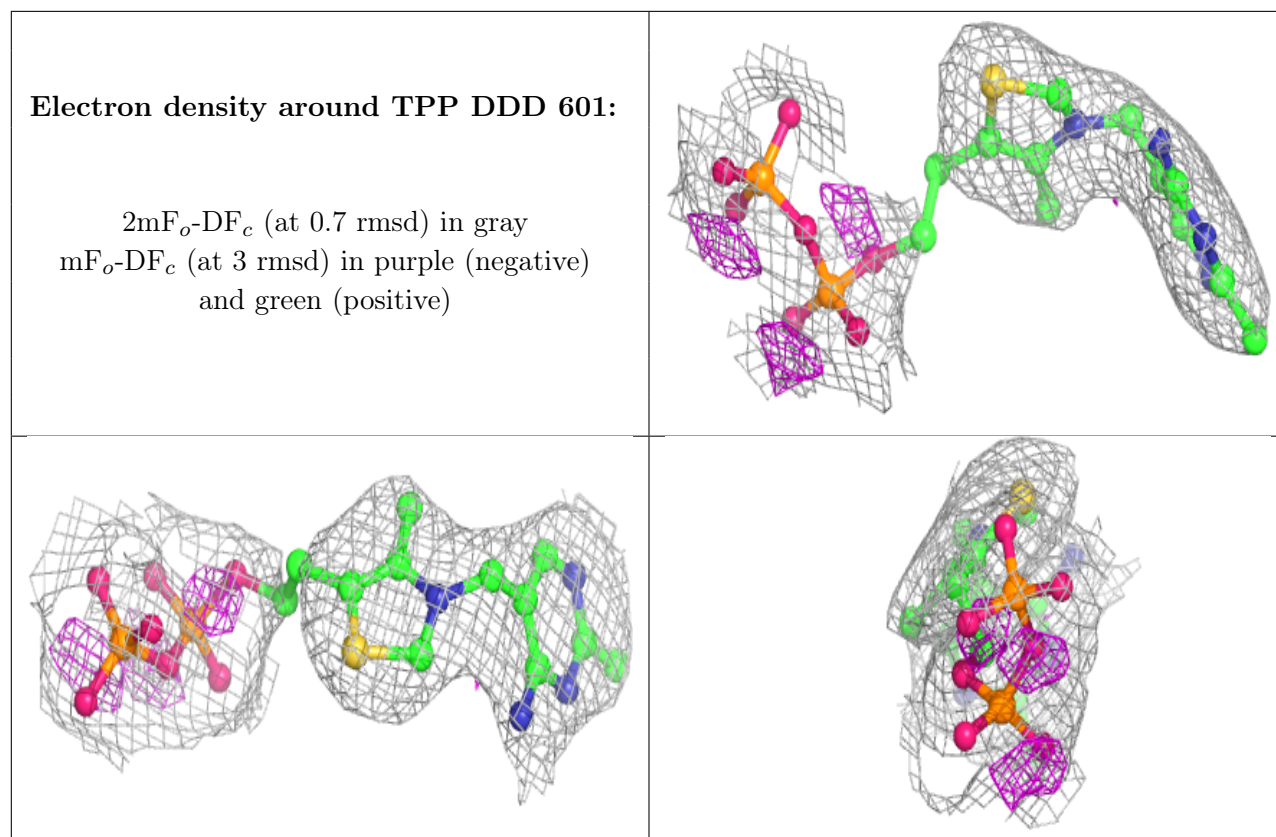
Electron density around TPP AAA 601:

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

**Electron density around TPP BBB 601:**

$2mF_o-DF_c$ (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.