



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:27 PM UTC

PDB ID : 2W93 / pdb_00002w93
Title : Crystal structure of the *Saccharomyces cerevisiae* pyruvate decarboxylase variant E477Q in complex with the surrogate pyruvamide
Authors : Kutter, S.; Weiss, M.S.; Konig, S.
Deposited on : 2009-01-21
Resolution : 1.60 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

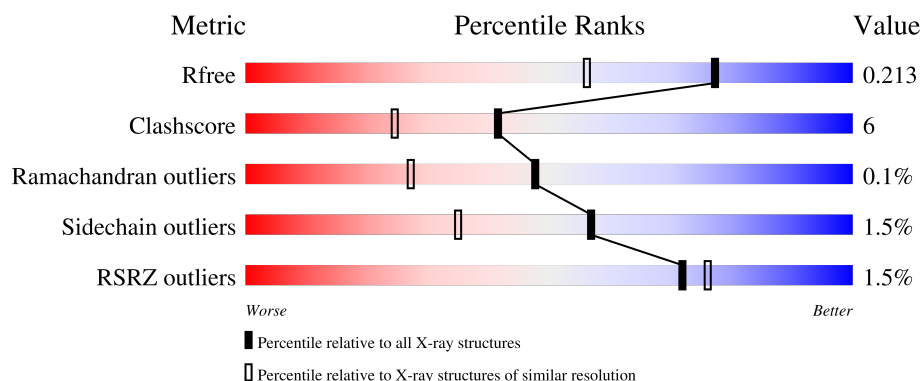
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	A	563	
1	B	563	
1	C	563	
1	D	563	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TPP	B	600	-	-	X	-
2	TPP	D	600	-	-	X	-
4	PY0	A	603	-	-	X	-
4	PY0	A	604	X	-	-	-
4	PY0	B	602	-	-	X	-
4	PY0	C	602	-	-	X	-
4	PY0	D	602	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18690 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.

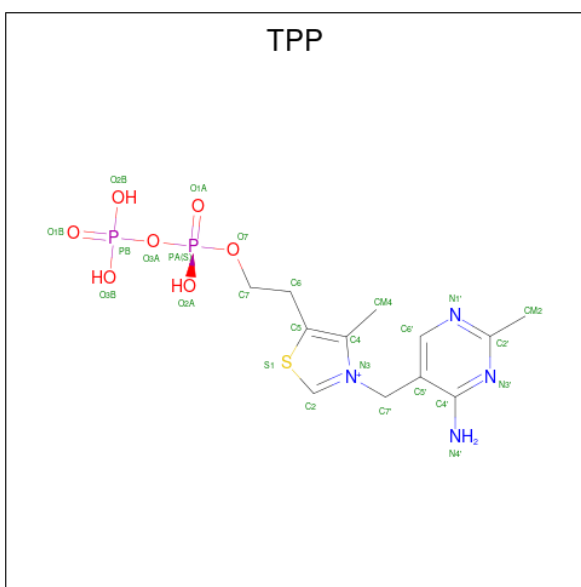
- Molecule 1 is a protein called PYRUVATE DECARBOXYLASE ISOZYME 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	544	Total	C	N	O	S	0	0	0
			4179	2668	703	792	16			
1	B	562	Total	C	N	O	S	0	0	0
			4324	2760	726	822	16			
1	C	557	Total	C	N	O	S	0	0	0
			4286	2738	718	814	16			
1	D	562	Total	C	N	O	S	0	0	0
			4324	2760	726	822	16			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	SER	ALA	conflict	UNP P06169
A	336	ASN	THR	conflict	UNP P06169
A	477	GLN	GLU	engineered mutation	UNP P06169
A	538	VAL	ILE	conflict	UNP P06169
B	106	SER	ALA	conflict	UNP P06169
B	336	ASN	THR	conflict	UNP P06169
B	477	GLN	GLU	engineered mutation	UNP P06169
B	538	VAL	ILE	conflict	UNP P06169
C	106	SER	ALA	conflict	UNP P06169
C	336	ASN	THR	conflict	UNP P06169
C	477	GLN	GLU	engineered mutation	UNP P06169
C	538	VAL	ILE	conflict	UNP P06169
D	106	SER	ALA	conflict	UNP P06169
D	336	ASN	THR	conflict	UNP P06169
D	477	GLN	GLU	engineered mutation	UNP P06169
D	538	VAL	ILE	conflict	UNP P06169

- Molecule 2 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).

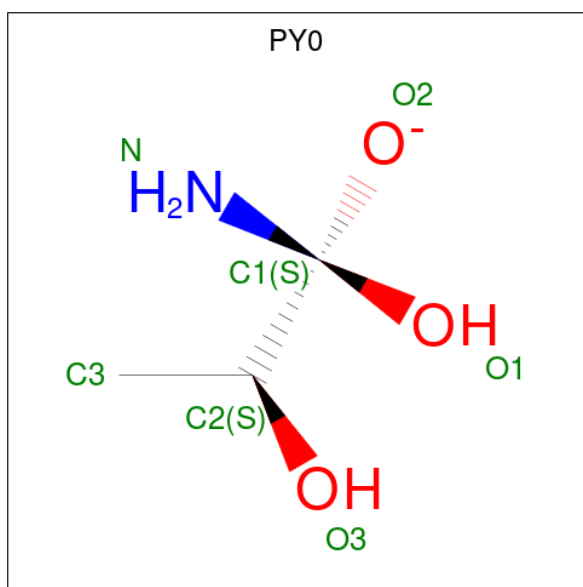


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	C	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	D	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is (1S,2S)-1-amino-1,2-dihydroxypropan-1-olate (CCD ID: PY0) (formula: $\text{C}_3\text{H}_8\text{NO}_3$).



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

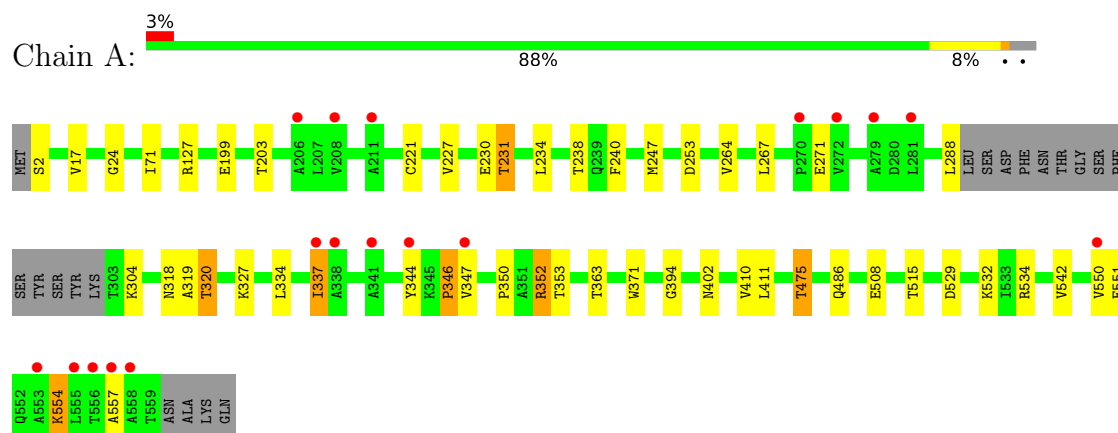
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	353	Total	O	0	0
			353	353		
5	B	409	Total	O	0	0
			409	409		
5	C	353	Total	O	0	0
			353	353		
5	D	298	Total	O	0	0
			298	298		

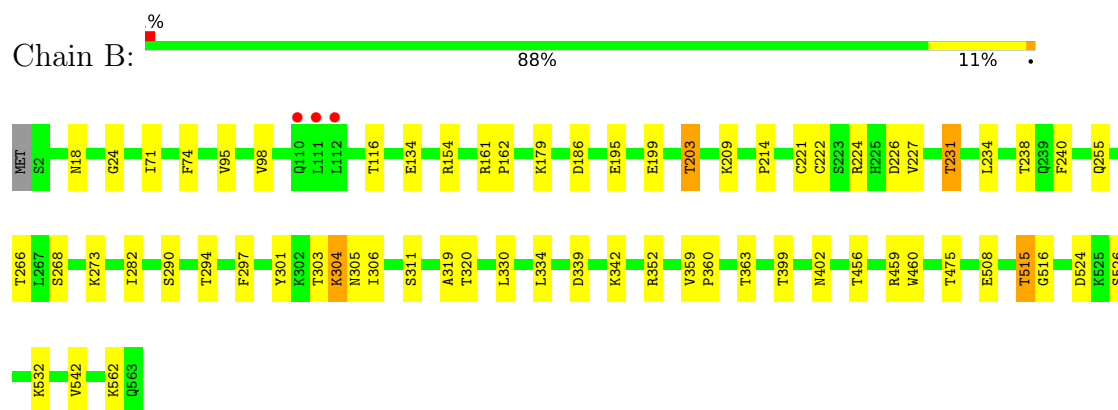
3 Residue-property plots

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.

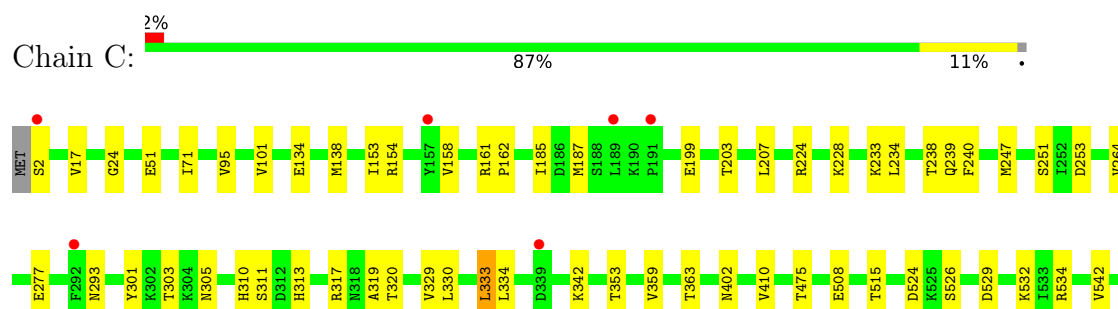
• Molecule 1: PYRUVATE DECARBOXYLASE ISOZYME 1

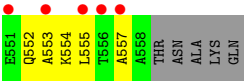


• Molecule 1: PYRUVATE DECARBOXYLASE ISOZYME 1

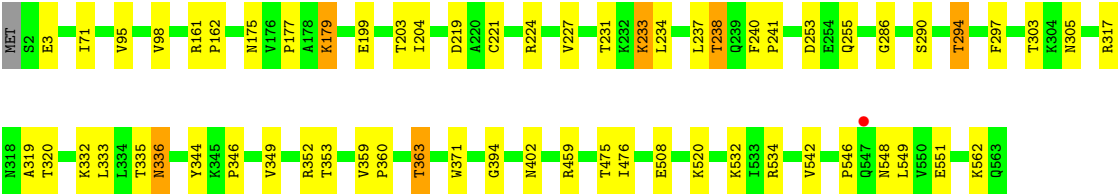
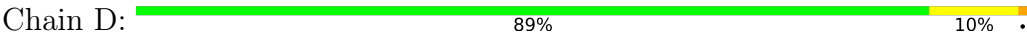


• Molecule 1: PYRUVATE DECARBOXYLASE ISOZYME 1





● Molecule 1: PYRUVATE DECARBOXYLASE ISOZYME 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.05Å 79.22Å 109.09Å 89.23° 73.32° 62.43°	Depositor
Resolution (Å)	103.70 – 1.60 103.46 – 1.60	Depositor EDS
% Data completeness (in resolution range)	96.0 (103.70-1.60) 93.9 (103.46-1.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.181 , 0.213 0.181 , 0.213	Depositor DCC
R_{free} test set	1054 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18690	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: PY0, 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	A	0.74	5/4265 (0.1%)	0.84	1/5800 (0.0%)
1	B	0.71	2/4415 (0.0%)	0.82	0/6003
1	C	0.68	0/4377	0.84	0/5952
1	D	0.67	0/4415	0.83	0/6003
All	All	0.70	7/17472 (0.0%)	0.83	1/23758 (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	A	5	0
1	B	6	0
1	C	6	0
1	D	6	0
All	All	23	0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	231	THR	C-O	-6.92	1.15	1.24
1	A	127	ARG	C-O	-6.07	1.17	1.24
1	B	515	THR	C-O	-5.99	1.17	1.24
1	A	475	THR	C-O	-5.95	1.17	1.24
1	A	486	GLN	C-O	-5.56	1.17	1.24
1	A	231	THR	C-O	-5.14	1.18	1.24
1	A	320	THR	C-O	-5.00	1.17	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	ILE	N-CA-C	5.66	118.13	111.05

All (23) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	203	THR	CB
1	A	231	THR	CB
1	A	320	THR	CB
1	A	475	THR	CB
1	A	515	THR	CB
1	B	231	THR	CB
1	B	238	THR	CB
1	B	294	THR	CB
1	B	303	THR	CB
1	B	475	THR	CB
1	B	515	THR	CB
1	C	203	THR	CB
1	C	238	THR	CB
1	C	303	THR	CB
1	C	320	THR	CB
1	C	475	THR	CB
1	C	515	THR	CB
1	D	203	THR	CB
1	D	231	THR	CB
1	D	303	THR	CB
1	D	335	THR	CB
1	D	475	THR	CB
1	D	515	THR	CB

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4179	0	4200	35	0
1	B	4324	0	4332	60	0
1	C	4286	0	4293	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4324	0	4332	54	0
2	A	26	0	16	1	0
2	B	26	0	16	9	0
2	C	26	0	16	6	0
2	D	26	0	16	9	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	14	0	16	7	0
4	B	14	0	14	10	0
4	C	14	0	15	7	0
4	D	14	0	14	8	0
5	A	353	0	0	2	0
5	B	409	0	0	11	0
5	C	353	0	0	3	0
5	D	298	0	0	3	0
All	All	18690	0	17280	220	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 6.

All (220) 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:C:600:TPP:H2	4:C:602:PY0:C2	1.32	1.58
2:C:600:TPP:C2	4:C:602:PY0:H2	1.22	1.57
2:D:600:TPP:H2	4:D:602:PY0:C2	1.10	1.56
2:D:600:TPP:C2	4:D:602:PY0:H2	1.05	1.52
2:B:600:TPP:H2	4:B:602:PY0:C2	1.00	1.44
2:B:600:TPP:C2	4:B:602:PY0:H2	0.88	1.34
1:B:303:THR:HG22	1:B:305:ASN:H	1.00	1.14
1:D:303:THR:HG22	1:D:305:ASN:H	1.18	1.08
1:C:303:THR:HG22	1:C:305:ASN:H	1.23	1.04
1:C:17:VAL:HG11	1:C:187:MET:HE3	1.37	1.03
2:D:600:TPP:H2	4:D:602:PY0:C3	1.88	1.02
1:B:294:THR:HG23	1:B:297:PHE:H	1.27	0.99
2:B:600:TPP:S1	4:B:602:PY0:H2	2.04	0.97
1:B:238:THR:HG23	1:B:240:PHE:H	1.29	0.95
1:B:303:THR:HG22	1:B:305:ASN:N	1.85	0.92
1:C:238:THR:HG23	1:C:240:PHE:H	1.35	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:600:TPP:C2	4:B:602:PY0:C2	1.83	0.90
2:B:600:TPP:H2	4:B:602:PY0:C3	2.01	0.90
1:B:203:THR:HG21	5:B:2138:HOH:O	1.71	0.90
2:B:600:TPP:H2	4:B:602:PY0:O3	1.71	0.90
1:C:153:ILE:HG22	1:C:187:MET:HE1	1.57	0.87
1:D:233:LYS:HE3	1:D:237:LEU:HG	1.58	0.86
1:B:227:VAL:O	1:B:231:THR:HG23	1.76	0.85
1:B:311:SER:H	4:B:603:PY0:HN2	1.25	0.84
1:D:227:VAL:O	1:D:231:THR:HG23	1.75	0.84
1:C:203:THR:HG21	5:C:2138:HOH:O	1.78	0.83
1:D:332:LYS:O	1:D:335:THR:HG22	1.79	0.83
1:B:363:THR:OG1	1:B:515:THR:CG2	2.26	0.81
1:D:294:THR:HG23	1:D:297:PHE:H	1.45	0.81
1:B:363:THR:HG22	5:B:2249:HOH:O	1.81	0.79
1:B:363:THR:OG1	1:B:515:THR:HG22	1.82	0.79
1:A:238:THR:HG23	1:A:240:PHE:H	1.49	0.78
2:D:600:TPP:C2	4:D:602:PY0:C2	1.98	0.78
1:C:311:SER:H	4:C:603:PY0:HN2	1.30	0.77
1:D:294:THR:CG2	1:D:297:PHE:H	1.95	0.77
1:A:221:CYS:CB	4:A:603:PY0:O2	2.33	0.76
1:A:227:VAL:O	1:A:231:THR:HG23	1.86	0.76
1:B:18:ASN:HB2	5:B:2013:HOH:O	1.84	0.76
1:B:508:GLU:HG3	1:B:532:LYS:HD2	1.69	0.75
1:C:234:LEU:O	1:C:238:THR:HG22	1.87	0.75
1:D:360:PRO:O	1:D:363:THR:HG23	1.85	0.75
1:D:199:GLU:O	1:D:203:THR:HG23	1.87	0.75
1:C:17:VAL:CG1	1:C:187:MET:HE3	2.15	0.74
1:C:303:THR:HG22	1:C:305:ASN:N	2.02	0.74
2:C:600:TPP:S1	4:C:602:PY0:H2	2.22	0.74
1:C:185:ILE:HB	1:C:187:MET:HE2	1.71	0.73
1:C:329:VAL:O	1:C:333:LEU:HB2	1.88	0.72
1:A:320:THR:HG22	1:D:320:THR:O	1.90	0.71
1:D:238:THR:HG23	1:D:240:PHE:H	1.55	0.71
1:D:233:LYS:HE3	1:D:237:LEU:CG	2.20	0.70
1:D:233:LYS:HD2	1:D:233:LYS:O	1.91	0.70
1:A:221:CYS:SG	4:A:603:PY0:O2	2.50	0.69
1:B:475:THR:HG22	1:B:542:VAL:O	1.93	0.69
1:B:290:SER:O	1:B:294:THR:HG22	1.91	0.69
2:C:600:TPP:H2	4:C:602:PY0:O3	1.91	0.67
2:C:600:TPP:C2	4:C:602:PY0:C2	2.16	0.67
1:D:234:LEU:O	1:D:238:THR:HB	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:THR:CG2	1:B:297:PHE:H	2.07	0.65
1:B:234:LEU:O	1:B:238:THR:HG22	1.97	0.64
1:B:363:THR:OG1	1:B:515:THR:HG21	1.96	0.64
1:C:524:ASP:OD2	1:C:526:SER:OG	2.13	0.64
1:D:303:THR:HG22	1:D:305:ASN:N	2.03	0.64
1:D:303:THR:HG23	5:D:2141:HOH:O	1.97	0.64
1:D:294:THR:HG23	1:D:297:PHE:N	2.13	0.63
1:A:221:CYS:HB3	4:A:603:PY0:O2	1.99	0.63
1:C:199:GLU:O	1:C:203:THR:HG23	1.99	0.62
1:C:207:LEU:HD21	1:C:317:ARG:HH11	1.66	0.61
2:D:600:TPP:C2	4:D:602:PY0:C3	2.62	0.61
1:C:529:ASP:O	1:C:529:ASP:OD2	2.19	0.61
1:D:475:THR:HG22	1:D:542:VAL:O	2.02	0.60
1:C:207:LEU:HD21	1:C:317:ARG:NH1	2.16	0.60
1:C:138:MET:HE2	5:C:2101:HOH:O	2.01	0.59
1:C:508:GLU:HG3	1:C:532:LYS:HD2	1.84	0.59
1:D:335:THR:HG23	1:D:336:ASN:CG	2.27	0.59
1:D:238:THR:CG2	1:D:240:PHE:H	2.16	0.58
1:B:339:ASP:OD1	1:B:342:LYS:HE3	2.04	0.57
1:B:154:ARG:NH1	1:B:186:ASP:O	2.31	0.57
1:B:515:THR:HG23	5:B:2248:HOH:O	2.04	0.57
1:A:221:CYS:SG	4:A:603:PY0:C1	2.93	0.56
1:C:553:ALA:O	1:C:554:LYS:HB2	2.04	0.56
1:B:320:THR:O	1:C:320:THR:HG22	2.05	0.55
1:B:360:PRO:O	1:B:363:THR:HG23	2.07	0.55
1:D:233:LYS:CE	1:D:237:LEU:HG	2.33	0.55
1:D:290:SER:O	1:D:294:THR:HB	2.07	0.55
1:D:233:LYS:HE3	1:D:237:LEU:CD2	2.36	0.55
1:B:359:VAL:HB	1:B:363:THR:HG21	1.89	0.54
1:A:475:THR:HG22	1:A:542:VAL:O	2.09	0.53
1:B:352:ARG:HE	1:B:399:THR:HG21	1.73	0.53
1:C:363:THR:HB	1:C:515:THR:HG22	1.90	0.53
2:D:600:TPP:H2	4:D:602:PY0:O3	1.96	0.53
1:C:475:THR:HG22	1:C:542:VAL:O	2.09	0.53
1:C:101:VAL:HG21	1:C:138:MET:HE1	1.91	0.53
1:D:508:GLU:HG3	1:D:532:LYS:HD2	1.90	0.53
1:A:253:ASP:HB3	1:A:402:ASN:OD1	2.10	0.52
1:D:359:VAL:HB	1:D:363:THR:HG21	1.91	0.52
1:A:234:LEU:O	1:A:238:THR:HG22	2.08	0.52
2:C:600:TPP:H2	4:C:602:PY0:H2	0.54	0.52
1:B:475:THR:CG2	1:B:542:VAL:O	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:ASP:HB3	5:A:2342:HOH:O	2.10	0.51
1:A:271:GLU:HB3	1:A:350:PRO:HB3	1.91	0.51
1:C:253:ASP:HB3	1:C:402:ASN:OD1	2.11	0.51
1:B:282:ILE:HD13	1:B:301:TYR:CE2	2.46	0.50
1:C:277:GLU:HA	1:C:301:TYR:HB3	1.93	0.50
1:C:359:VAL:HG23	1:C:515:THR:HG21	1.94	0.50
1:B:74:PHE:HE2	1:B:116:THR:HG22	1.77	0.50
1:C:247:MET:HE2	1:C:410:VAL:HB	1.93	0.50
1:D:476:ILE:HG13	1:D:549:LEU:HD11	1.94	0.50
1:B:199:GLU:O	1:B:203:THR:CG2	2.60	0.49
1:B:319:ALA:HB1	1:C:319:ALA:HB1	1.93	0.49
1:A:508:GLU:HB2	1:A:534:ARG:HG2	1.95	0.49
1:B:95:VAL:O	1:B:162:PRO:HA	2.13	0.49
1:B:304:LYS:HD3	5:B:2224:HOH:O	2.13	0.49
1:D:253:ASP:HB3	1:D:402:ASN:OD1	2.13	0.49
2:B:600:TPP:S1	4:B:602:PY0:C2	2.83	0.48
1:B:303:THR:HG21	1:B:305:ASN:HB2	1.94	0.48
1:B:304:LYS:HA	1:B:304:LYS:HE3	1.96	0.48
1:C:363:THR:HB	1:C:515:THR:CG2	2.43	0.48
1:D:508:GLU:HB2	1:D:534:ARG:HG2	1.95	0.48
1:A:221:CYS:SG	4:A:603:PY0:C2	3.02	0.48
1:D:71:ILE:HG12	1:D:98:VAL:HB	1.96	0.48
1:D:238:THR:HG23	1:D:240:PHE:CG	2.50	0.47
1:B:266:THR:HA	1:B:273:LYS:HE2	1.96	0.47
1:B:339:ASP:HA	1:B:342:LYS:HG3	1.94	0.47
1:C:555:LEU:C	1:C:557:ALA:H	2.23	0.47
1:B:195:GLU:HG2	5:B:2136:HOH:O	2.15	0.47
1:B:524:ASP:OD2	1:B:526:SER:HB3	2.15	0.47
1:A:508:GLU:HG3	1:A:532:LYS:HD2	1.96	0.47
1:B:214:PRO:HG2	1:B:240:PHE:CE1	2.50	0.47
1:B:134:GLU:HB2	1:B:161:ARG:HB2	1.96	0.46
1:B:456:THR:HA	1:B:459:ARG:HG2	1.97	0.46
1:C:224:ARG:CZ	1:C:224:ARG:HA	2.44	0.46
1:D:335:THR:HG23	1:D:336:ASN:ND2	2.30	0.46
1:A:238:THR:OG1	1:A:240:PHE:CZ	2.68	0.46
1:B:199:GLU:O	1:B:203:THR:HG22	2.15	0.46
1:C:475:THR:CG2	1:C:542:VAL:O	2.63	0.46
1:B:363:THR:HG1	1:B:515:THR:CG2	2.28	0.46
1:B:515:THR:HG23	1:B:516:GLY:N	2.31	0.46
1:C:228:LYS:HE3	1:C:251:SER:HA	1.98	0.46
1:C:320:THR:O	1:C:320:THR:HG23	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:THR:HB	1:A:515:THR:HG22	1.97	0.46
1:B:255:GLN:HB2	1:B:402:ASN:OD1	2.16	0.46
1:C:247:MET:HE3	1:C:293:ASN:CG	2.41	0.46
2:D:600:TPP:S1	4:D:602:PY0:C3	3.04	0.46
1:B:515:THR:CG2	5:B:2248:HOH:O	2.63	0.46
1:B:18:ASN:CB	5:B:2013:HOH:O	2.53	0.46
1:C:51:GLU:OE2	2:D:600:TPP:N1'	2.50	0.45
1:D:255:GLN:HB2	1:D:402:ASN:OD1	2.16	0.45
1:D:161:ARG:NH2	5:D:2089:HOH:O	2.34	0.45
1:B:359:VAL:HG23	1:B:515:THR:HG21	1.99	0.45
1:C:185:ILE:CB	1:C:187:MET:HE2	2.44	0.45
1:D:344:TYR:CE2	1:D:346:PRO:HA	2.52	0.45
2:B:600:TPP:C2	4:B:602:PY0:C3	2.74	0.45
1:B:222:CYS:SG	1:B:231:THR:HG21	2.57	0.45
1:B:224:ARG:CZ	1:B:224:ARG:HA	2.48	0.44
1:A:363:THR:HB	1:A:515:THR:CG2	2.47	0.44
1:D:294:THR:HG23	1:D:297:PHE:CA	2.48	0.44
1:D:459:ARG:NH1	5:D:2208:HOH:O	2.50	0.44
1:B:24:GLY:HA3	1:B:71:ILE:O	2.18	0.44
1:D:221:CYS:HB2	1:D:286:GLY:CA	2.48	0.44
1:D:317:ARG:HE	1:D:317:ARG:HB3	1.56	0.44
1:A:319:ALA:HB1	1:D:319:ALA:HB1	2.00	0.44
1:C:95:VAL:O	1:C:162:PRO:HA	2.18	0.43
1:D:3:GLU:HB3	1:D:175:ASN:HB3	2.01	0.43
1:C:154:ARG:O	1:C:158:VAL:HG22	2.18	0.43
1:D:371:TRP:CE2	1:D:394:GLY:HA3	2.54	0.43
1:B:268:SER:HB2	1:B:273:LYS:HB2	2.00	0.43
1:D:241:PRO:HB3	1:D:349:VAL:HG12	2.00	0.43
1:A:199:GLU:O	1:A:203:THR:HG23	2.16	0.43
1:C:310:HIS:HB2	1:C:313:HIS:O	2.19	0.43
1:A:230:GLU:OE2	1:A:327:LYS:NZ	2.37	0.43
1:A:334:LEU:HA	1:A:337:ILE:HG22	2.00	0.43
1:C:553:ALA:O	1:C:554:LYS:CB	2.67	0.43
2:D:600:TPP:S1	4:D:602:PY0:H31C	2.59	0.43
1:B:459:ARG:HG3	1:B:460:TRP:CD1	2.54	0.43
1:C:247:MET:HE3	1:C:293:ASN:HB2	2.00	0.43
1:C:247:MET:CE	1:C:293:ASN:HB2	2.49	0.43
1:D:204:ILE:HG21	1:D:333:LEU:HD11	2.01	0.43
1:B:209:LYS:HE3	5:B:2146:HOH:O	2.19	0.42
1:C:515:THR:HG23	5:C:2219:HOH:O	2.19	0.42
1:A:344:TYR:CE2	1:A:346:PRO:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ARG:HG3	1:A:353:THR:N	2.33	0.42
1:A:550:VAL:O	1:A:554:LYS:HG2	2.19	0.42
1:D:352:ARG:HG2	1:D:353:THR:N	2.34	0.42
1:A:318:ASN:HB2	1:D:199:GLU:OE1	2.20	0.42
1:C:134:GLU:HB2	1:C:161:ARG:HB2	2.01	0.42
1:C:529:ASP:OD2	1:C:529:ASP:C	2.62	0.42
1:A:221:CYS:SG	4:A:603:PY0:N	2.92	0.42
1:D:219:ASP:HB3	1:D:286:GLY:O	2.20	0.42
1:A:17:VAL:HA	4:A:604:PY0:H33C	2.02	0.41
1:B:456:THR:O	1:B:459:ARG:HG2	2.20	0.41
1:C:24:GLY:HA3	1:C:71:ILE:O	2.19	0.41
1:D:233:LYS:HE3	1:D:237:LEU:HD21	2.01	0.41
1:B:221:CYS:HB3	4:B:603:PY0:HN1	1.85	0.41
1:C:247:MET:HG3	1:C:410:VAL:HB	2.02	0.41
1:D:224:ARG:CZ	1:D:224:ARG:HA	2.49	0.41
1:D:546:PRO:HB2	1:D:548:ASN:OD1	2.20	0.41
1:A:515:THR:HG23	5:A:2197:HOH:O	2.20	0.41
1:B:330:LEU:O	1:B:334:LEU:HG	2.21	0.41
1:A:371:TRP:CE2	1:A:394:GLY:HA3	2.56	0.41
1:D:520:LYS:HA	1:D:520:LYS:HD3	1.88	0.41
1:A:288:LEU:CD2	1:A:411:LEU:HD22	2.51	0.41
1:B:306:ILE:HD11	5:B:2213:HOH:O	2.20	0.41
1:C:330:LEU:O	1:C:334:LEU:HG	2.21	0.41
1:A:247:MET:HG3	1:A:410:VAL:HB	2.03	0.41
1:C:508:GLU:HB2	1:C:534:ARG:HG2	2.01	0.41
1:D:95:VAL:O	1:D:162:PRO:HA	2.21	0.41
1:B:294:THR:HG23	1:B:297:PHE:N	2.12	0.40
2:B:600:TPP:C6'	2:B:600:TPP:HM41	2.51	0.40
1:D:294:THR:CG2	1:D:297:PHE:N	2.72	0.40
1:C:238:THR:HG23	1:C:239:GLN:N	2.35	0.40
2:A:600:TPP:H2	5:B:2021:HOH:O	2.22	0.40
1:D:177:PRO:HB3	1:D:179:LYS:HE2	2.04	0.40
1:A:24:GLY:HA3	1:A:71:ILE:O	2.21	0.40
1:A:230:GLU:OE1	1:A:230:GLU:N	2.52	0.40
1:D:475:THR:CG2	1:D:542:VAL:O	2.69	0.40
1:A:475:THR:CG2	1:A:542:VAL:O	2.69	0.40
1:B:71:ILE:HA	1:B:98:VAL:O	2.21	0.40
1:B:363:THR:HG1	1:B:515:THR:HG21	1.82	0.40
1:C:185:ILE:CG2	1:C:187:MET:HE2	2.51	0.40
1:D:294:THR:HG23	1:D:297:PHE:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	540/563 (96%)	527 (98%)	11 (2%)	2 (0%)	30	14
1	B	560/563 (100%)	546 (98%)	13 (2%)	1 (0%)	43	24
1	C	555/563 (99%)	540 (97%)	15 (3%)	0	100	100
1	D	560/563 (100%)	546 (98%)	14 (2%)	0	100	100
All	All	2215/2252 (98%)	2159 (98%)	53 (2%)	3 (0%)	48	27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	226	ASP
1	A	557	ALA
1	A	346	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	451/468 (96%)	443 (98%)	8 (2%)	51	28
1	B	467/468 (100%)	463 (99%)	4 (1%)	70	55
1	C	463/468 (99%)	456 (98%)	7 (2%)	57	35
1	D	467/468 (100%)	459 (98%)	8 (2%)	53	30
All	All	1848/1872 (99%)	1821 (98%)	27 (2%)	57	35

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	264	VAL
1	A	267	LEU
1	A	304	LYS
1	A	347	VAL
1	A	352	ARG
1	A	551	GLU
1	A	554	LYS
1	B	179	LYS
1	B	203	THR
1	B	304	LYS
1	B	562	LYS
1	C	2	SER
1	C	233	LYS
1	C	264	VAL
1	C	333	LEU
1	C	342	LYS
1	C	353	THR
1	C	552	GLN
1	D	179	LYS
1	D	233	LYS
1	D	238	THR
1	D	294	THR
1	D	336	ASN
1	D	363	THR
1	D	551	GLU
1	D	562	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	239	GLN
1	A	397	GLN
1	B	397	GLN
1	B	477	GLN
1	C	175	ASN
1	D	325	GLN
1	D	477	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	26,27,27	1.59	7 (26%)	38,40,40	1.96	12 (31%)
4	PY0	C	603	1	4,6,6	1.51	1 (25%)	1,9,9	2.05	1 (100%)
4	PY0	C	602	-	4,6,6	1.41	1 (25%)	1,9,9	0.71	0
4	PY0	A	604	-	4,6,6	2.62	2 (50%)	1,9,9	0.79	0
4	PY0	D	603	1	4,6,6	1.05	0	1,9,9	2.30	1 (100%)
4	PY0	B	603	1	4,6,6	1.32	0	1,9,9	1.27	0
4	PY0	B	602	-	4,6,6	2.41	1 (25%)	1,9,9	0.13	0
2	TPP	D	600	3	26,27,27	1.65	8 (30%)	38,40,40	1.83	10 (26%)
4	PY0	A	603	-	4,6,6	1.54	1 (25%)	1,9,9	0.01	0
2	TPP	A	600	3	26,27,27	1.53	4 (15%)	38,40,40	1.71	8 (21%)
2	TPP	C	600	3	26,27,27	1.70	6 (23%)	38,40,40	1.49	7 (18%)
4	PY0	D	602	-	4,6,6	2.37	1 (25%)	1,9,9	0.69	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	B	600	3	-	2/17/17/17	0/2/2/2
4	PY0	C	603	1	-	0/0/6/6	-
4	PY0	C	602	-	-	0/0/6/6	-
4	PY0	A	604	-	1/1/2/2	0/0/6/6	-
4	PY0	D	603	1	-	0/0/6/6	-
4	PY0	B	603	1	-	0/0/6/6	-
4	PY0	B	602	-	-	0/0/6/6	-
2	TPP	D	600	3	-	3/17/17/17	0/2/2/2
4	PY0	A	603	-	-	0/0/6/6	-
2	TPP	A	600	3	-	2/17/17/17	0/2/2/2
2	TPP	C	600	3	-	2/17/17/17	0/2/2/2
4	PY0	D	602	-	-	0/0/6/6	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	PY0	O2-C1	4.61	1.44	1.38
2	C	600	TPP	C5-S1	-4.60	1.60	1.72
4	D	602	PY0	O2-C1	4.54	1.44	1.38
2	D	600	TPP	C5-S1	-4.14	1.61	1.72
2	A	600	TPP	C5-S1	-4.07	1.62	1.72
2	B	600	TPP	C5-S1	-3.83	1.62	1.72
4	A	604	PY0	O1-C1	3.76	1.43	1.38
4	A	604	PY0	O2-C1	3.62	1.43	1.38
2	A	600	TPP	C2-N3	3.15	1.40	1.32
2	C	600	TPP	C4'-N3'	3.12	1.39	1.35
2	B	600	TPP	C6'-N1'	3.06	1.40	1.34
4	A	603	PY0	O2-C1	-2.93	1.34	1.38
2	C	600	TPP	C2-N3	2.79	1.39	1.32
2	C	600	TPP	C6'-N1'	2.65	1.39	1.34
2	B	600	TPP	C2-S1	-2.63	1.61	1.69
2	A	600	TPP	C6'-N1'	2.63	1.39	1.34
2	D	600	TPP	C2-N3	2.60	1.38	1.32
2	B	600	TPP	C2-N3	2.57	1.38	1.32
2	A	600	TPP	C4'-N3'	2.54	1.38	1.35
2	C	600	TPP	C2'-N1'	2.52	1.38	1.34
4	C	603	PY0	O2-C1	2.49	1.41	1.38
2	C	600	TPP	C2-S1	-2.33	1.62	1.69
2	D	600	TPP	C6'-N1'	2.33	1.39	1.34
2	D	600	TPP	C2'-N3'	2.33	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	TPP	C2-S1	-2.30	1.62	1.69
4	C	602	PY0	O2-C1	2.14	1.41	1.38
2	D	600	TPP	C2'-N1'	2.09	1.37	1.34
2	B	600	TPP	C5-C4	2.08	1.39	1.35
2	D	600	TPP	C5-C4	2.07	1.39	1.35
2	B	600	TPP	C2'-N1'	2.06	1.37	1.34
2	D	600	TPP	C4-N3	-2.06	1.35	1.39
2	B	600	TPP	C4-N3	-2.01	1.35	1.39

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	TPP	C2-N3-C4	-5.03	107.27	114.06
2	D	600	TPP	C2-N3-C4	-4.66	107.76	114.06
2	A	600	TPP	C2-N3-C4	-4.47	108.02	114.06
2	B	600	TPP	S1-C2-N3	4.26	117.69	112.30
2	B	600	TPP	C6'-C5'-C4'	4.20	120.71	115.55
2	D	600	TPP	S1-C2-N3	3.98	117.33	112.30
2	D	600	TPP	N1'-C2'-N3'	-3.64	119.47	125.53
2	A	600	TPP	C5'-C6'-N1'	-3.55	118.06	123.83
2	C	600	TPP	C2-N3-C4	-3.43	109.43	114.06
2	A	600	TPP	C6'-N1'-C2'	3.41	121.68	116.07
2	A	600	TPP	C6'-C5'-C4'	3.38	119.70	115.55
2	D	600	TPP	C2-S1-C5	-3.34	89.00	91.22
2	C	600	TPP	N1'-C2'-N3'	-3.32	120.01	125.53
2	C	600	TPP	CM2-C2'-N3'	3.20	121.91	117.13
2	A	600	TPP	CM2-C2'-N1'	3.14	120.54	117.20
2	A	600	TPP	N1'-C2'-N3'	-3.11	120.35	125.53
2	D	600	TPP	C4-C5-S1	2.99	115.22	110.56
2	B	600	TPP	CM2-C2'-N1'	2.98	120.37	117.20
2	B	600	TPP	C5'-C6'-N1'	-2.94	119.04	123.83
2	B	600	TPP	N1'-C2'-N3'	-2.93	120.66	125.53
2	C	600	TPP	C2'-N3'-C4'	2.92	122.59	118.10
2	D	600	TPP	C2'-N3'-C4'	2.72	122.28	118.10
2	B	600	TPP	C2-S1-C5	-2.70	89.43	91.22
2	D	600	TPP	CM2-C2'-N3'	2.66	121.11	117.13
2	B	600	TPP	C2'-N3'-C4'	2.58	122.06	118.10
2	C	600	TPP	N4'-C4'-N3'	2.50	120.41	117.03
2	B	600	TPP	C5'-C4'-N3'	-2.34	117.88	121.31
4	D	603	PY0	O3-C2-C3	-2.30	103.63	108.92
2	B	600	TPP	C4-C5-S1	2.29	114.14	110.56
2	B	600	TPP	O3B-PB-O2B	2.17	115.96	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	TPP	CM4-C4-N3	2.16	125.56	120.57
2	D	600	TPP	C6'-N1'-C2'	2.14	119.59	116.07
2	A	600	TPP	CM4-C4-C5	-2.13	122.30	127.75
2	D	600	TPP	C6'-C5'-C4'	2.12	118.15	115.55
2	B	600	TPP	C6'-N1'-C2'	2.11	119.54	116.07
2	D	600	TPP	CM2-C2'-N1'	2.08	119.42	117.20
4	C	603	PY0	O3-C2-C3	2.05	113.62	108.92
2	C	600	TPP	C4-C5-S1	2.04	113.75	110.56
2	C	600	TPP	O3B-PB-O2B	2.03	115.40	107.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	604	PY0	C2

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	TPP	PA-O3A-PB-O3B
2	B	600	TPP	PA-O3A-PB-O3B
2	C	600	TPP	PA-O3A-PB-O3B
2	D	600	TPP	PA-O3A-PB-O3B
2	A	600	TPP	PA-O3A-PB-O2B
2	B	600	TPP	PA-O3A-PB-O2B
2	C	600	TPP	PA-O3A-PB-O2B
2	D	600	TPP	PA-O3A-PB-O2B
2	D	600	TPP	PA-O3A-PB-O1B

There are no ring outliers.

11 monomers are involved in 35 short contacts:

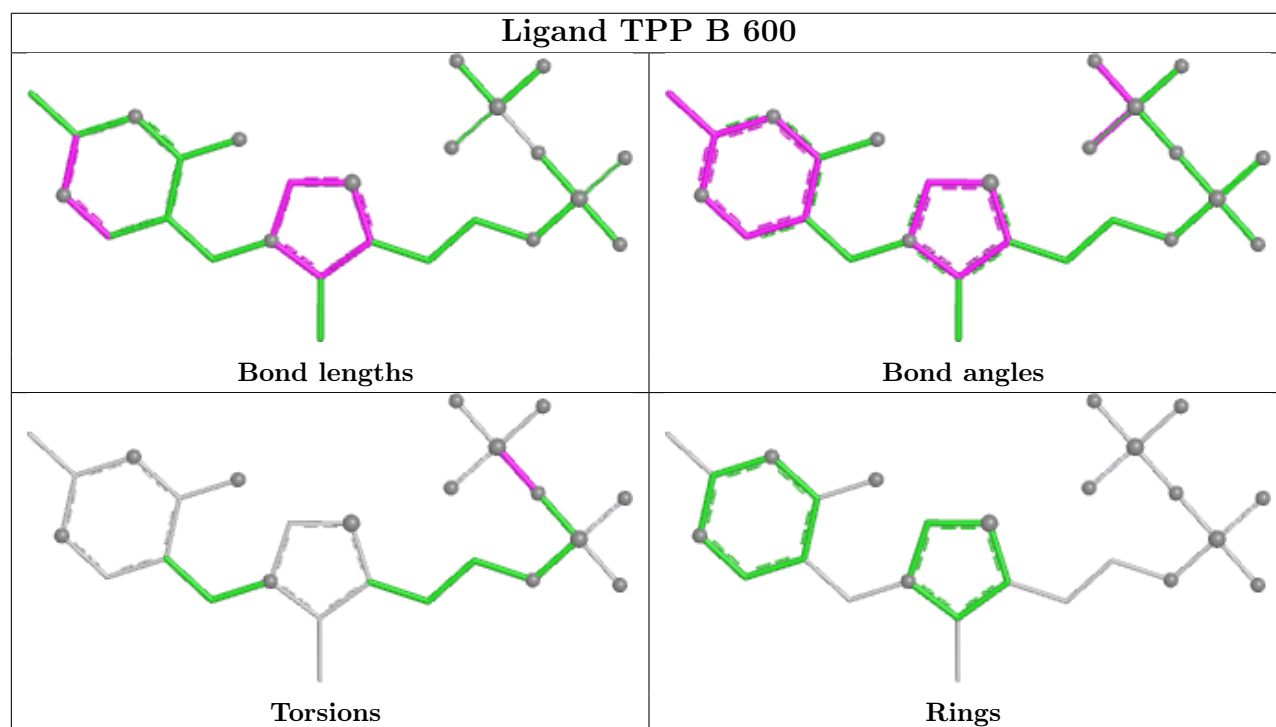
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	TPP	9	0
4	C	603	PY0	1	0
4	C	602	PY0	6	0
4	A	604	PY0	1	0
4	B	603	PY0	2	0
4	B	602	PY0	8	0
2	D	600	TPP	9	0
4	A	603	PY0	6	0
2	A	600	TPP	1	0

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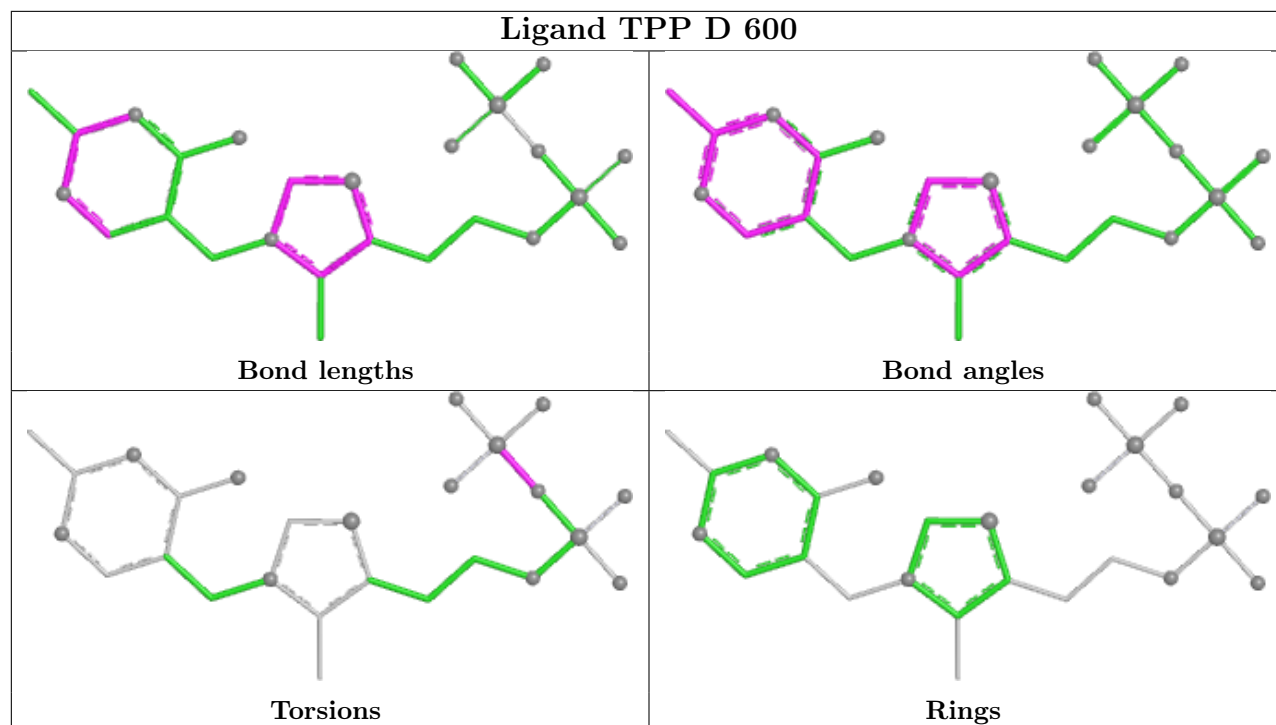
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	600	TPP	6	0
4	D	602	PY0	8	0

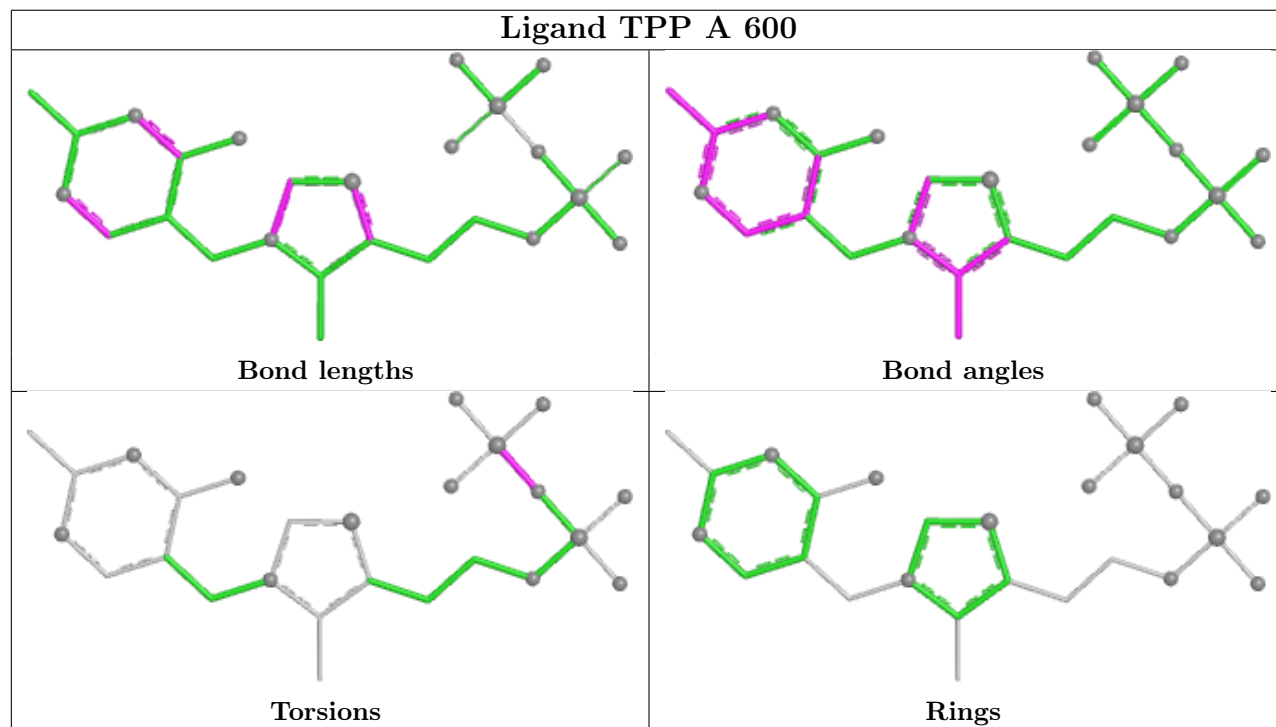
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

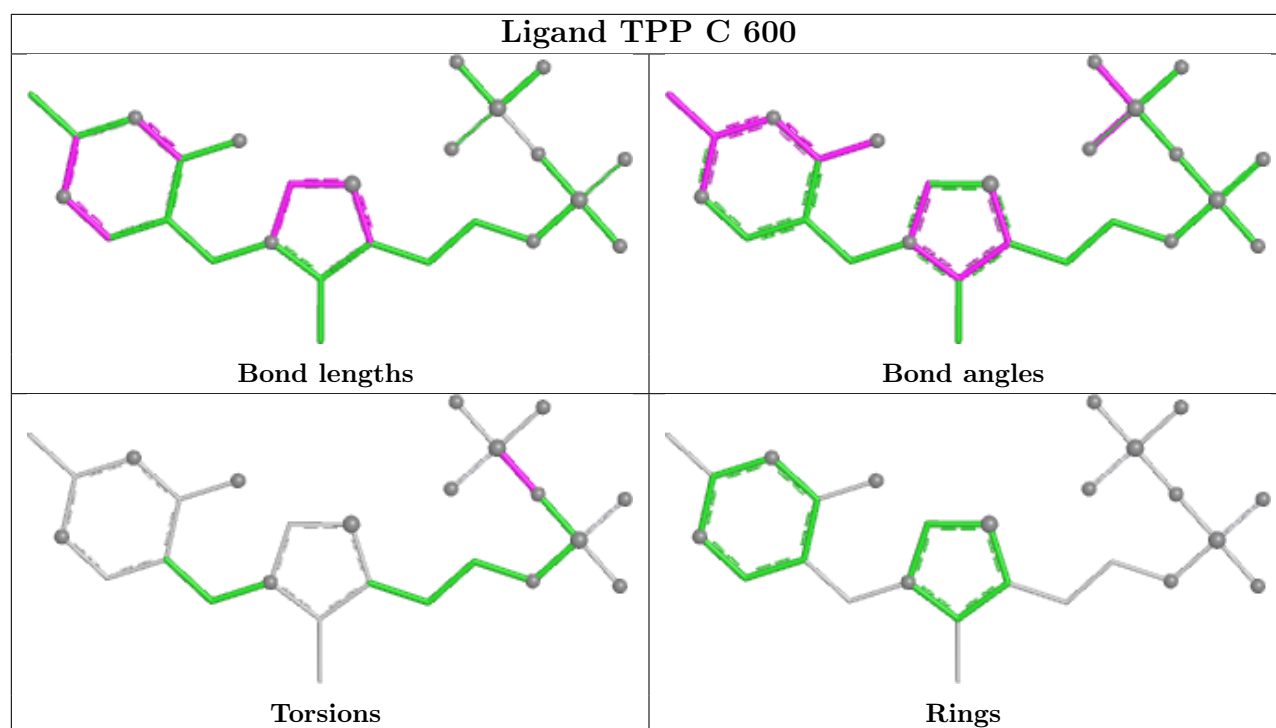


Ligand TPP D 600



Ligand TPP A 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	544/563 (96%)	-0.18	18 (3%) 49 52	11, 20, 46, 73	0
1	B	562/563 (99%)	-0.32	3 (0%) 87 90	11, 20, 32, 54	0
1	C	557/563 (98%)	-0.18	11 (1%) 65 69	13, 22, 39, 69	0
1	D	562/563 (99%)	-0.13	1 (0%) 91 92	13, 24, 40, 48	0
All	All	2225/2252 (98%)	-0.20	33 (1%) 72 76	11, 22, 40, 73	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	558	ALA	3.5
1	A	211	ALA	3.3
1	A	555	LEU	3.2
1	C	553	ALA	3.2
1	C	292	PHE	3.2
1	B	111	LEU	3.0
1	A	557	ALA	3.0
1	C	189	LEU	3.0
1	A	550	VAL	2.9
1	A	206	ALA	2.9
1	A	279	ALA	2.8
1	C	557	ALA	2.8
1	A	344	TYR	2.8
1	B	112	LEU	2.8
1	C	551	GLU	2.7
1	C	555	LEU	2.7
1	A	341	ALA	2.6
1	A	553	ALA	2.6
1	A	281	LEU	2.4
1	C	157	TYR	2.4
1	C	556	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	339	ASP	2.4
1	A	208	VAL	2.4
1	A	272	VAL	2.3
1	A	556	THR	2.3
1	D	547	GLN	2.3
1	B	110	GLN	2.2
1	C	2	SER	2.2
1	A	347	VAL	2.2
1	A	337	ILE	2.2
1	A	270	PRO	2.1
1	A	338	ALA	2.0
1	C	191	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PY0	A	603	7/7	0.60	0.35	21,22,23,43	7
4	PY0	C	602	7/7	0.72	0.27	37,38,38,39	7
4	PY0	C	603	7/7	0.76	0.33	22,23,25,26	7
4	PY0	A	604	7/7	0.83	0.14	57,57,58,58	0
4	PY0	B	602	7/7	0.84	0.13	22,24,28,29	0
4	PY0	D	602	7/7	0.87	0.12	29,30,32,35	0
4	PY0	B	603	7/7	0.94	0.10	11,18,21,29	0
4	PY0	D	603	7/7	0.94	0.10	14,22,23,26	0
3	MG	C	601	1/1	0.98	0.04	16,16,16,16	0
2	TPP	C	600	26/26	0.99	0.04	14,16,17,18	0
2	TPP	D	600	26/26	0.99	0.04	14,16,18,18	0

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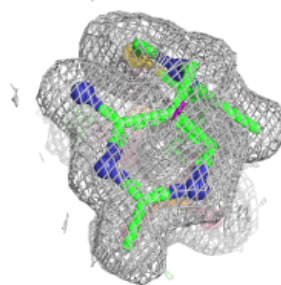
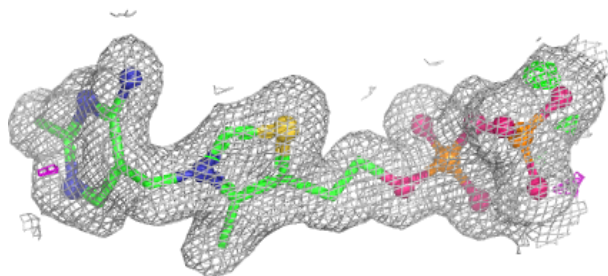
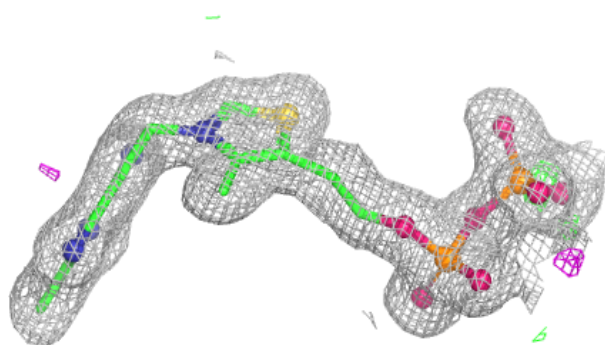
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	601	1/1	0.99	0.03	16,16,16,16	0
3	MG	B	601	1/1	0.99	0.02	14,14,14,14	0
2	TPP	A	600	26/26	0.99	0.04	12,13,15,17	0
3	MG	D	601	1/1	0.99	0.03	17,17,17,17	0
2	TPP	B	600	26/26	0.99	0.04	11,13,15,16	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.

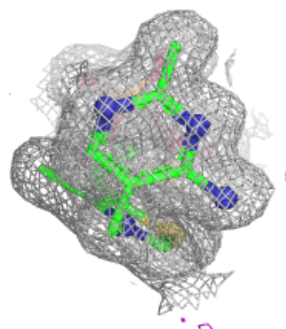
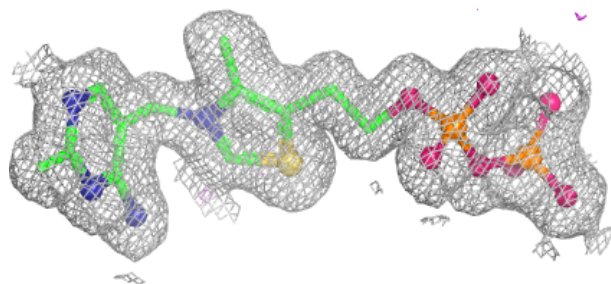
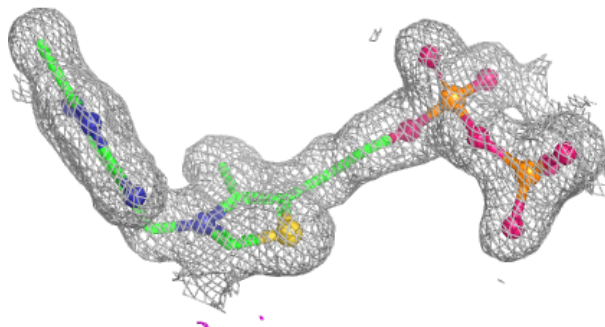
Electron density around TPP C 600:

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

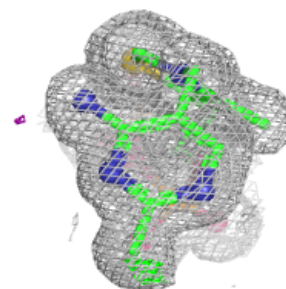
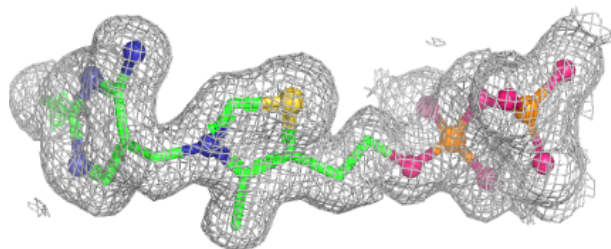
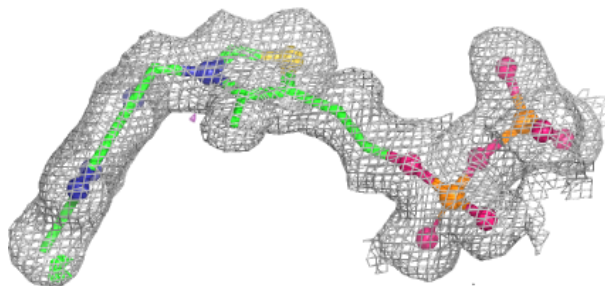


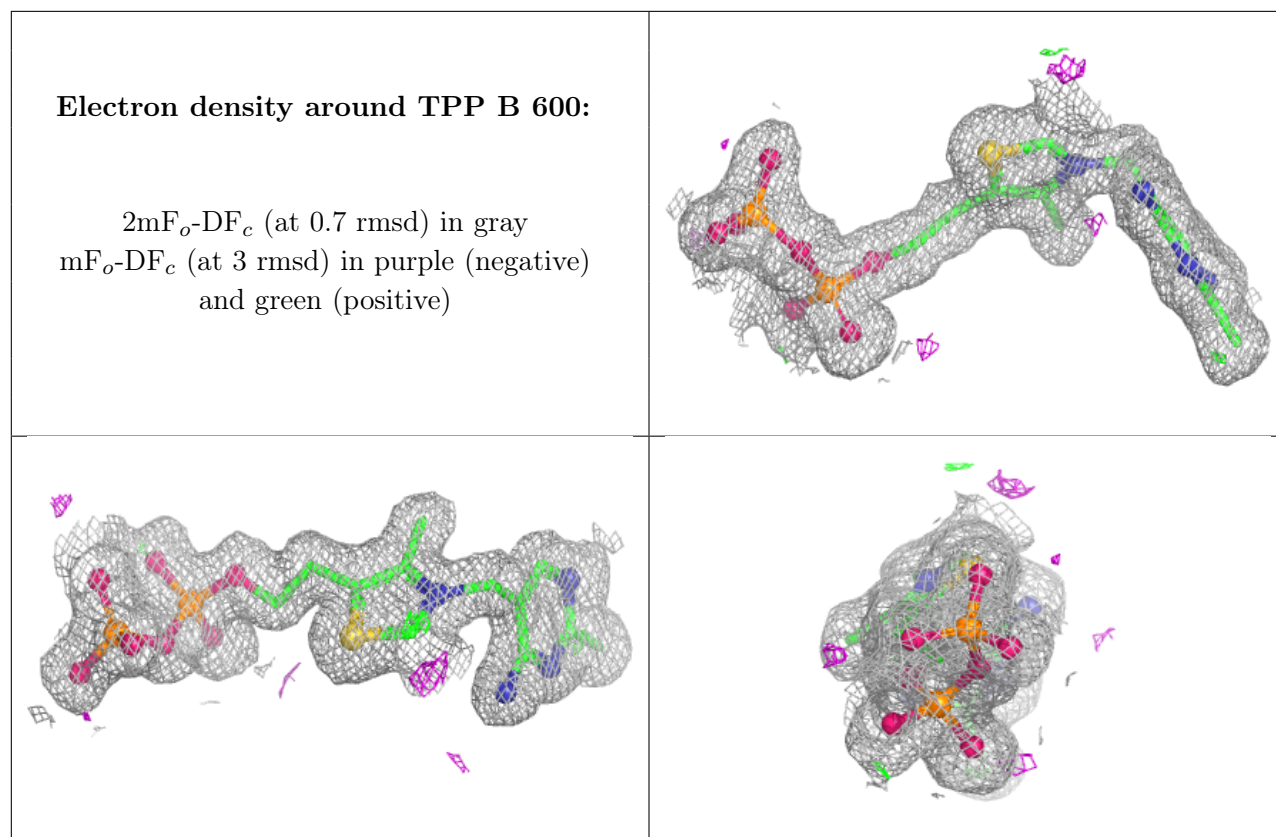
Electron density around TPP D 600:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.