



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:24 AM UTC

PDB ID : 2WVA / pdb_00002wva
Title : Structural insights into the pre-reaction state of pyruvate decarboxylase from *Zymomonas mobilis*
Authors : Pei, X.Y.; Erixon, K.; Luisi, B.F.; Leeper, F.J.
Deposited on : 2009-10-15
Resolution : 2.20 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

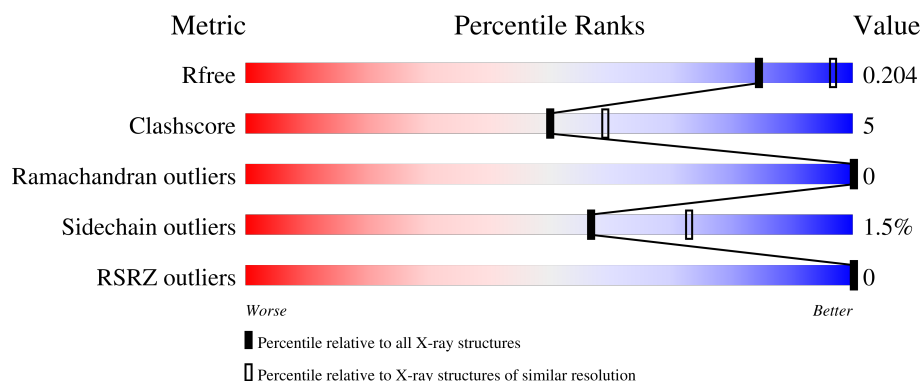
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	568	
1	B	568	
1	E	568	
1	F	568	
1	V	568	

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Mol	Chain	Length	Quality of chain
1	X	568	 90% 9%
1	Y	568	 88% 11% .
1	Z	568	 88% 10% ..

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
4	PYR	Z	602	-	X	-	-

2 Entry composition

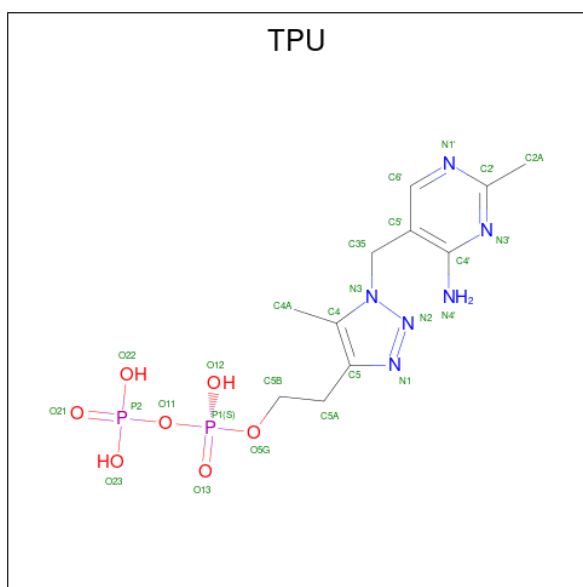
There are 5 unique types of molecules in this entry. The entry contains 37053 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	565	Total	C	N	O	S	0	2	0
			4274	2719	727	810	18			
1	B	565	Total	C	N	O	S	0	0	0
			4266	2714	727	807	18			
1	E	565	Total	C	N	O	S	0	1	0
			4269	2716	727	808	18			
1	F	565	Total	C	N	O	S	0	1	0
			4269	2716	727	808	18			
1	V	565	Total	C	N	O	S	0	1	0
			4269	2716	727	808	18			
1	X	566	Total	C	N	O	S	0	0	0
			4274	2719	728	808	19			
1	Y	565	Total	C	N	O	S	0	1	0
			4269	2716	727	808	18			
1	Z	565	Total	C	N	O	S	0	0	0
			4266	2714	727	807	18			

- Molecule 2 is 2-{1-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-5-METHYL-1H-1,2,3-TRIAZOL-4-YL}ETHYL TRIHYDROGEN DIPHOSPHATE (CCD ID: TPU) (formula: C₁₁H₁₈N₆O₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			26	11	6	7	2		
2	B	1	Total	C	N	O	P	0	0
			26	11	6	7	2		
2	E	1	Total	C	N	O	P	0	0
			26	11	6	7	2		
2	F	1	Total	C	N	O	P	0	0
			26	11	6	7	2		
2	V	1	Total	C	N	O	P	0	0
			26	11	6	7	2		
2	X	1	Total	C	N	O	P	0	0
			26	11	6	7	2		
2	Y	1	Total	C	N	O	P	0	0
			26	11	6	7	2		
2	Z	1	Total	C	N	O	P	0	0
			26	11	6	7	2		

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

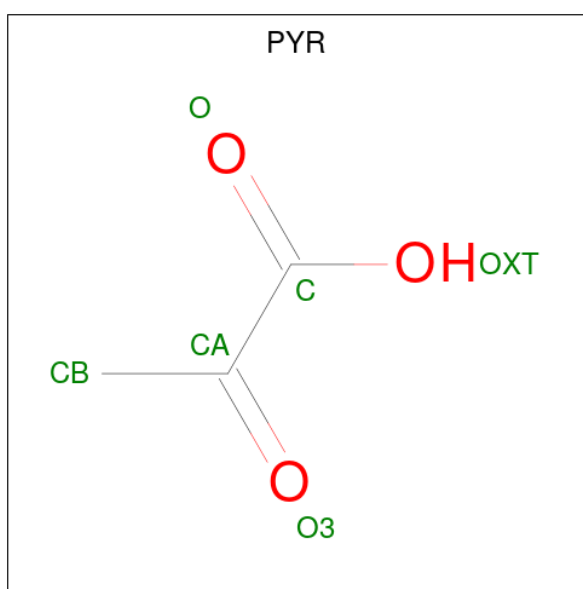
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	V	1	Total	Mg	0	0
			1	1		
3	X	1	Total	Mg	0	0
			1	1		
3	Y	1	Total	Mg	0	0
			1	1		
3	Z	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PYRUVIC ACID (CCD ID: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			6	3	3		
4	V	1	Total	C	O	0	0
			6	3	3		
4	Z	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	388	Total	O	0	0
			388	388		
5	B	293	Total	O	0	0
			293	293		

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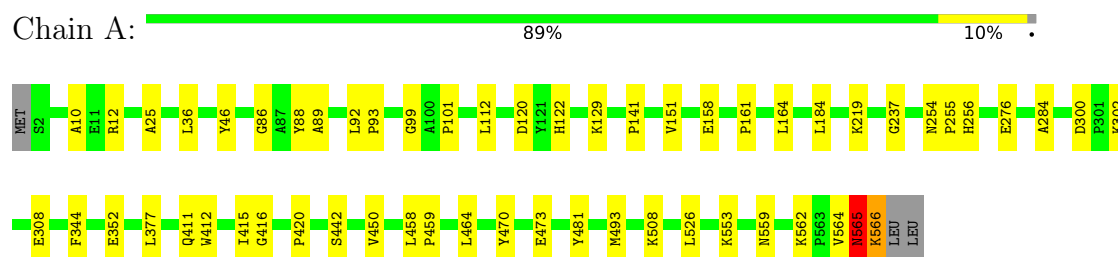
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	295	Total 295	O 295	0	0
5	F	334	Total 334	O 334	0	0
5	V	344	Total 344	O 344	0	0
5	X	357	Total 357	O 357	0	0
5	Y	317	Total 317	O 317	0	0
5	Z	335	Total 335	O 335	0	0

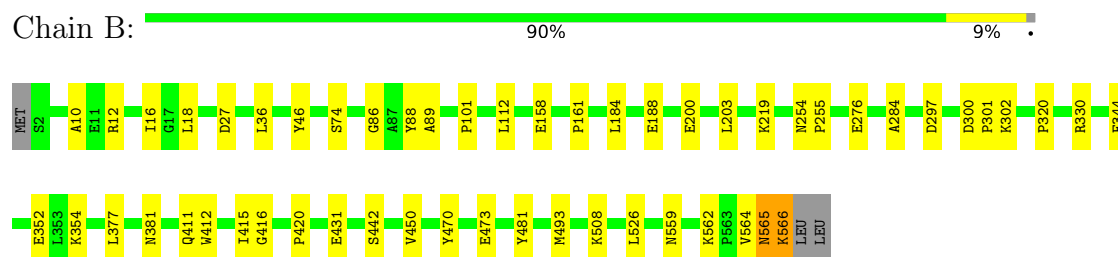
3 Residue-property plots

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.

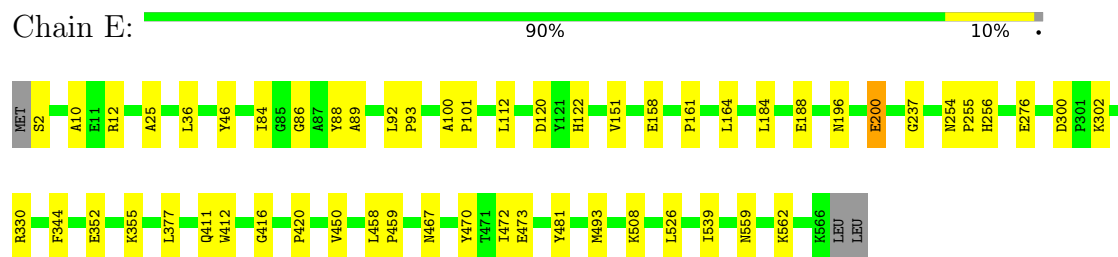
• Molecule 1: PYRUVATE DECARBOXYLASE



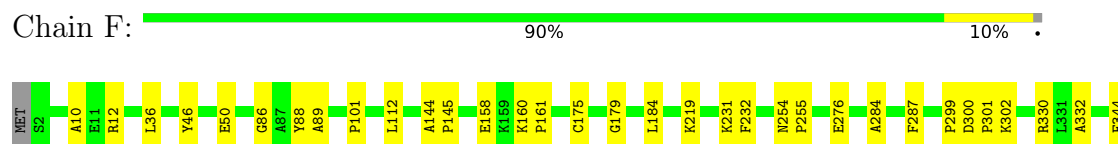
• Molecule 1: PYRUVATE DECARBOXYLASE



• Molecule 1: PYRUVATE DECARBOXYLASE



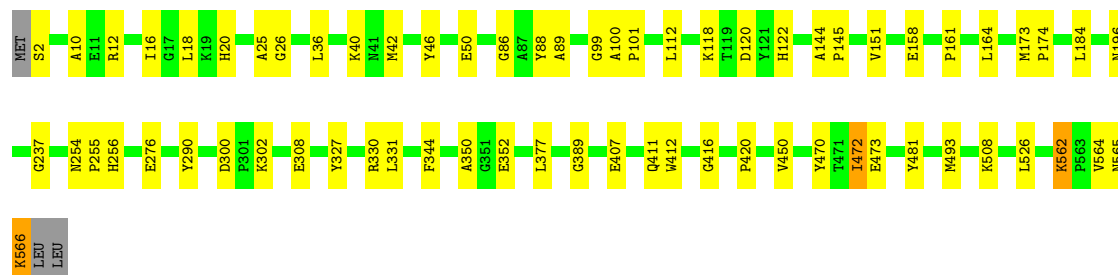
• Molecule 1: PYRUVATE DECARBOXYLASE





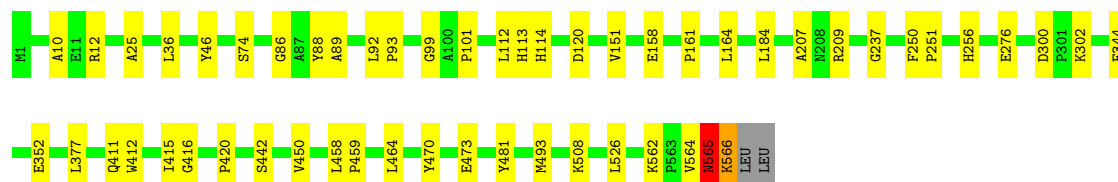
• Molecule 1: PYRUVATE DECARBOXYLASE

Chain V: 88% 11% ..



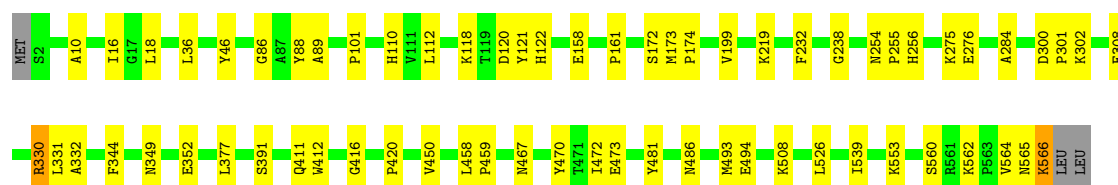
• Molecule 1: PYRUVATE DECARBOXYLASE

Chain X: 90% 9%



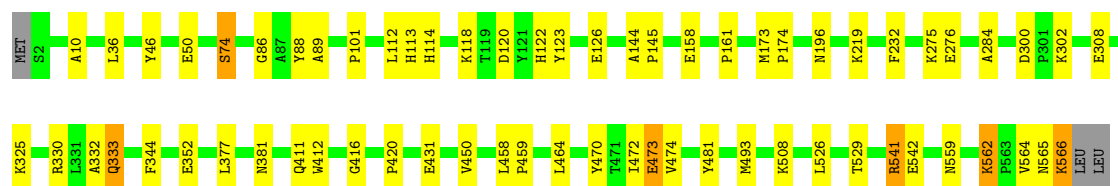
• Molecule 1: PYRUVATE DECARBOXYLASE

Chain Y: 88% 11% .



• Molecule 1: PYRUVATE DECARBOXYLASE

Chain Z: 88% 10% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.62Å 111.58Å 167.43Å 89.82° 90.11° 78.94°	Depositor
Resolution (Å)	34.65 – 2.20 34.65 – 2.20	Depositor EDS
% Data completeness (in resolution range)	82.4 (34.65-2.20) 80.5 (34.65-2.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.20Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.194 , 0.213 0.187 , 0.204	Depositor DCC
R_{free} test set	10462 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.810	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.448 for -h,-k,l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	37053	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.14% 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: PYR, MG, TPU

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	0.53	0/4372	0.77	2/5944 (0.0%)
1	B	0.53	0/4358	0.78	1/5925 (0.0%)
1	E	0.53	0/4364	0.77	0/5933
1	F	0.52	0/4364	0.77	2/5933 (0.0%)
1	V	0.56	0/4364	0.78	1/5933 (0.0%)
1	X	0.54	0/4366	0.77	2/5935 (0.0%)
1	Y	0.56	0/4363	0.78	0/5930
1	Z	0.58	0/4358	0.78	0/5925
All	All	0.54	0/34909	0.78	8/47458 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	565	ASN	N-CA-C	7.08	120.47	109.07
1	A	565	ASN	N-CA-C	6.24	118.90	108.73
1	A	99	GLY	N-CA-C	-5.74	106.01	112.33
1	V	99	GLY	N-CA-C	-5.74	105.19	112.54
1	F	179	GLY	CA-C-N	5.35	125.27	119.76
1	F	179	GLY	C-N-CA	5.35	125.27	119.76
1	X	99	GLY	N-CA-C	-5.35	105.69	112.54
1	X	565	ASN	N-CA-C	5.30	117.88	109.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4274	0	4245	45	0
1	B	4266	0	4236	42	0
1	E	4269	0	4241	38	0
1	F	4269	0	4241	46	0
1	V	4269	0	4241	55	0
1	X	4274	0	4248	36	0
1	Y	4269	0	4240	66	0
1	Z	4266	0	4236	52	0
2	A	26	0	15	2	0
2	B	26	0	15	2	0
2	E	26	0	15	4	0
2	F	26	0	15	4	0
2	V	26	0	15	4	0
2	X	26	0	15	2	0
2	Y	26	0	15	2	0
2	Z	26	0	15	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	V	1	0	0	0	0
3	X	1	0	0	0	0
3	Y	1	0	0	0	0
3	Z	1	0	0	0	0
4	F	6	0	0	0	0
4	V	6	0	0	0	0
4	Z	6	0	0	3	0
5	A	388	0	0	7	0
5	B	293	0	0	4	0
5	E	295	0	0	4	0
5	F	334	0	0	7	0
5	V	344	0	0	14	0
5	X	357	0	0	4	0
5	Y	317	0	0	14	0
5	Z	335	0	0	8	0
All	All	37053	0	34048	359	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 5.

All (359) 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:Y:565:ASN:C	1:Y:566:LYS:HB3	1.67	1.19
1:X:450:VAL:HG11	1:X:493:MET:HE1	1.26	1.14
1:F:565:ASN:ND2	1:F:566:LYS:H	1.45	1.14
1:Y:450:VAL:HG11	1:Y:493:MET:HE1	1.31	1.12
1:E:450:VAL:HG11	1:E:493:MET:HE1	1.30	1.12
1:Z:450:VAL:HG11	1:Z:493:MET:HE1	1.32	1.11
1:A:450:VAL:HG11	1:A:493:MET:HE1	1.28	1.11
1:B:450:VAL:HG11	1:B:493:MET:HE1	1.30	1.09
1:V:450:VAL:HG11	1:V:493:MET:HE1	1.30	1.09
1:F:565:ASN:CG	1:F:566:LYS:H	1.59	1.06
1:F:450:VAL:HG11	1:F:493:MET:HE1	1.33	1.06
1:Y:565:ASN:O	1:Y:566:LYS:HB3	1.59	1.02
1:F:564:VAL:HG12	1:F:565:ASN:H	1.21	1.01
1:F:541:ARG:HD3	5:F:2290:HOH:O	1.60	1.01
1:Y:565:ASN:CG	1:Y:566:LYS:HB2	1.91	0.95
1:Y:565:ASN:ND2	1:Y:566:LYS:CB	2.30	0.94
1:F:413:GLY:HA2	5:F:2265:HOH:O	1.68	0.93
1:B:381:ASN:HB2	1:Z:431:GLU:HB2	1.49	0.92
1:B:566:LYS:NZ	1:B:566:LYS:HB2	1.80	0.91
1:B:566:LYS:HB2	1:B:566:LYS:HZ2	1.33	0.91
1:Y:565:ASN:HD21	1:Y:566:LYS:HG2	1.36	0.88
1:V:566:LYS:HE3	5:V:2168:HOH:O	1.75	0.87
1:Y:565:ASN:ND2	1:Y:566:LYS:HG2	1.91	0.86
1:F:565:ASN:CG	1:F:566:LYS:N	2.29	0.85
1:Y:565:ASN:CG	1:Y:566:LYS:CB	2.49	0.84
1:F:566:LYS:O	1:F:566:LYS:HG2	1.74	0.84
1:B:565:ASN:ND2	1:B:566:LYS:HG2	1.91	0.84
1:V:566:LYS:HA	5:Y:2072:HOH:O	1.76	0.84
1:Y:566:LYS:HE3	1:Y:566:LYS:HA	1.61	0.81
1:Z:566:LYS:O	1:Z:566:LYS:HG2	1.80	0.80
1:F:566:LYS:O	1:F:566:LYS:CG	2.29	0.80
1:Y:565:ASN:O	1:Y:566:LYS:CB	2.30	0.80
1:V:566:LYS:CG	1:V:566:LYS:O	2.30	0.80
1:Y:566:LYS:HE3	1:Y:566:LYS:CA	2.13	0.79
1:Y:565:ASN:ND2	1:Y:566:LYS:CG	2.47	0.77
1:A:450:VAL:CG1	1:A:493:MET:HE1	2.14	0.77
2:V:600:TPU:H351	4:Z:602:PYR:OXT	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:VAL:CG1	1:B:493:MET:HE1	2.14	0.77
1:X:450:VAL:CG1	1:X:493:MET:HE1	2.11	0.77
1:Z:562:LYS:HD2	5:Z:2333:HOH:O	1.85	0.76
1:E:450:VAL:CG1	1:E:493:MET:HE1	2.14	0.76
1:F:564:VAL:HG12	1:F:565:ASN:N	1.96	0.76
1:V:566:LYS:CE	5:V:2168:HOH:O	2.34	0.74
1:F:565:ASN:ND2	1:F:566:LYS:N	2.29	0.74
1:V:42:MET:SD	5:V:2016:HOH:O	2.45	0.74
1:X:566:LYS:HD3	1:X:566:LYS:C	2.12	0.73
1:F:10:ALA:HB2	1:F:36:LEU:HD23	1.71	0.73
1:V:450:VAL:CG1	1:V:493:MET:HE1	2.15	0.73
1:B:566:LYS:NZ	1:B:566:LYS:CB	2.51	0.73
1:Y:276:GLU:HG3	1:Y:344:PHE:CZ	2.25	0.71
1:Y:565:ASN:ND2	1:Y:566:LYS:HB3	2.04	0.71
1:F:276:GLU:HG3	1:F:344:PHE:CZ	2.25	0.71
1:Z:276:GLU:HG3	1:Z:344:PHE:CZ	2.25	0.71
1:Z:450:VAL:CG1	1:Z:493:MET:HE1	2.16	0.71
1:V:276:GLU:HG3	1:V:344:PHE:CZ	2.26	0.71
1:Y:553:LYS:HG3	5:Y:2305:HOH:O	1.90	0.70
1:B:276:GLU:HG3	1:B:344:PHE:CZ	2.26	0.70
1:Y:565:ASN:OD1	1:Y:566:LYS:HB2	1.92	0.70
1:V:566:LYS:O	1:V:566:LYS:HG3	1.89	0.70
1:X:276:GLU:HG3	1:X:344:PHE:CZ	2.27	0.70
1:Y:450:VAL:CG1	1:Y:493:MET:HE1	2.16	0.70
1:F:450:VAL:CG1	1:F:493:MET:HE1	2.17	0.70
1:A:276:GLU:HG3	1:A:344:PHE:CZ	2.26	0.70
1:V:10:ALA:HB2	1:V:36:LEU:HD23	1.74	0.69
1:Y:565:ASN:O	1:Y:566:LYS:CA	2.41	0.68
1:Z:10:ALA:HB2	1:Z:36:LEU:HD23	1.75	0.68
1:E:276:GLU:HG3	1:E:344:PHE:CZ	2.29	0.66
1:V:196:ASN:OD1	1:V:330:ARG:NH1	2.28	0.66
1:Y:565:ASN:HD21	1:Y:566:LYS:CG	2.05	0.66
1:Y:308:GLU:HG3	5:Y:2220:HOH:O	1.95	0.66
1:Y:172:SER:HB2	5:Y:2135:HOH:O	1.95	0.66
1:B:10:ALA:HB2	1:B:36:LEU:HD23	1.79	0.65
1:V:562:LYS:HB2	5:V:2335:HOH:O	1.95	0.65
1:A:120[B]:ASP:OD2	1:E:122:HIS:HE1	1.79	0.65
1:F:564:VAL:CG1	1:F:565:ASN:H	2.02	0.65
1:Y:565:ASN:O	1:Y:566:LYS:N	2.29	0.65
1:A:10:ALA:HB2	1:A:36:LEU:HD23	1.80	0.64
1:X:10:ALA:HB2	1:X:36:LEU:HD23	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:HIS:HE1	1:E:120:ASP:OD2	1.82	0.63
1:E:10:ALA:HB2	1:E:36:LEU:HD23	1.80	0.63
1:A:565:ASN:O	1:A:565:ASN:ND2	2.32	0.63
1:B:354:LYS:NZ	5:B:2222:HOH:O	2.33	0.62
1:V:42:MET:HB2	5:V:2016:HOH:O	1.99	0.61
1:Y:377:LEU:HG	5:Y:2243:HOH:O	1.99	0.61
1:Y:10:ALA:HB2	1:Y:36:LEU:HD23	1.81	0.61
1:Y:566:LYS:HE3	1:Y:566:LYS:C	2.26	0.60
1:A:565:ASN:ND2	1:A:566:LYS:HE3	2.17	0.59
1:Z:275:LYS:HE2	5:Z:2207:HOH:O	2.02	0.59
1:F:330:ARG:NH2	5:F:2240:HOH:O	2.35	0.58
1:E:196:ASN:O	1:E:200:GLU:HG2	2.04	0.58
1:V:20:HIS:C	5:V:2016:HOH:O	2.46	0.57
1:Z:474:VAL:HG21	1:Z:541:ARG:HD2	1.85	0.57
1:A:565:ASN:HD21	1:A:566:LYS:CE	2.18	0.57
1:Y:470:TYR:HB3	2:Y:600:TPU:H5A1	1.87	0.57
1:Y:565:ASN:CG	1:Y:566:LYS:HB3	2.28	0.56
1:Z:566:LYS:O	1:Z:566:LYS:CG	2.49	0.56
1:A:129:LYS:NZ	5:A:2108:HOH:O	2.39	0.56
1:F:470:TYR:HB3	2:F:600:TPU:H5A1	1.88	0.56
1:Y:565:ASN:C	1:Y:566:LYS:CB	2.61	0.56
1:E:355:LYS:HB3	5:E:2214:HOH:O	2.05	0.56
1:A:566:LYS:O	1:A:566:LYS:HG2	2.02	0.56
5:Y:2044:HOH:O	1:Z:118:LYS:HD3	2.05	0.56
1:Y:110:HIS:O	1:Y:121:TYR:OH	2.23	0.56
1:A:566:LYS:NZ	5:A:2386:HOH:O	2.38	0.55
1:Y:275:LYS:NZ	5:Y:2202:HOH:O	2.40	0.55
1:Y:122:HIS:HE1	1:Z:120:ASP:OD2	1.89	0.55
1:F:175:CYS:HA	5:F:2145:HOH:O	2.06	0.55
1:B:470:TYR:HB3	2:B:600:TPU:H5A1	1.90	0.54
1:X:564:VAL:HG12	1:X:565:ASN:N	2.23	0.54
1:V:481:TYR:HB3	1:Z:46:TYR:CE1	2.42	0.54
1:A:481:TYR:HB3	1:B:46:TYR:CE1	2.43	0.54
1:E:2:SER:N	5:E:2002:HOH:O	2.40	0.54
1:A:565:ASN:ND2	1:A:565:ASN:C	2.66	0.53
1:V:46:TYR:CE1	1:Z:481:TYR:HB3	2.44	0.53
1:Z:566:LYS:HD3	1:Z:566:LYS:C	2.33	0.53
1:A:89:ALA:HB1	1:A:411:GLN:HG3	1.89	0.52
1:X:207:ALA:HB3	5:X:2157:HOH:O	2.10	0.52
1:Z:114:HIS:NE2	4:Z:602:PYR:O3	2.42	0.52
1:V:562:LYS:HD3	5:V:2335:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:199:VAL:HG21	1:Y:330:ARG:HG2	1.92	0.52
1:B:564:VAL:HG12	1:B:565:ASN:N	2.25	0.51
1:A:565:ASN:HD21	1:A:566:LYS:HE3	1.76	0.51
1:X:470:TYR:CD1	2:X:600:TPU:H5A2	2.45	0.51
1:Y:391:SER:HA	5:Y:2254:HOH:O	2.09	0.51
1:Y:118:LYS:NZ	5:Y:2087:HOH:O	2.29	0.51
1:F:231:LYS:HD3	5:F:2189:HOH:O	2.09	0.51
1:V:122:HIS:HE1	1:X:120:ASP:OD2	1.93	0.51
1:B:86:GLY:HA2	1:B:412:TRP:CG	2.46	0.51
1:E:89:ALA:HB1	1:E:411:GLN:HG3	1.92	0.51
1:A:120[B]:ASP:OD2	1:E:122:HIS:CE1	2.62	0.51
1:Z:565:ASN:O	1:Z:566:LYS:C	2.54	0.51
1:X:151:VAL:HG21	1:X:164:LEU:HG	1.92	0.50
1:X:89:ALA:HB1	1:X:411:GLN:HG3	1.93	0.50
1:X:209:ARG:NH2	5:X:2163:HOH:O	2.31	0.50
1:E:470:TYR:HB3	2:E:600:TPU:H5A1	1.93	0.50
1:Z:325:LYS:HE3	5:Z:2067:HOH:O	2.11	0.50
1:Z:559:ASN:ND2	5:Z:2328:HOH:O	2.44	0.50
1:A:470:TYR:CD1	2:A:600:TPU:H5A2	2.46	0.49
1:E:481:TYR:HB3	1:F:46:TYR:CE1	2.48	0.49
1:X:481:TYR:HB3	1:Y:46:TYR:CE1	2.47	0.49
5:X:2321:HOH:O	1:Y:486:ASN:HB3	2.10	0.49
1:Y:199:VAL:HG13	1:Y:331:LEU:CD1	2.42	0.49
1:Y:472:ILE:HG22	2:Y:600:TPU:H5B2	1.95	0.49
1:A:101:PRO:HB3	1:A:112:LEU:CD1	2.42	0.49
1:V:89:ALA:HB1	1:V:411:GLN:HG3	1.94	0.49
1:Z:472:ILE:HG22	2:Z:600:TPU:H5B2	1.95	0.49
1:B:101:PRO:HB3	1:B:112:LEU:CD1	2.43	0.49
1:E:472:ILE:HG22	2:E:600:TPU:H5B2	1.94	0.48
1:Y:89:ALA:HB1	1:Y:411:GLN:HG3	1.95	0.48
1:B:200:GLU:CD	1:B:203:LEU:HD12	2.37	0.48
1:V:118:LYS:HB3	5:V:2032:HOH:O	2.13	0.48
1:V:26:GLY:HA2	2:Z:600:TPU:H352	1.95	0.48
1:F:300:ASP:OD1	1:F:302:LYS:HD3	2.13	0.48
1:Y:86:GLY:HA2	1:Y:412:TRP:CG	2.48	0.48
1:E:86:GLY:HA2	1:E:412:TRP:CG	2.49	0.48
1:Z:300:ASP:OD1	1:Z:302:LYS:HD3	2.13	0.48
1:X:12:ARG:HD2	1:X:184:LEU:HD11	1.95	0.48
1:Z:89:ALA:HB1	1:Z:411:GLN:HG3	1.95	0.48
1:A:46:TYR:CE1	1:B:481:TYR:HB3	2.49	0.48
1:F:89:ALA:HB1	1:F:411:GLN:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ARG:HD2	1:A:184:LEU:HD11	1.96	0.47
1:B:89:ALA:HB1	1:B:411:GLN:HG3	1.96	0.47
1:B:431:GLU:HB2	1:Z:381:ASN:HB2	1.95	0.47
1:X:416:GLY:O	1:X:420:PRO:HD2	2.14	0.47
1:A:141:PRO:HD3	5:A:2078:HOH:O	2.12	0.47
1:A:566:LYS:CE	1:A:566:LYS:C	2.87	0.47
1:B:88:TYR:HA	1:B:161:PRO:HD2	1.97	0.47
1:X:86:GLY:HA2	1:X:412:TRP:CG	2.49	0.47
1:F:470:TYR:CD1	2:F:600:TPU:H5A2	2.49	0.47
1:A:564:VAL:HG12	1:A:565:ASN:N	2.29	0.47
1:E:25:ALA:HB2	1:F:481:TYR:HB2	1.96	0.47
1:X:101:PRO:HB3	1:X:112:LEU:CD1	2.44	0.47
1:Z:88:TYR:HA	1:Z:161:PRO:HD2	1.97	0.47
1:A:86:GLY:HA2	1:A:412:TRP:CG	2.49	0.47
1:E:559:ASN:ND2	5:E:2285:HOH:O	2.48	0.47
1:X:209:ARG:NE	5:X:2163:HOH:O	2.40	0.47
1:Z:114:HIS:CE1	4:Z:602:PYR:O3	2.68	0.47
1:A:300:ASP:OD1	1:A:302:LYS:HD3	2.15	0.47
1:V:389:GLY:HA2	1:V:472:ILE:HG21	1.97	0.47
1:X:88:TYR:HA	1:X:161:PRO:HD2	1.97	0.47
1:V:12:ARG:HD2	1:V:184:LEU:HD11	1.97	0.46
1:Z:122:HIS:HD2	1:Z:126:GLU:OE2	1.97	0.46
1:V:40:LYS:NZ	5:V:2027:HOH:O	2.48	0.46
1:V:300:ASP:OD1	1:V:302:LYS:HD3	2.16	0.46
1:V:470:TYR:CD1	2:V:600:TPU:H5A2	2.50	0.46
1:A:25:ALA:HB2	1:B:481:TYR:HB2	1.97	0.46
1:A:416:GLY:O	1:A:420:PRO:HD2	2.15	0.46
1:F:101:PRO:HB3	1:F:112:LEU:CD1	2.45	0.46
1:Z:86:GLY:HA2	1:Z:412:TRP:CG	2.51	0.46
1:Z:308:GLU:HG3	5:Z:2228:HOH:O	2.16	0.46
1:A:88:TYR:HA	1:A:161:PRO:HD2	1.98	0.46
1:B:565:ASN:HD21	1:B:566:LYS:HG2	1.73	0.46
1:E:493:MET:HG3	1:E:508:LYS:C	2.40	0.46
1:F:471:THR:N	2:F:600:TPU:O21	2.47	0.46
1:Y:349:ASN:HA	5:Y:2238:HOH:O	2.16	0.46
1:X:46:TYR:CE1	1:Y:481:TYR:HB3	2.50	0.46
1:B:219:LYS:HB2	1:B:284:ALA:HB1	1.97	0.46
1:E:101:PRO:HB3	1:E:112:LEU:CD1	2.46	0.46
1:V:416:GLY:O	1:V:420:PRO:HD2	2.16	0.46
1:Y:300:ASP:OD1	1:Y:302:LYS:HD3	2.16	0.46
1:B:300:ASP:OD1	1:B:302:LYS:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:377:LEU:HD21	1:X:526:LEU:HD11	1.99	0.45
1:F:88:TYR:HA	1:F:161:PRO:HD2	1.98	0.45
1:Y:377:LEU:HD21	1:Y:526:LEU:HD11	1.98	0.45
1:Y:458:LEU:HA	1:Y:459:PRO:HD3	1.79	0.45
1:Z:470:TYR:HB3	2:Z:600:TPU:H5A1	1.98	0.45
1:V:565:ASN:O	1:V:566:LYS:C	2.59	0.45
1:Y:219:LYS:HB2	1:Y:284:ALA:HB1	1.98	0.45
1:B:377:LEU:HD21	1:B:526:LEU:HD11	1.97	0.45
1:F:377:LEU:HD21	1:F:526:LEU:HD11	1.98	0.45
1:V:237:GLY:HA2	1:V:256:HIS:CE1	2.52	0.45
1:V:493:MET:HG3	1:V:508:LYS:C	2.41	0.45
1:A:151:VAL:HG21	1:A:164:LEU:HG	1.97	0.45
1:A:377:LEU:HD21	1:A:526:LEU:HD11	1.98	0.45
1:B:565:ASN:HD22	1:B:566:LYS:HG2	1.75	0.45
1:E:88:TYR:HA	1:E:161:PRO:HD2	1.98	0.45
1:E:151:VAL:HG21	1:E:164:LEU:HG	1.96	0.45
1:Y:232:PHE:HA	1:Y:332:ALA:HB2	1.98	0.45
1:A:566:LYS:HE3	1:A:566:LYS:C	2.41	0.45
1:E:300:ASP:OD1	1:E:302:LYS:HD3	2.16	0.45
1:V:101:PRO:HB3	1:V:112:LEU:CD1	2.47	0.45
1:V:254:ASN:HA	1:V:255:PRO:HD3	1.88	0.45
1:X:300:ASP:OD1	1:X:302:LYS:HD3	2.17	0.45
5:A:2336:HOH:O	1:B:27:ASP:HB3	2.16	0.45
1:B:559:ASN:ND2	5:B:2285:HOH:O	2.50	0.45
1:E:377:LEU:HD21	1:E:526:LEU:HD11	1.99	0.45
1:V:377:LEU:HD21	1:V:526:LEU:HD11	1.99	0.45
1:A:254:ASN:HA	1:A:255:PRO:HD3	1.87	0.44
1:E:458:LEU:HA	1:E:459:PRO:HD3	1.81	0.44
1:V:86:GLY:HA2	1:V:412:TRP:CG	2.53	0.44
1:V:151:VAL:HG21	1:V:164:LEU:HG	1.99	0.44
1:V:564:VAL:HG12	1:V:565:ASN:N	2.31	0.44
1:E:196:ASN:OD1	1:E:330:ARG:NH1	2.51	0.44
1:F:458:LEU:HA	1:F:459:PRO:HD3	1.79	0.44
1:Z:529:THR:HG22	5:Z:2311:HOH:O	2.17	0.44
1:B:416:GLY:O	1:B:420:PRO:HD2	2.18	0.44
1:F:86:GLY:HA2	1:F:412:TRP:CG	2.53	0.44
1:V:566:LYS:CD	5:V:2168:HOH:O	2.64	0.44
1:Y:101:PRO:HB3	1:Y:112:LEU:CD1	2.48	0.44
1:F:473:GLU:OE2	1:F:473:GLU:HA	2.18	0.44
1:Y:416:GLY:O	1:Y:420:PRO:HD2	2.17	0.44
1:Y:494:GLU:HG2	5:Y:2284:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:308:GLU:CG	5:Y:2220:HOH:O	2.60	0.44
1:E:470:TYR:CD1	2:E:600:TPU:H5A2	2.53	0.44
2:E:600:TPU:N1'	1:F:50:GLU:OE2	2.51	0.44
1:A:237:GLY:HA2	1:A:256:HIS:CE1	2.52	0.44
1:Y:88:TYR:HA	1:Y:161:PRO:HD2	2.00	0.43
1:E:92:LEU:HA	1:E:93:PRO:HD3	1.89	0.43
1:F:160:LYS:NZ	5:F:2135:HOH:O	2.51	0.43
1:V:100:ALA:HB1	1:V:101:PRO:HD2	2.00	0.43
1:Z:101:PRO:HB3	1:Z:112:LEU:CD1	2.49	0.43
1:Z:377:LEU:HD21	1:Z:526:LEU:HD11	1.99	0.43
1:F:472:ILE:HG22	2:F:600:TPU:H5B2	2.00	0.43
1:A:493:MET:HG3	1:A:508:LYS:C	2.43	0.43
1:Z:565:ASN:ND2	1:Z:565:ASN:C	2.76	0.43
1:A:470:TYR:HB3	2:A:600:TPU:H5A1	2.01	0.43
1:F:416:GLY:O	1:F:420:PRO:HD2	2.18	0.43
1:F:493:MET:HG3	1:F:508:LYS:C	2.43	0.43
1:V:350:ALA:HB3	5:V:2200:HOH:O	2.17	0.43
1:Z:458:LEU:HA	1:Z:459:PRO:HD3	1.82	0.43
1:E:46:TYR:CE1	1:F:481:TYR:HB3	2.53	0.43
1:V:173:MET:HA	1:V:174:PRO:HD3	1.89	0.43
1:X:566:LYS:C	1:X:566:LYS:CD	2.88	0.43
1:V:144:ALA:HB3	1:V:145:PRO:HD3	2.01	0.43
1:X:415:ILE:HB	1:X:442:SER:OG	2.19	0.43
1:Y:560:SER:OG	5:Y:2313:HOH:O	2.21	0.43
1:Z:333:GLN:HE21	1:Z:333:GLN:HB3	1.60	0.43
1:Z:493:MET:HG3	1:Z:508:LYS:C	2.43	0.43
1:Z:564:VAL:HG12	1:Z:565:ASN:N	2.34	0.43
1:B:200:GLU:OE2	1:B:203:LEU:HD12	2.19	0.43
1:X:564:VAL:CG1	1:X:565:ASN:N	2.81	0.42
1:Y:565:ASN:CA	1:Y:566:LYS:HB3	2.42	0.42
1:X:237:GLY:HA2	1:X:256:HIS:CE1	2.55	0.42
1:Z:113:HIS:O	1:Z:114:HIS:HB2	2.20	0.42
1:V:254:ASN:OD1	1:V:256:HIS:CD2	2.73	0.42
1:X:113:HIS:O	1:X:114:HIS:HB2	2.19	0.42
1:X:493:MET:HG3	1:X:508:LYS:C	2.45	0.42
1:Y:173:MET:HA	1:Y:174:PRO:HD3	1.89	0.42
1:Y:238:GLY:N	5:Y:2186:HOH:O	2.45	0.42
1:Z:416:GLY:O	1:Z:420:PRO:HD2	2.18	0.42
1:E:254:ASN:HA	1:E:255:PRO:HD3	1.88	0.42
1:E:416:GLY:O	1:E:420:PRO:HD2	2.18	0.42
1:E:493:MET:HG3	1:E:508:LYS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:2:SER:N	5:V:2001:HOH:O	2.52	0.42
1:V:327:TYR:O	1:V:331:LEU:HB2	2.20	0.42
1:V:88:TYR:HA	1:V:161:PRO:HD2	2.01	0.42
1:Y:564:VAL:HG12	1:Y:565:ASN:N	2.33	0.42
1:Z:74:SER:OG	1:Z:123:TYR:OH	2.37	0.42
1:B:493:MET:HG3	1:B:508:LYS:C	2.44	0.42
1:F:564:VAL:CG1	1:F:565:ASN:N	2.67	0.42
1:V:290:TYR:CZ	1:Z:113:HIS:CD2	3.07	0.42
1:A:464:LEU:HD13	1:A:464:LEU:C	2.45	0.42
1:F:12:ARG:HD2	1:F:184:LEU:HD11	2.01	0.42
1:Y:16:ILE:HG13	1:Y:18:LEU:HD13	2.02	0.42
1:V:564:VAL:CG1	1:V:565:ASN:N	2.83	0.42
1:Z:219:LYS:HD3	5:Z:2211:HOH:O	2.19	0.42
1:A:566:LYS:NZ	1:A:566:LYS:C	2.78	0.42
1:E:12:ARG:HD2	1:E:184:LEU:HD11	2.02	0.42
1:V:122:HIS:CE1	1:X:120:ASP:OD2	2.72	0.42
2:V:600:TPU:N1'	1:Z:50:GLU:OE2	2.53	0.42
1:Y:565:ASN:HA	1:Y:566:LYS:N	2.35	0.42
1:Z:196:ASN:OD1	1:Z:330:ARG:NH1	2.52	0.42
1:B:300:ASP:HA	1:B:301:PRO:HD3	1.93	0.41
1:F:232:PHE:HA	1:F:332:ALA:HB2	2.00	0.41
1:E:237:GLY:HA2	1:E:256:HIS:CE1	2.54	0.41
1:E:254:ASN:OD1	1:E:256:HIS:CD2	2.73	0.41
1:Y:493:MET:HG3	1:Y:508:LYS:C	2.44	0.41
1:Z:464:LEU:C	1:Z:464:LEU:HD13	2.45	0.41
1:A:559:ASN:ND2	5:A:2379:HOH:O	2.54	0.41
1:V:493:MET:HG3	1:V:508:LYS:O	2.19	0.41
1:X:458:LEU:HA	1:X:459:PRO:HD3	1.79	0.41
1:X:565:ASN:ND2	1:X:565:ASN:C	2.78	0.41
1:Z:173:MET:HA	1:Z:174:PRO:HD3	1.89	0.41
1:Z:473:GLU:OE2	1:Z:473:GLU:HA	2.20	0.41
1:B:415:ILE:HB	1:B:442:SER:OG	2.21	0.41
1:B:565:ASN:ND2	1:B:565:ASN:C	2.78	0.41
1:E:100:ALA:HB1	1:E:101:PRO:HD2	2.02	0.41
1:V:25:ALA:HB2	1:Z:481:TYR:HB2	2.03	0.41
1:B:16:ILE:HG13	1:B:18:LEU:HD13	2.02	0.41
1:F:287:PHE:CZ	1:F:299:PRO:HG2	2.56	0.41
1:X:25:ALA:HB2	1:Y:481:TYR:HB2	2.03	0.41
1:X:250:PHE:HA	1:X:251:PRO:HD3	1.94	0.41
1:B:12:ARG:HD2	1:B:184:LEU:HD11	2.02	0.41
1:A:553:LYS:HG3	5:A:2372:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:ASN:HA	1:B:255:PRO:HD3	1.83	0.41
1:F:254:ASN:HA	1:F:255:PRO:HD3	1.83	0.41
1:V:308:GLU:OE1	5:V:2225:HOH:O	2.22	0.41
1:Z:144:ALA:HB3	1:Z:145:PRO:HD3	2.03	0.41
1:A:92:LEU:HA	1:A:93:PRO:HD3	1.95	0.41
1:A:308:GLU:HG3	5:A:2257:HOH:O	2.21	0.41
1:A:415:ILE:HB	1:A:442:SER:OG	2.19	0.41
1:Z:118:LYS:HB3	5:Z:2096:HOH:O	2.20	0.41
1:Z:232:PHE:HA	1:Z:332:ALA:HB2	2.03	0.41
1:B:188:GLU:HA	1:E:188:GLU:HA	2.03	0.40
1:E:467:ASN:HA	1:E:539:ILE:O	2.21	0.40
1:X:92:LEU:HA	1:X:93:PRO:HD3	1.94	0.40
1:X:470:TYR:CG	2:X:600:TPU:H5A2	2.56	0.40
1:Y:254:ASN:OD1	1:Y:256:HIS:CD2	2.74	0.40
1:B:470:TYR:CD1	2:B:600:TPU:H5A2	2.56	0.40
1:F:219:LYS:HB2	1:F:284:ALA:HB1	2.02	0.40
1:X:464:LEU:C	1:X:464:LEU:HD13	2.46	0.40
1:Y:254:ASN:HA	1:Y:255:PRO:HD3	1.82	0.40
1:Y:564:VAL:CG1	1:Y:565:ASN:N	2.84	0.40
1:A:458:LEU:HA	1:A:459:PRO:HD3	1.80	0.40
1:E:84:ILE:HD13	1:E:84:ILE:HA	1.90	0.40
1:F:144:ALA:HB3	1:F:145:PRO:HD3	2.03	0.40
1:V:470:TYR:HB3	2:V:600:TPU:H5A1	2.02	0.40
1:Y:467:ASN:HA	1:Y:539:ILE:O	2.21	0.40
1:Z:219:LYS:HB2	1:Z:284:ALA:HB1	2.04	0.40
1:A:219:LYS:HB2	1:A:284:ALA:HB1	2.04	0.40
1:B:320:PRO:HD2	5:E:2005:HOH:O	2.20	0.40
1:F:300:ASP:HA	1:F:301:PRO:HD3	1.94	0.40
1:F:541:ARG:CD	5:F:2290:HOH:O	2.37	0.40
1:B:297:ASP:HB3	5:B:2198:HOH:O	2.21	0.40
1:B:381:ASN:HB3	5:B:2229:HOH:O	2.21	0.40
1:V:16:ILE:HG13	1:V:18:LEU:HD13	2.03	0.40
1:V:50:GLU:OE2	2:Z:600:TPU:N1'	2.55	0.40
1:V:407:GLU:HA	5:V:2271:HOH:O	2.21	0.40
1:Y:300:ASP:HA	1:Y:301:PRO:HD3	1.94	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	565/568 (100%)	555 (98%)	10 (2%)	0	100	100
1	B	563/568 (99%)	554 (98%)	9 (2%)	0	100	100
1	E	564/568 (99%)	554 (98%)	10 (2%)	0	100	100
1	F	564/568 (99%)	552 (98%)	12 (2%)	0	100	100
1	V	564/568 (99%)	555 (98%)	9 (2%)	0	100	100
1	X	564/568 (99%)	555 (98%)	9 (2%)	0	100	100
1	Y	563/568 (99%)	553 (98%)	10 (2%)	0	100	100
1	Z	563/568 (99%)	552 (98%)	11 (2%)	0	100	100
All	All	4510/4544 (99%)	4430 (98%)	80 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	436/437 (100%)	430 (99%)	6 (1%)	59	75
1	B	434/437 (99%)	427 (98%)	7 (2%)	55	71
1	E	435/437 (100%)	430 (99%)	5 (1%)	65	79
1	F	435/437 (100%)	430 (99%)	5 (1%)	65	79
1	V	435/437 (100%)	428 (98%)	7 (2%)	55	71
1	X	435/437 (100%)	428 (98%)	7 (2%)	55	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Y	435/437 (100%)	428 (98%)	7 (2%)	55	71
1	Z	434/437 (99%)	425 (98%)	9 (2%)	47	63
All	All	3479/3496 (100%)	3426 (98%)	53 (2%)	57	73

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	GLU
1	A	352	GLU
1	A	473	GLU
1	A	562	LYS
1	A	565	ASN
1	A	566	LYS
1	B	74	SER
1	B	158	GLU
1	B	330	ARG
1	B	352	GLU
1	B	473	GLU
1	B	562	LYS
1	B	566	LYS
1	E	158	GLU
1	E	200	GLU
1	E	352	GLU
1	E	473	GLU
1	E	562	LYS
1	F	158	GLU
1	F	352	GLU
1	F	473	GLU
1	F	541	ARG
1	F	562	LYS
1	V	120	ASP
1	V	158	GLU
1	V	352	GLU
1	V	472	ILE
1	V	473	GLU
1	V	562	LYS
1	V	566	LYS
1	X	74	SER
1	X	158	GLU
1	X	352	GLU
1	X	473	GLU

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Mol	Chain	Res	Type
1	X	562	LYS
1	X	565	ASN
1	X	566	LYS
1	Y	120	ASP
1	Y	158	GLU
1	Y	330	ARG
1	Y	352	GLU
1	Y	473	GLU
1	Y	562	LYS
1	Y	566	LYS
1	Z	74	SER
1	Z	158	GLU
1	Z	333	GLN
1	Z	352	GLU
1	Z	473	GLU
1	Z	541	ARG
1	Z	542	GLU
1	Z	562	LYS
1	Z	566	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	HIS
1	A	256	HIS
1	A	323	HIS
1	A	559	ASN
1	A	565	ASN
1	B	44	GLN
1	B	122	HIS
1	B	256	HIS
1	B	323	HIS
1	B	434	ASN
1	B	559	ASN
1	B	565	ASN
1	E	35	ASN
1	E	122	HIS
1	E	256	HIS
1	E	323	HIS
1	E	559	ASN
1	F	122	HIS
1	F	256	HIS

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Mol	Chain	Res	Type
1	F	323	HIS
1	F	559	ASN
1	F	565	ASN
1	V	35	ASN
1	V	122	HIS
1	V	256	HIS
1	V	323	HIS
1	V	559	ASN
1	V	565	ASN
1	X	122	HIS
1	X	256	HIS
1	X	323	HIS
1	X	559	ASN
1	X	565	ASN
1	Y	122	HIS
1	Y	256	HIS
1	Y	323	HIS
1	Y	434	ASN
1	Y	559	ASN
1	Y	565	ASN
1	Z	122	HIS
1	Z	256	HIS
1	Z	323	HIS
1	Z	333	GLN
1	Z	434	ASN
1	Z	559	ASN
1	Z	565	ASN

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 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 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	TPU	F	600	3	26,27,27	2.43	11 (42%)	35,40,40	3.23	14 (40%)
2	TPU	E	600	3	26,27,27	2.29	11 (42%)	35,40,40	3.33	14 (40%)
2	TPU	Y	600	3	26,27,27	2.47	10 (38%)	35,40,40	2.78	11 (31%)
2	TPU	V	600	3	26,27,27	2.27	12 (46%)	35,40,40	3.40	11 (31%)
2	TPU	X	600	3	26,27,27	2.47	11 (42%)	35,40,40	3.37	14 (40%)
2	TPU	Z	600	3	26,27,27	2.47	11 (42%)	35,40,40	3.77	12 (34%)
4	PYR	Z	602	-	5,5,5	3.02	3 (60%)	3,6,6	1.56	1 (33%)
4	PYR	V	602	-	5,5,5	3.11	3 (60%)	3,6,6	1.31	0
2	TPU	B	600	3	26,27,27	2.58	12 (46%)	35,40,40	2.99	12 (34%)
4	PYR	F	602	-	5,5,5	3.12	3 (60%)	3,6,6	1.30	0
2	TPU	A	600	3	26,27,27	2.40	10 (38%)	35,40,40	3.58	15 (42%)

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	TPU	F	600	3	-	7/17/17/17	0/2/2/2
2	TPU	E	600	3	-	6/17/17/17	0/2/2/2
2	TPU	Y	600	3	-	9/17/17/17	0/2/2/2
2	TPU	V	600	3	-	6/17/17/17	0/2/2/2
2	TPU	X	600	3	-	3/17/17/17	0/2/2/2
2	TPU	Z	600	3	-	8/17/17/17	0/2/2/2
4	PYR	Z	602	-	-	2/4/4/4	-
4	PYR	V	602	-	-	1/4/4/4	-
2	TPU	B	600	3	-	5/17/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PYR	F	602	-	-	0/4/4/4	-
2	TPU	A	600	3	-	5/17/17/17	0/2/2/2

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	TPU	P1-O11	5.81	1.65	1.59
2	Z	600	TPU	P1-O11	5.28	1.65	1.59
2	F	600	TPU	P1-O11	5.24	1.65	1.59
2	X	600	TPU	C4'-N4'	5.20	1.47	1.34
2	A	600	TPU	P1-O11	5.18	1.65	1.59
2	X	600	TPU	P1-O11	5.12	1.65	1.59
2	Y	600	TPU	P1-O11	4.78	1.64	1.59
4	V	602	PYR	CA-C	-4.76	1.38	1.54
2	E	600	TPU	P1-O11	4.65	1.64	1.59
2	A	600	TPU	C4'-N4'	4.59	1.45	1.34
2	B	600	TPU	C2'-N1'	4.57	1.41	1.34
2	B	600	TPU	C4'-N4'	4.55	1.45	1.34
2	V	600	TPU	C4'-N4'	4.51	1.45	1.34
2	E	600	TPU	C4'-N4'	4.50	1.45	1.34
2	Z	600	TPU	C2'-N1'	4.50	1.41	1.34
4	F	602	PYR	CA-C	-4.49	1.39	1.54
4	Z	602	PYR	CA-C	-4.49	1.39	1.54
2	Y	600	TPU	C2'-N1'	4.46	1.41	1.34
2	Y	600	TPU	C4'-N4'	4.45	1.45	1.34
2	F	600	TPU	C4'-N4'	4.39	1.45	1.34
2	F	600	TPU	C2'-N1'	4.32	1.40	1.34
2	Z	600	TPU	C4'-N4'	4.22	1.45	1.34
2	V	600	TPU	P1-O11	4.18	1.64	1.59
2	B	600	TPU	N3-N2	4.15	1.41	1.35
2	Y	600	TPU	N3-N2	4.11	1.41	1.35
2	Y	600	TPU	C5-N1	4.07	1.41	1.36
2	E	600	TPU	C2'-N1'	3.99	1.40	1.34
2	X	600	TPU	C5-N1	3.98	1.41	1.36
2	B	600	TPU	C5-N1	3.91	1.41	1.36
2	A	600	TPU	C2'-N1'	3.88	1.40	1.34
4	F	602	PYR	O3-CA	3.79	1.31	1.23
2	X	600	TPU	N3-N2	3.75	1.40	1.35
4	F	602	PYR	O-C	3.74	1.31	1.22
2	A	600	TPU	C5-N1	3.73	1.41	1.36
2	B	600	TPU	C2'-N3'	3.67	1.40	1.34
2	V	600	TPU	C2'-N1'	3.64	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Z	602	PYR	O-C	3.63	1.31	1.22
4	V	602	PYR	O3-CA	3.61	1.31	1.23
4	V	602	PYR	O-C	3.53	1.31	1.22
4	Z	602	PYR	O3-CA	3.50	1.31	1.23
2	F	600	TPU	C5-N1	3.48	1.41	1.36
2	Y	600	TPU	C2'-N3'	3.45	1.40	1.34
2	X	600	TPU	C2'-N1'	3.43	1.39	1.34
2	Z	600	TPU	N3-N2	3.40	1.40	1.35
2	Z	600	TPU	C5'-C4'	3.29	1.48	1.42
2	E	600	TPU	P2-O23	3.28	1.67	1.54
2	F	600	TPU	N3-N2	3.18	1.39	1.35
2	A	600	TPU	C2'-N3'	3.17	1.39	1.34
2	V	600	TPU	P2-O23	3.16	1.66	1.54
2	Z	600	TPU	C5-N1	3.10	1.40	1.36
2	E	600	TPU	C2'-N3'	3.08	1.39	1.34
2	A	600	TPU	N3-N2	3.02	1.39	1.35
2	X	600	TPU	C2'-N3'	2.99	1.39	1.34
2	Y	600	TPU	P2-O23	2.96	1.65	1.54
2	E	600	TPU	N3-N2	2.92	1.39	1.35
2	V	600	TPU	C2'-N3'	2.84	1.38	1.34
2	Z	600	TPU	C2'-N3'	2.83	1.38	1.34
2	Z	600	TPU	P2-O23	2.81	1.65	1.54
2	X	600	TPU	P2-O22	2.79	1.65	1.54
2	F	600	TPU	C4A-C4	2.78	1.53	1.49
2	X	600	TPU	P2-O23	2.77	1.65	1.54
2	A	600	TPU	P2-O22	2.76	1.65	1.54
2	A	600	TPU	P2-O23	2.75	1.65	1.54
2	V	600	TPU	C5'-C4'	2.75	1.47	1.42
2	V	600	TPU	C4'-N3'	-2.74	1.31	1.35
2	V	600	TPU	P2-O22	2.74	1.65	1.54
2	F	600	TPU	C5'-C4'	2.70	1.47	1.42
2	E	600	TPU	P2-O22	2.70	1.64	1.54
2	Z	600	TPU	P2-O22	2.69	1.64	1.54
2	F	600	TPU	P2-O22	2.68	1.64	1.54
2	Y	600	TPU	P2-O22	2.68	1.64	1.54
2	F	600	TPU	C2'-N3'	2.68	1.38	1.34
2	V	600	TPU	P1-O12	2.66	1.67	1.55
2	E	600	TPU	C5-N1	2.65	1.40	1.36
2	X	600	TPU	C5'-C4'	2.65	1.47	1.42
2	B	600	TPU	C5'-C4'	2.63	1.47	1.42
2	A	600	TPU	C4'-N3'	-2.63	1.31	1.35
2	F	600	TPU	C4'-N3'	-2.63	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	600	TPU	P2-O23	2.56	1.64	1.54
2	V	600	TPU	C5-N1	2.55	1.39	1.36
2	B	600	TPU	P2-O22	2.53	1.64	1.54
2	Z	600	TPU	C4'-N3'	-2.53	1.31	1.35
2	B	600	TPU	P2-O23	2.52	1.64	1.54
2	V	600	TPU	N3-N2	2.46	1.38	1.35
2	Y	600	TPU	C5'-C4'	2.40	1.46	1.42
2	A	600	TPU	C5'-C4'	2.26	1.46	1.42
2	V	600	TPU	C6'-C5'	-2.24	1.33	1.37
2	E	600	TPU	C4'-N3'	-2.24	1.32	1.35
2	E	600	TPU	C6'-C5'	-2.22	1.33	1.37
2	Z	600	TPU	C4A-C4	2.21	1.52	1.49
2	B	600	TPU	C4A-C4	2.19	1.52	1.49
2	E	600	TPU	C5'-C4'	2.17	1.46	1.42
2	B	600	TPU	C4'-N3'	-2.14	1.32	1.35
2	Y	600	TPU	C4A-C4	2.09	1.52	1.49
2	X	600	TPU	C4A-C4	2.06	1.52	1.49
2	X	600	TPU	C4'-N3'	-2.04	1.32	1.35
2	B	600	TPU	P1-O12	2.02	1.64	1.55

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	600	TPU	C4-N3-N2	-19.08	106.31	111.50
2	V	600	TPU	C4-N3-N2	-16.93	106.90	111.50
2	A	600	TPU	C4-N3-N2	-16.68	106.97	111.50
2	E	600	TPU	C4-N3-N2	-15.86	107.19	111.50
2	X	600	TPU	C4-N3-N2	-15.42	107.31	111.50
2	F	600	TPU	C4-N3-N2	-15.22	107.36	111.50
2	B	600	TPU	C4-N3-N2	-13.45	107.84	111.50
2	Y	600	TPU	C4-N3-N2	-12.36	108.14	111.50
2	X	600	TPU	C35-N3-N2	5.69	126.73	119.35
2	E	600	TPU	C35-N3-N2	5.42	126.37	119.35
2	B	600	TPU	C35-N3-N2	5.22	126.11	119.35
2	A	600	TPU	C35-N3-N2	5.08	125.94	119.35
2	Y	600	TPU	C35-N3-N2	4.75	125.51	119.35
2	F	600	TPU	C35-N3-N2	4.03	124.58	119.35
2	A	600	TPU	C35-C5'-C4'	-4.00	118.51	122.56
2	Z	600	TPU	N3-N2-N1	3.95	110.20	107.34
2	B	600	TPU	N1'-C2'-N3'	-3.94	118.97	125.53
2	A	600	TPU	N4'-C4'-N3'	3.92	122.31	117.03
2	Z	600	TPU	C35-N3-N2	3.83	124.32	119.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	600	TPU	N1'-C2'-N3'	-3.79	119.22	125.53
2	Y	600	TPU	N1'-C2'-N3'	-3.74	119.31	125.53
2	A	600	TPU	C6'-C5'-C4'	3.72	120.12	115.55
2	X	600	TPU	N1'-C2'-N3'	-3.71	119.36	125.53
2	Z	600	TPU	O12-P1-O11	3.67	117.18	107.27
2	Z	600	TPU	N1'-C2'-N3'	-3.61	119.53	125.53
2	E	600	TPU	C6'-C5'-C4'	3.61	119.98	115.55
2	X	600	TPU	C4A-C4-C5	-3.58	124.06	131.68
2	E	600	TPU	N1'-C2'-N3'	-3.54	119.64	125.53
2	V	600	TPU	C2A-C2'-N3'	3.50	122.37	117.13
2	A	600	TPU	C4A-C4-C5	-3.50	124.23	131.68
2	V	600	TPU	N1'-C2'-N3'	-3.47	119.76	125.53
2	F	600	TPU	C2A-C2'-N1'	3.43	120.86	117.20
2	F	600	TPU	O12-P1-O11	3.43	116.55	107.27
2	V	600	TPU	C4A-C4-C5	-3.35	124.54	131.68
2	V	600	TPU	C35-N3-N2	3.35	123.69	119.35
2	E	600	TPU	C2A-C2'-N3'	3.32	122.10	117.13
2	Z	600	TPU	C4A-C4-C5	-3.27	124.72	131.68
2	X	600	TPU	C4A-C4-N3	3.26	127.99	123.00
2	X	600	TPU	N4'-C4'-N3'	3.21	121.36	117.03
2	A	600	TPU	C5'-C4'-N4'	-3.19	117.84	122.14
2	A	600	TPU	N1'-C2'-N3'	-3.17	120.25	125.53
2	Y	600	TPU	C6'-C5'-C4'	3.14	119.41	115.55
2	F	600	TPU	N3-N2-N1	3.13	109.61	107.34
2	B	600	TPU	C2A-C2'-N3'	3.09	121.75	117.13
2	B	600	TPU	C6'-C5'-C4'	3.08	119.34	115.55
2	V	600	TPU	N3-N2-N1	3.06	109.56	107.34
2	E	600	TPU	N4'-C4'-N3'	3.06	121.15	117.03
2	V	600	TPU	C4A-C4-N3	3.04	127.65	123.00
2	Z	600	TPU	C2A-C2'-N1'	3.03	120.42	117.20
2	Z	600	TPU	C5'-C35-N3	-2.98	110.22	113.08
2	V	600	TPU	C6'-C5'-C4'	2.91	119.12	115.55
2	F	600	TPU	C4A-C4-C5	-2.91	125.50	131.68
2	X	600	TPU	C2A-C2'-N3'	2.88	121.44	117.13
2	E	600	TPU	C4A-C4-C5	-2.85	125.61	131.68
2	V	600	TPU	C35-C5'-C6'	-2.84	117.23	121.30
2	Z	600	TPU	C4A-C4-N3	2.82	127.31	123.00
2	X	600	TPU	C6'-C5'-C4'	2.80	118.99	115.55
2	B	600	TPU	C6'-N1'-C2'	2.80	120.66	116.07
2	F	600	TPU	C6'-C5'-C4'	2.76	118.94	115.55
2	F	600	TPU	C4A-C4-N3	2.74	127.19	123.00
2	A	600	TPU	C4A-C4-N3	2.71	127.15	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	600	TPU	C6'-N1'-C2'	2.71	120.52	116.07
2	A	600	TPU	C6'-N1'-C2'	2.70	120.50	116.07
2	V	600	TPU	C6'-N1'-C2'	2.66	120.44	116.07
2	X	600	TPU	C5-N1-N2	-2.65	106.16	109.13
2	Y	600	TPU	C4A-C4-C5	-2.62	126.11	131.68
2	Z	600	TPU	C6'-N1'-C2'	2.61	120.36	116.07
2	B	600	TPU	C5-N1-N2	-2.56	106.26	109.13
2	A	600	TPU	C5'-C6'-N1'	-2.55	119.69	123.83
2	Y	600	TPU	C2A-C2'-N1'	2.54	119.91	117.20
2	F	600	TPU	C6'-N1'-C2'	2.52	120.22	116.07
2	A	600	TPU	C5'-C35-N3	-2.51	110.66	113.08
2	X	600	TPU	N3-N2-N1	2.51	109.16	107.34
2	X	600	TPU	C6'-N1'-C2'	2.49	120.17	116.07
2	B	600	TPU	C4A-C4-C5	-2.47	126.42	131.68
2	F	600	TPU	C5'-C35-N3	-2.47	110.70	113.08
2	Y	600	TPU	C2A-C2'-N3'	2.44	120.78	117.13
2	B	600	TPU	N3-N2-N1	2.40	109.08	107.34
2	E	600	TPU	N3-N2-N1	2.37	109.06	107.34
2	Y	600	TPU	C6'-N1'-C2'	2.37	119.96	116.07
2	Y	600	TPU	C4A-C4-N3	2.30	126.53	123.00
2	A	600	TPU	O22-P2-O11	2.28	112.30	104.64
2	A	600	TPU	C2A-C2'-N3'	2.28	120.55	117.13
4	Z	602	PYR	OXT-C-CA	2.23	119.77	113.59
2	B	600	TPU	C4A-C4-N3	2.22	126.39	123.00
2	F	600	TPU	C5-N1-N2	-2.22	106.64	109.13
2	E	600	TPU	C5'-C6'-N1'	-2.19	120.26	123.83
2	A	600	TPU	N3-N2-N1	2.19	108.93	107.34
2	B	600	TPU	C35-C5'-C6'	-2.19	118.16	121.30
2	E	600	TPU	C35-C5'-C6'	-2.19	118.17	121.30
2	X	600	TPU	O12-P1-O11	2.17	113.14	107.27
2	X	600	TPU	C5A-C5-N1	2.17	126.97	120.86
2	E	600	TPU	C4A-C4-N3	2.11	126.23	123.00
2	Z	600	TPU	C6'-C5'-C4'	2.11	118.14	115.55
2	E	600	TPU	C5'-C4'-N4'	-2.09	119.32	122.14
2	Y	600	TPU	C35-C5'-C6'	-2.08	118.32	121.30
2	E	600	TPU	C5-N1-N2	-2.04	106.84	109.13
2	B	600	TPU	O12-P1-O11	2.04	112.78	107.27
2	V	600	TPU	C5'-C6'-N1'	-2.02	120.54	123.83
2	Y	600	TPU	O23-P2-O11	2.02	111.39	104.64
2	F	600	TPU	C5'-C6'-N1'	-2.01	120.56	123.83
2	F	600	TPU	C2'-N3'-C4'	2.01	121.19	118.10
2	X	600	TPU	C2'-N3'-C4'	2.01	121.19	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	600	TPU	C5-N1-N2	-2.00	106.89	109.13

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	TPU	C5B-O5G-P1-O11
2	A	600	TPU	C5B-O5G-P1-O12
2	A	600	TPU	C5B-O5G-P1-O13
2	B	600	TPU	C5B-O5G-P1-O11
2	B	600	TPU	C5B-O5G-P1-O13
2	E	600	TPU	C5B-O5G-P1-O11
2	E	600	TPU	C5B-O5G-P1-O12
2	E	600	TPU	C5B-O5G-P1-O13
2	E	600	TPU	C5-C5A-C5B-O5G
2	F	600	TPU	C5-C5A-C5B-O5G
2	V	600	TPU	P1-O11-P2-O22
2	V	600	TPU	C5B-O5G-P1-O13
2	X	600	TPU	P1-O11-P2-O23
2	Y	600	TPU	C5-C5A-C5B-O5G
2	Z	600	TPU	C5-C5A-C5B-O5G
4	V	602	PYR	OXT-C-CA-CB
4	Z	602	PYR	OXT-C-CA-CB
2	A	600	TPU	P2-O11-P1-O5G
2	B	600	TPU	P2-O11-P1-O13
2	E	600	TPU	P2-O11-P1-O12
2	F	600	TPU	P2-O11-P1-O12
2	Z	600	TPU	P2-O11-P1-O12
2	V	600	TPU	C5-C5A-C5B-O5G
2	X	600	TPU	C5-C5A-C5B-O5G
2	F	600	TPU	C5B-O5G-P1-O11
2	F	600	TPU	C5B-O5G-P1-O12
2	F	600	TPU	C5B-O5G-P1-O13
2	V	600	TPU	C5B-O5G-P1-O11
2	X	600	TPU	C5B-O5G-P1-O12
2	Y	600	TPU	C5B-O5G-P1-O11
2	Y	600	TPU	C5B-O5G-P1-O12
2	Y	600	TPU	C5B-O5G-P1-O13
2	Z	600	TPU	C5B-O5G-P1-O11
2	Z	600	TPU	C5B-O5G-P1-O12
2	Z	600	TPU	C5B-O5G-P1-O13
2	V	600	TPU	P2-O11-P1-O12

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Mol	Chain	Res	Type	Atoms
2	E	600	TPU	N1-C5-C5A-C5B
2	Y	600	TPU	N1-C5-C5A-C5B
2	Z	600	TPU	N1-C5-C5A-C5B
2	Y	600	TPU	P2-O11-P1-O13
2	Y	600	TPU	C4-C5-C5A-C5B
2	Z	600	TPU	C4-C5-C5A-C5B
4	Z	602	PYR	O-C-CA-CB
2	B	600	TPU	P1-O11-P2-O22
2	Y	600	TPU	P1-O11-P2-O22
2	F	600	TPU	P2-O11-P1-O13
2	Y	600	TPU	P2-O11-P1-O12
2	Z	600	TPU	P2-O11-P1-O13
2	F	600	TPU	N1-C5-C5A-C5B
2	A	600	TPU	C5-C5A-C5B-O5G
2	B	600	TPU	C5-C5A-C5B-O5G
2	V	600	TPU	P2-O11-P1-O13

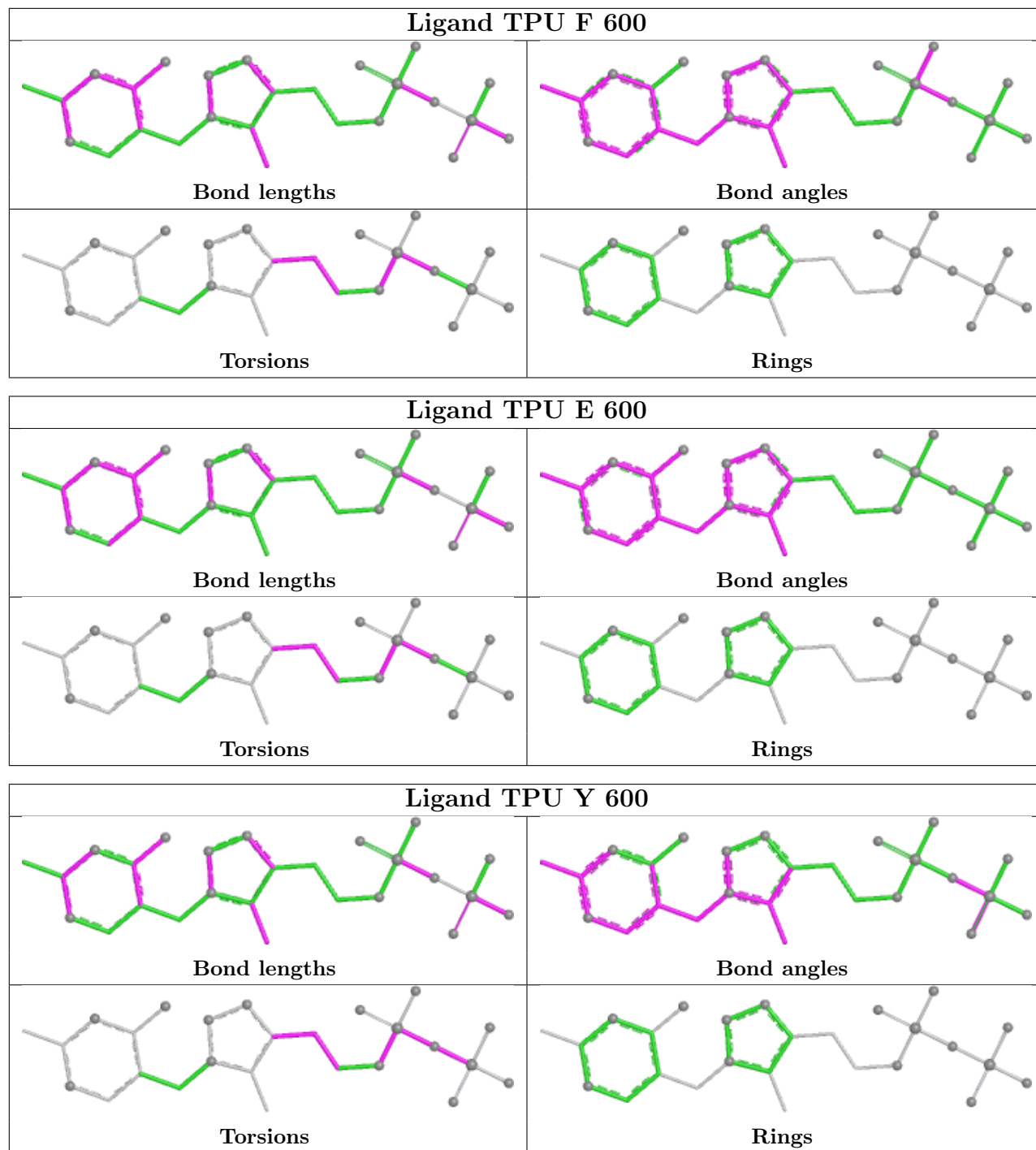
There are no ring outliers.

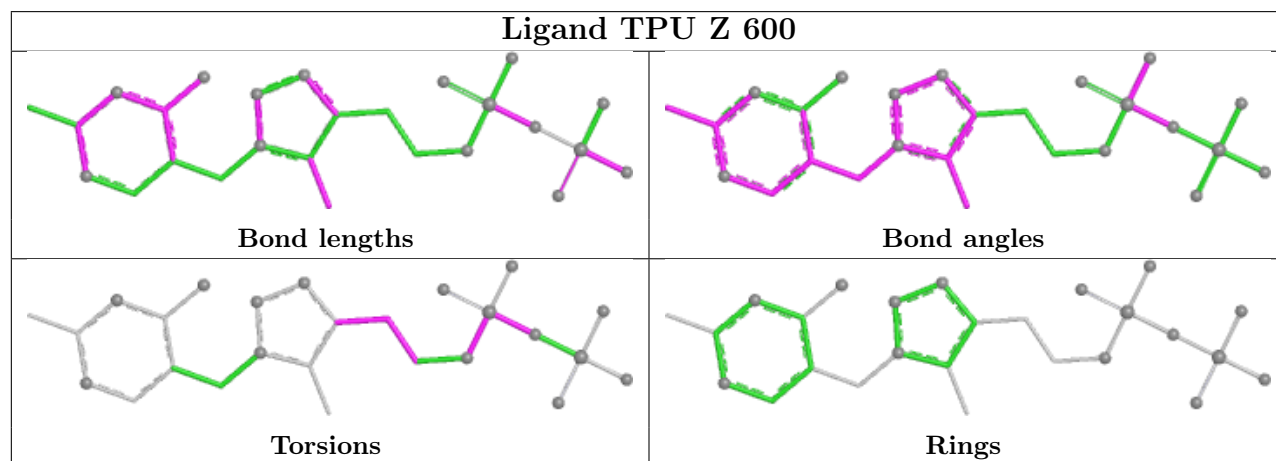
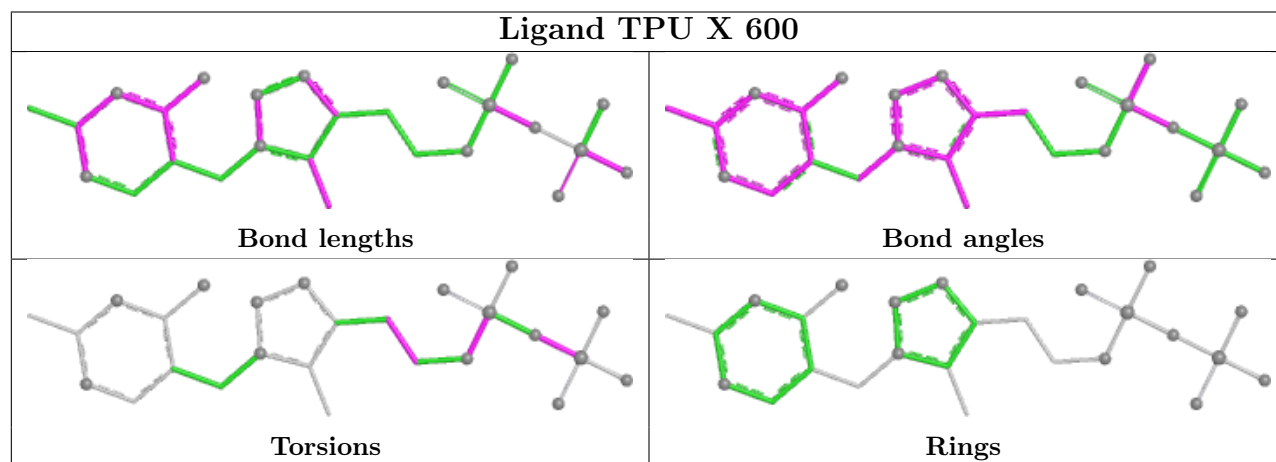
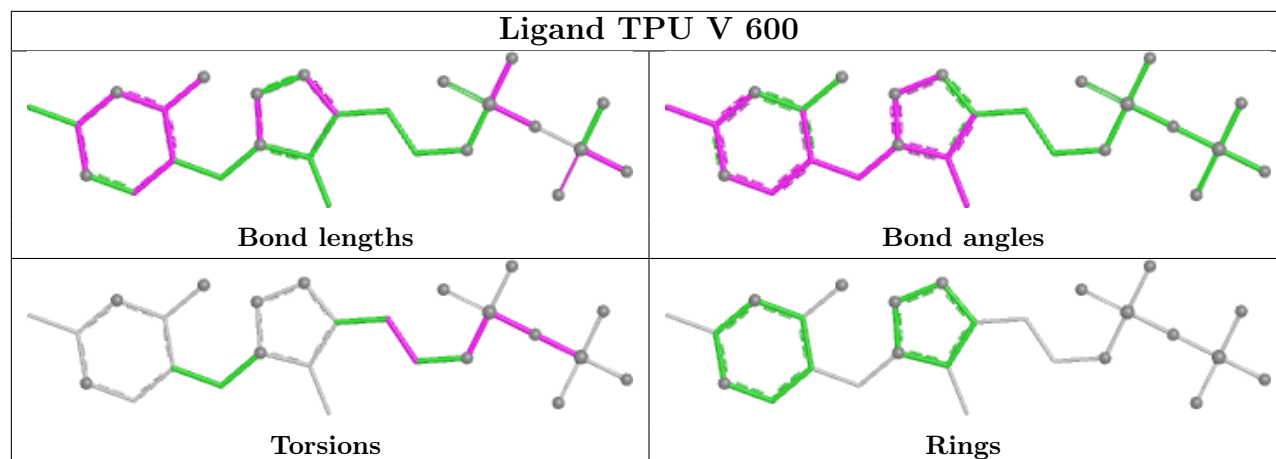
9 monomers are involved in 26 short contacts:

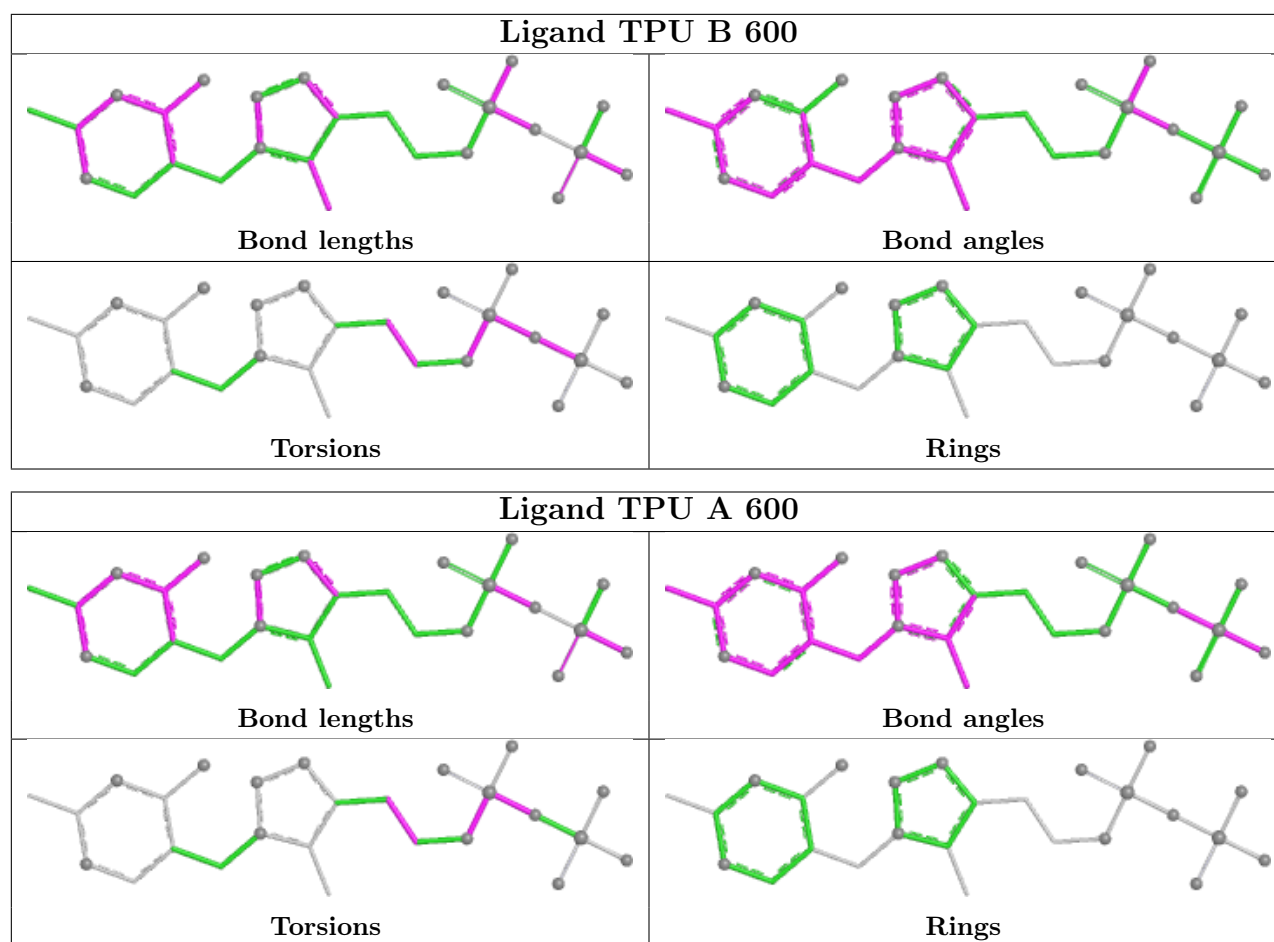
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	600	TPU	4	0
2	E	600	TPU	4	0
2	Y	600	TPU	2	0
2	V	600	TPU	4	0
2	X	600	TPU	2	0
2	Z	600	TPU	4	0
4	Z	602	PYR	3	0
2	B	600	TPU	2	0
2	A	600	TPU	2	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	Y	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Y	565:ASN	C	566:LYS	N	3.00

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	565/568 (99%)	-1.44	0 100 100	24, 51, 74, 93	3 (0%)
1	B	565/568 (99%)	-1.28	0 100 100	32, 56, 83, 104	1 (0%)
1	E	565/568 (99%)	-1.44	0 100 100	25, 54, 81, 110	2 (0%)
1	F	565/568 (99%)	-1.36	0 100 100	24, 53, 78, 98	2 (0%)
1	V	565/568 (99%)	-1.44	0 100 100	26, 53, 80, 100	2 (0%)
1	X	566/568 (99%)	-1.46	0 100 100	30, 50, 76, 99	1 (0%)
1	Y	565/568 (99%)	-1.32	0 100 100	21, 54, 84, 104	2 (0%)
1	Z	565/568 (99%)	-1.39	0 100 100	30, 52, 79, 99	1 (0%)
All	All	4521/4544 (99%)	-1.39	0 100 100	21, 53, 80, 110	14 (0%)

There are no RSRZ outliers to report.

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](#)

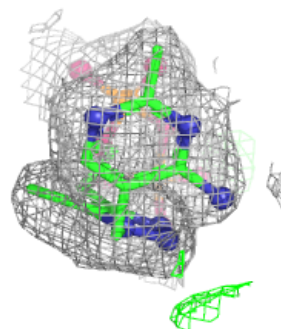
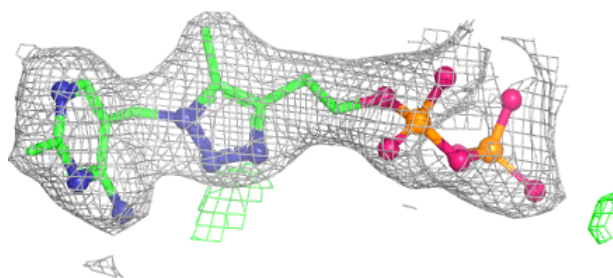
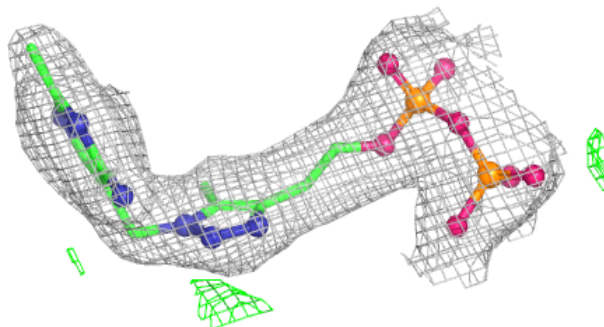
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TPU	A	600	26/26	0.99	0.03	41,46,49,50	0
2	TPU	Y	600	26/26	0.99	0.03	49,52,58,58	0
4	PYR	F	602	6/6	0.99	0.04	98,99,99,100	0
4	PYR	V	602	6/6	0.99	0.04	103,103,104,104	0
4	PYR	Z	602	6/6	0.99	0.06	112,112,113,113	0
2	TPU	X	600	26/26	1.00	0.03	38,41,44,45	0
2	TPU	B	600	26/26	1.00	0.02	47,49,54,55	0
2	TPU	Z	600	26/26	1.00	0.03	50,54,58,59	0
3	MG	A	601	1/1	1.00	0.01	50,50,50,50	0
3	MG	B	601	1/1	1.00	0.03	57,57,57,57	0
3	MG	E	601	1/1	1.00	0.01	60,60,60,60	0
3	MG	F	569	1/1	1.00	0.01	52,52,52,52	0
3	MG	V	601	1/1	1.00	0.05	51,51,51,51	0
3	MG	X	601	1/1	1.00	0.02	54,54,54,54	0
3	MG	Y	601	1/1	1.00	0.02	63,63,63,63	0
3	MG	Z	569	1/1	1.00	0.02	55,55,55,55	0
2	TPU	E	600	26/26	1.00	0.02	42,44,48,48	0
2	TPU	F	600	26/26	1.00	0.02	48,50,53,54	0
2	TPU	V	600	26/26	1.00	0.03	35,38,42,43	0

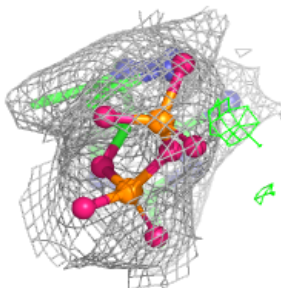
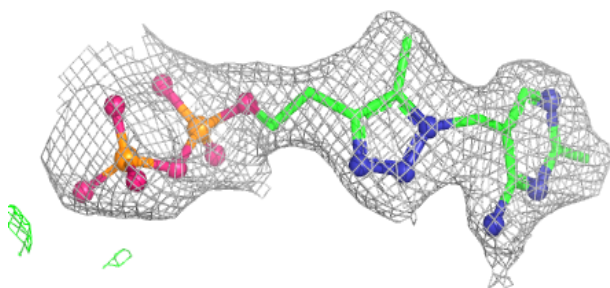
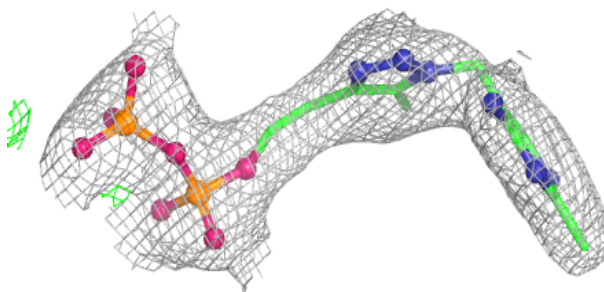
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPU A 600:

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

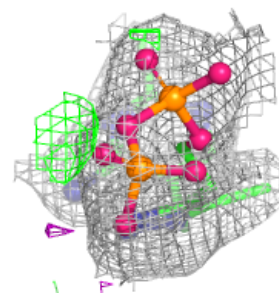
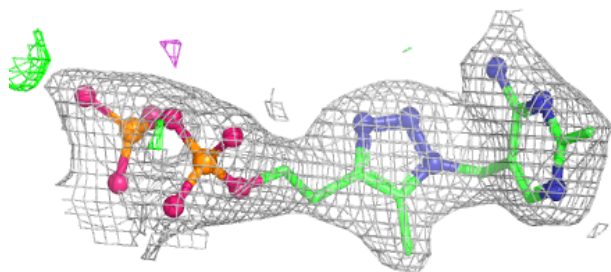
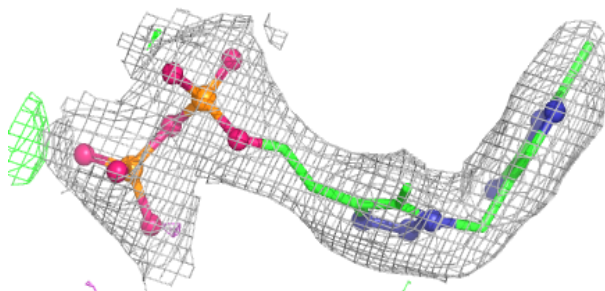
**Electron density around TPU Y 600:**

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

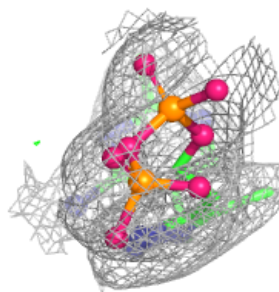
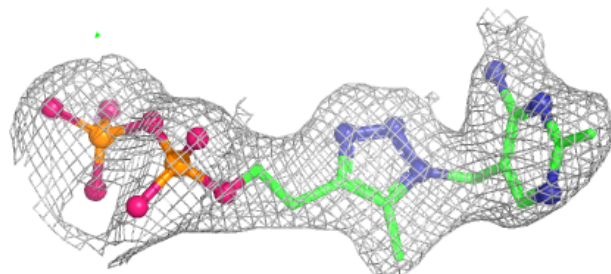
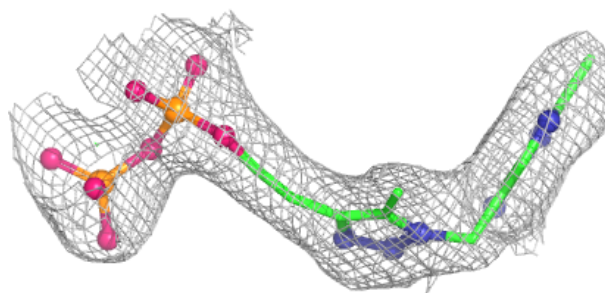


Electron density around TPU X 600:

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

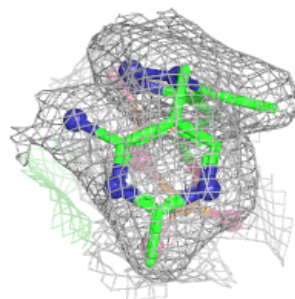
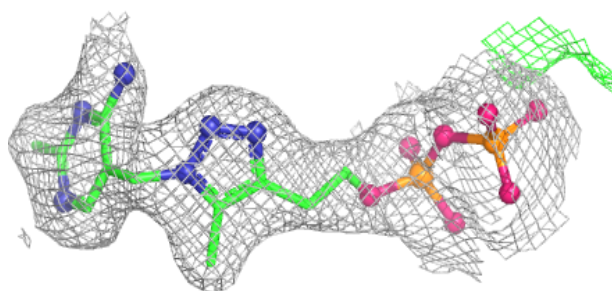
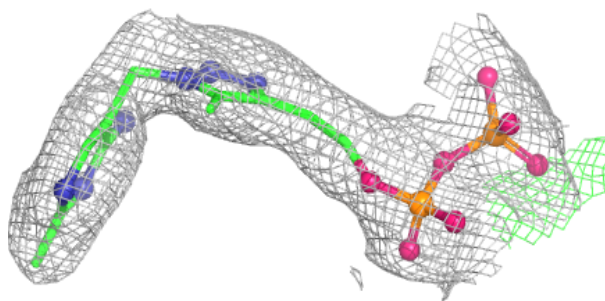
**Electron density around TPU B 600:**

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

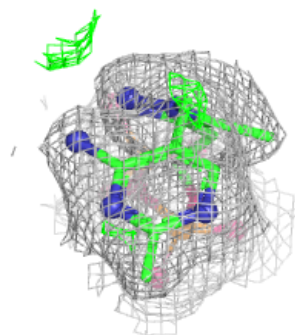
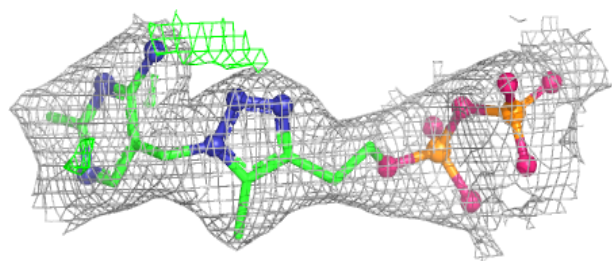
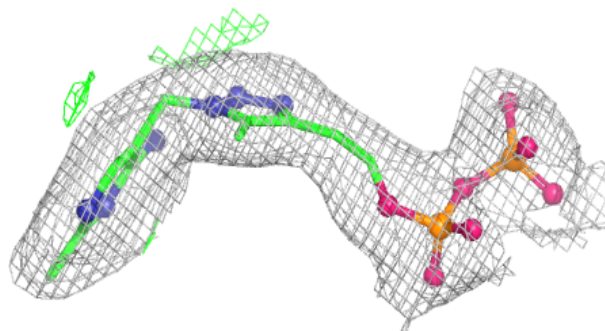


Electron density around TPU Z 600:

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

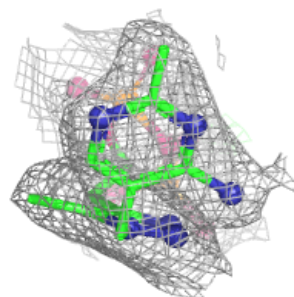
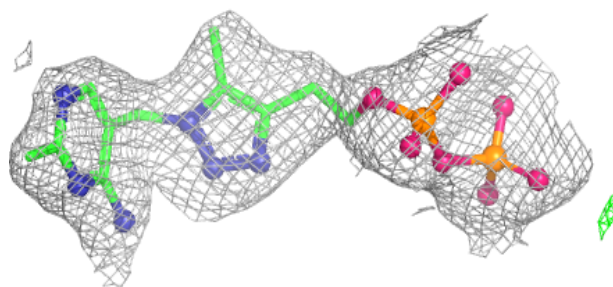
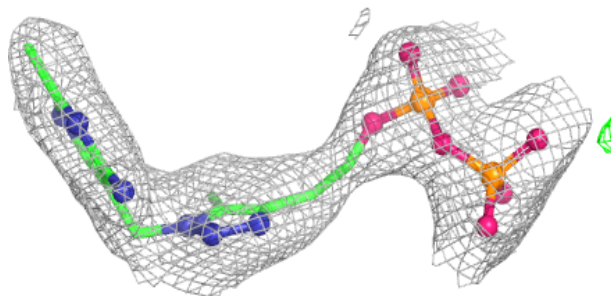
**Electron density around TPU E 600:**

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

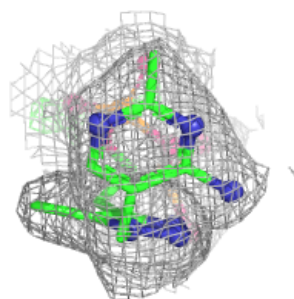
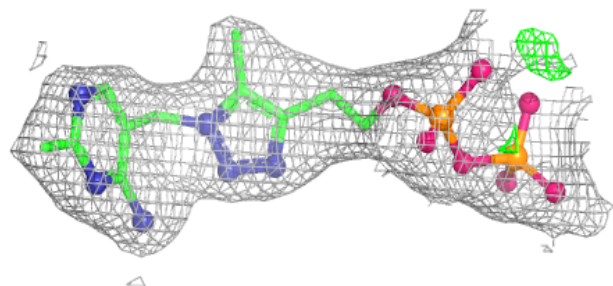
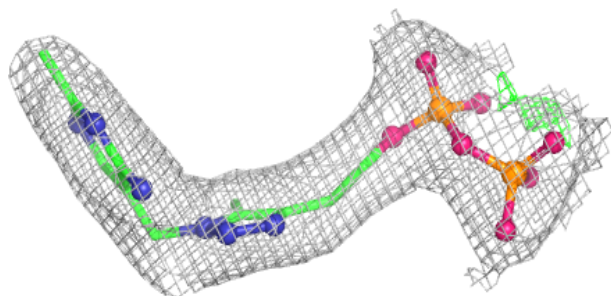


Electron density around TPU F 600:

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

**Electron density around TPU V 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.