



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:46 PM UTC

PDB ID : 1H5S / pdb_00001h5s
Title : Thymidyltransferase complexed with TMP
Authors : Rosano, C.; Zuccotti, S.; Bolognesi, M.
Deposited on : 2001-05-25
Resolution : 2.30 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

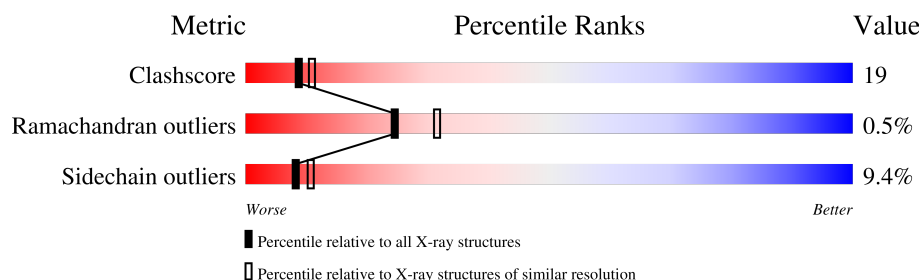
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	293	 70% 26% . .
2	B	293	 62% 31% 5% . .
3	C	293	 66% 25% 7% . .
4	D	293	 67% 27% 5% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9667 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 Glucose-1-phosphate thymidyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	26	0	0
			2276	1461	377	428	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	185	LEU	GLN	conflict	UNP P37744
A	217	LEU	MET	conflict	UNP P37744

- Molecule 2 is a protein called Glucose-1-phosphate thymidyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	291	Total	C	N	O	S	13	0	0
			2280	1461	380	429	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	217	LEU	MET	conflict	UNP P37744
B	288	GLN	MET	conflict	UNP P37744

- Molecule 3 is a protein called Glucose-1-phosphate thymidyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	290	Total	C	N	O	S	13	0	0
			2277	1459	378	429	11			

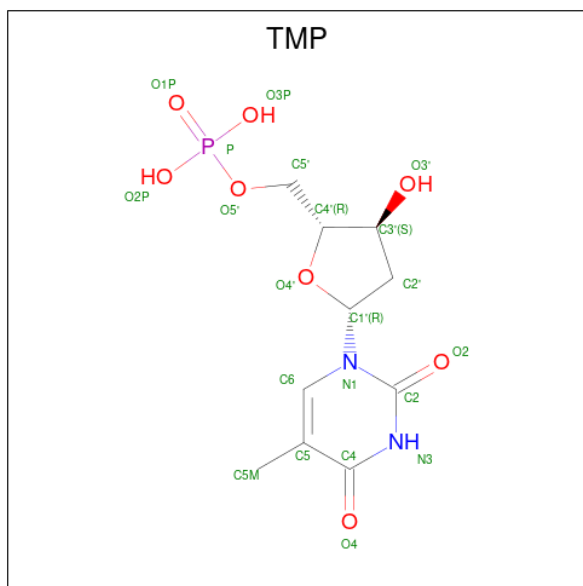
- Molecule 4 is a protein called Glucose-1-phosphate thymidyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	290	Total	C	N	O	S	13	0	0
			2274	1458	377	429	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	102	ALA	GLY	conflict	UNP P37744
D	217	LEU	MET	conflict	UNP P37744

- Molecule 5 is THYMIDINE-5'-PHOSPHATE (CCD ID: TMP) (formula: $C_{10}H_{15}N_2O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
5	A	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
5	B	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
5	B	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
5	C	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
5	C	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
5	D	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
5	D	1	Total	C	N	O	P	0	0
			21	10	2	8	1		

- Molecule 6 is water.

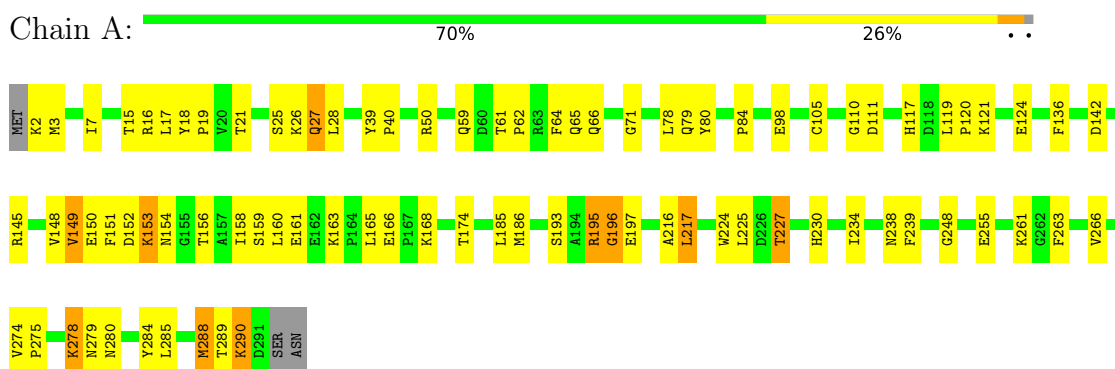
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	111	Total 111	O 111	0	0
6	B	71	Total 71	O 71	0	0
6	C	109	Total 109	O 109	0	0
6	D	101	Total 101	O 101	0	0

3 Residue-property plots [i](#)

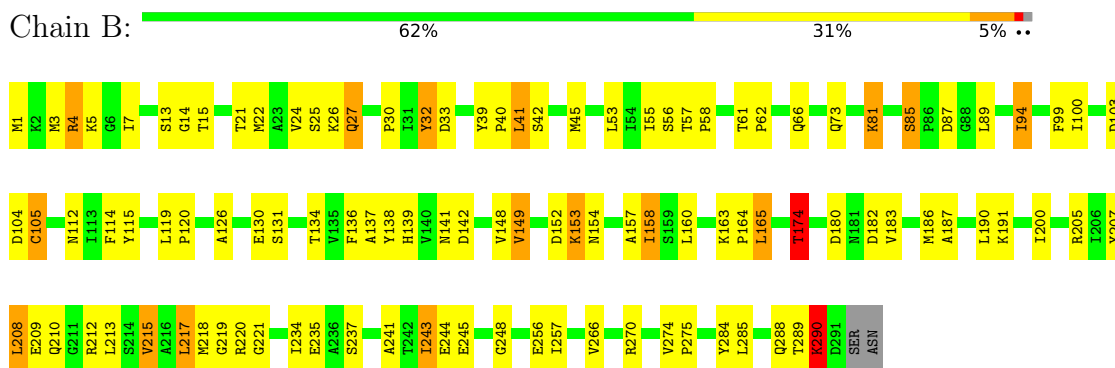
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

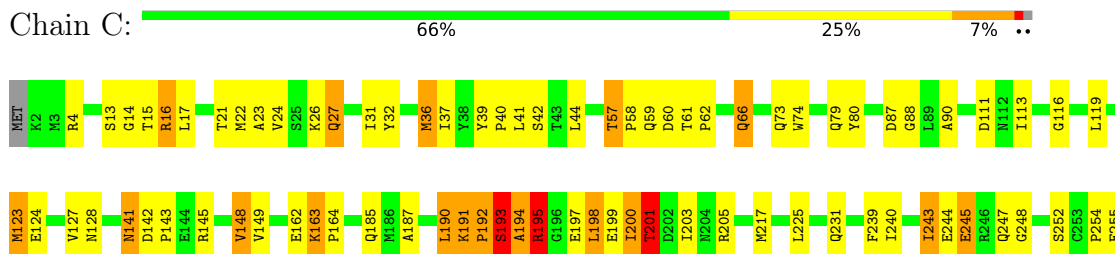
- Molecule 1: Glucose-1-phosphate thymidyltransferase 1



- Molecule 2: Glucose-1-phosphate thymidyltransferase 1



- Molecule 3: Glucose-1-phosphate thymidyltransferase 1





● Molecule 4: Glucose-1-phosphate thymidyltransferase 1



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.10Å 119.27Å 81.11Å 90.00° 112.66° 90.00°	Depositor
Resolution (Å)	12.00 – 2.30	Depositor
% Data completeness (in resolution range)	99.0 (12.00-2.30)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.176 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9667	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TMP

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	1.26	4/2323 (0.2%)	1.76	18/3145 (0.6%)
2	B	1.23	2/2327 (0.1%)	1.20	8/3150 (0.3%)
3	C	1.46	9/2324 (0.4%)	1.51	22/3145 (0.7%)
4	D	1.44	5/2321 (0.2%)	1.48	12/3144 (0.4%)
All	All	1.35	20/9295 (0.2%)	1.50	60/12584 (0.5%)

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	1	1
2	B	1	1
All	All	2	2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	290	LYS	C-N	46.72	1.98	1.33
4	D	290	LYS	C-N	40.02	1.89	1.33
2	B	290	LYS	C-N	-32.26	0.88	1.33
1	A	290	LYS	C-N	26.72	1.70	1.33
4	D	290	LYS	CA-CB	-24.85	1.19	1.52
1	A	290	LYS	CA-CB	-13.29	1.31	1.53
4	D	274	VAL	CA-CB	8.40	1.58	1.54
2	B	45	MET	SD-CE	-7.53	1.60	1.79
1	A	163	LYS	C-O	-6.89	1.20	1.23
3	C	217	MET	SD-CE	6.17	1.95	1.79
3	C	36	MET	SD-CE	5.88	1.94	1.79
1	A	3	MET	SD-CE	-5.66	1.65	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	119	LEU	C-O	-5.54	1.19	1.24
3	C	200	ILE	CA-CB	5.47	1.61	1.54
3	C	195	ARG	N-CA	5.32	1.52	1.46
4	D	102	ALA	CA-CB	-5.29	1.46	1.53
3	C	163	LYS	C-O	-5.26	1.21	1.23
3	C	123	MET	SD-CE	5.16	1.92	1.79
3	C	290	LYS	CA-CB	-5.16	1.43	1.54
4	D	223	ALA	CA-CB	-5.10	1.45	1.53

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	LYS	O-C-N	-67.54	32.76	122.59
4	D	290	LYS	O-C-N	-46.99	61.01	122.56
3	C	290	LYS	O-C-N	-45.06	61.72	122.10
1	A	124	GLU	CA-CB-CG	11.40	136.91	114.10
2	B	290	LYS	CA-CB-CG	11.29	136.68	114.10
2	B	290	LYS	CB-CA-C	10.42	131.16	110.42
4	D	290	LYS	N-CA-CB	10.32	126.18	110.60
1	A	197	GLU	N-CA-C	8.82	123.19	109.52
3	C	195	ARG	N-CA-C	8.73	123.47	112.03
3	C	269	VAL	N-CA-C	-7.89	103.11	110.53
3	C	194	ALA	N-CA-C	7.86	120.84	111.33
3	C	290	LYS	CA-CB-CG	-7.55	98.99	114.10
1	A	290	LYS	N-CA-CB	7.51	123.18	110.49
4	D	101	GLY	CA-C-N	-7.30	111.06	122.67
4	D	101	GLY	C-N-CA	-7.30	111.06	122.67
4	D	191	LYS	N-CA-C	-7.16	100.16	110.40
1	A	124	GLU	CB-CG-CD	7.16	124.77	112.60
3	C	290	LYS	CA-C-N	7.03	134.35	121.70
3	C	290	LYS	C-N-CA	7.03	134.35	121.70
3	C	201	THR	N-CA-C	6.90	119.83	111.82
1	A	290	LYS	CB-CA-C	6.87	124.08	110.42
3	C	148	VAL	N-CA-C	6.84	117.69	108.11
3	C	266	VAL	CB-CA-C	-6.58	103.46	111.88
2	B	183	VAL	N-CA-C	6.33	117.08	110.62
3	C	243	ILE	CB-CA-C	-6.19	104.04	111.97
1	A	217	LEU	CD1-CG-CD2	-6.18	97.20	110.80
1	A	121	LYS	CA-CB-CG	6.14	126.38	114.10
1	A	279	ASN	N-CA-C	6.09	117.83	109.18
3	C	22	MET	N-CA-C	-6.08	104.73	111.36
1	A	255	GLU	N-CA-C	-5.93	104.82	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	219	GLY	N-CA-C	5.85	118.76	112.33
3	C	57	THR	CA-C-N	5.63	124.82	118.97
3	C	57	THR	C-N-CA	5.63	124.82	118.97
2	B	66	GLN	N-CA-C	-5.56	105.23	112.23
3	C	199	GLU	N-CA-C	5.55	118.98	110.20
2	B	41	LEU	N-CA-C	-5.54	105.14	111.07
3	C	141	ASN	CA-C-N	-5.46	116.78	122.89
3	C	141	ASN	C-N-CA	-5.46	116.78	122.89
4	D	214	SER	CA-C-N	-5.38	115.57	123.10
4	D	214	SER	C-N-CA	-5.38	115.57	123.10
3	C	116	GLY	N-CA-C	5.32	117.29	110.96
1	A	16	ARG	CB-CG-CD	5.30	123.50	111.30
1	A	16	ARG	CG-CD-NE	-5.30	100.34	112.00
4	D	110	GLY	CA-C-N	-5.27	114.30	122.67
4	D	110	GLY	C-N-CA	-5.27	114.30	122.67
2	B	174	THR	N-CA-CB	-5.21	101.69	110.49
3	C	60	ASP	N-CA-C	5.21	119.72	112.90
3	C	200	ILE	CA-C-N	-5.20	112.41	120.31
3	C	200	ILE	C-N-CA	-5.20	112.41	120.31
4	D	5	LYS	N-CA-C	5.14	117.78	109.40
1	A	195	ARG	N-CA-C	-5.14	101.98	109.63
1	A	110	GLY	CA-C-N	-5.12	114.49	122.73
1	A	110	GLY	C-N-CA	-5.12	114.49	122.73
1	A	196	GLY	CA-C-N	-5.10	114.59	122.59
1	A	196	GLY	C-N-CA	-5.10	114.59	122.59
1	A	148	VAL	N-CA-C	5.05	115.18	108.11
4	D	124	GLU	N-CA-C	5.03	116.45	111.07
4	D	268	GLN	N-CA-C	5.03	117.15	111.02
2	B	30	PRO	CB-CA-C	-5.02	105.38	111.46
3	C	44	LEU	N-CA-C	-5.02	105.89	111.36

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	290	LYS	CA
2	B	290	LYS	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	GLY	Peptide
2	B	290	LYS	Mainchain

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	2276	0	2288	68	0
2	B	2280	0	2283	104	0
3	C	2277	0	2283	105	0
4	D	2274	0	2276	92	0
5	A	42	0	26	0	0
5	B	42	0	26	1	0
5	C	42	0	26	7	0
5	D	42	0	26	1	0
6	A	111	0	0	6	1
6	B	71	0	0	2	0
6	C	109	0	0	10	1
6	D	101	0	0	10	0
All	All	9667	0	9234	344	1

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 19.

All (344) 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:A:153:LYS:HD3	1:A:153:LYS:N	1.46	1.24
4:D:266:VAL:HG13	4:D:289:THR:HG23	1.25	1.17
3:C:16:ARG:HD2	3:C:16:ARG:N	1.62	1.14
3:C:16:ARG:H	3:C:16:ARG:CD	1.58	1.09
3:C:195:ARG:O	3:C:195:ARG:HG2	1.31	1.08
1:A:238:ASN:OD1	2:B:234:ILE:HG21	1.52	1.08
3:C:256:GLU:OE2	3:C:260:ARG:NH2	1.88	1.07
2:B:153:LYS:H	2:B:153:LYS:HD2	0.91	1.05
2:B:270:ARG:HG2	2:B:289:THR:HG21	1.37	1.05
3:C:245:GLU:N	3:C:245:GLU:OE1	1.88	1.05
3:C:195:ARG:O	3:C:195:ARG:CG	2.05	1.02
2:B:245:GLU:O	3:C:141:ASN:ND2	1.92	1.01
1:A:238:ASN:OD1	2:B:234:ILE:CG2	2.09	1.00
3:C:195:ARG:O	6:C:2061:HOH:O	1.81	0.98
2:B:153:LYS:HD2	2:B:153:LYS:N	1.77	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:124:GLU:OE1	4:D:124:GLU:HA	1.62	0.95
1:A:153:LYS:CD	1:A:153:LYS:H	1.77	0.94
4:D:119:LEU:HD13	4:D:123:MET:HE2	1.49	0.93
4:D:270:ARG:HH21	4:D:289:THR:HG22	1.31	0.93
3:C:16:ARG:HD2	3:C:16:ARG:H	0.78	0.93
2:B:100:ILE:HD11	2:B:105:CYS:SG	2.10	0.92
4:D:270:ARG:HE	4:D:289:THR:HG21	1.34	0.91
1:A:153:LYS:N	1:A:153:LYS:CD	2.29	0.91
4:D:270:ARG:NE	4:D:289:THR:HG21	1.87	0.90
1:A:153:LYS:HD3	1:A:153:LYS:H	1.07	0.89
5:C:1292:TMP:H3'	6:C:2106:HOH:O	1.73	0.89
3:C:27:GLN:HE21	3:C:27:GLN:H	1.21	0.89
4:D:266:VAL:HG13	4:D:289:THR:CG2	2.02	0.89
3:C:124:GLU:O	3:C:127:VAL:HG22	1.73	0.88
2:B:153:LYS:H	2:B:153:LYS:CD	1.76	0.87
4:D:152:ASP:O	4:D:154:ASN:O	1.92	0.87
4:D:2:LYS:HD2	4:D:77:ASN:HB2	1.56	0.86
3:C:59:GLN:HE22	4:D:63:ARG:NH1	1.76	0.84
3:C:205:ARG:HD2	6:C:2066:HOH:O	1.77	0.83
4:D:2:LYS:O	4:D:51:ASP:HB2	1.78	0.83
2:B:221:GLY:CA	5:C:1292:TMP:H5'1	2.09	0.83
2:B:42:SER:OG	2:B:257:ILE:CD1	2.27	0.82
1:A:111:ASP:HB2	1:A:227:THR:HG21	1.61	0.81
4:D:270:ARG:NH2	4:D:289:THR:HG22	1.97	0.80
1:A:225:LEU:O	6:A:2087:HOH:O	2.00	0.79
1:A:239:PHE:CE1	4:D:243:ILE:HD11	2.17	0.79
2:B:94:ILE:HD13	2:B:94:ILE:N	1.98	0.79
4:D:150:GLU:HG2	4:D:158:ILE:HG13	1.64	0.77
3:C:14:GLY:H	3:C:16:ARG:NH1	1.82	0.77
4:D:124:GLU:OE1	4:D:124:GLU:CA	2.33	0.77
3:C:163:LYS:NZ	3:C:195:ARG:HH22	1.83	0.77
3:C:27:GLN:H	3:C:27:GLN:NE2	1.82	0.76
1:A:117:HIS:CD2	4:D:222:TYR:OH	2.39	0.75
1:A:274:VAL:HB	1:A:275:PRO:HD3	1.69	0.74
3:C:268:GLN:HE21	3:C:268:GLN:HA	1.52	0.74
3:C:23:ALA:HB1	4:D:28:LEU:HD22	1.68	0.74
1:A:142:ASP:OD2	1:A:145:ARG:NH1	2.18	0.73
2:B:42:SER:OG	2:B:257:ILE:HD12	1.89	0.73
4:D:2:LYS:HA	4:D:50:ARG:HB2	1.71	0.72
4:D:286:TYR:CD1	6:D:2094:HOH:O	2.42	0.72
3:C:162:GLU:OE1	3:C:201:THR:CG2	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:TYR:O	3:C:42:SER:HB2	1.90	0.72
1:A:117:HIS:CD2	4:D:222:TYR:CZ	2.78	0.71
1:A:227:THR:O	1:A:227:THR:CG2	2.38	0.71
3:C:59:GLN:NE2	4:D:63:ARG:NH1	2.39	0.71
3:C:163:LYS:NZ	3:C:195:ARG:NH2	2.39	0.70
2:B:157:ALA:HB2	2:B:215:VAL:CG1	2.22	0.70
4:D:274:VAL:O	4:D:277:ILE:HG22	1.92	0.70
2:B:270:ARG:CG	2:B:289:THR:HG21	2.18	0.69
4:D:270:ARG:HE	4:D:289:THR:CG2	2.04	0.69
2:B:220:ARG:HH12	3:C:260:ARG:HH21	1.39	0.69
2:B:39:TYR:N	2:B:40:PRO:HD2	2.08	0.69
1:A:152:ASP:HB2	1:A:156:THR:H	1.57	0.69
1:A:227:THR:O	1:A:227:THR:HG23	1.92	0.69
4:D:142:ASP:OD2	4:D:145:ARG:NH2	2.23	0.68
2:B:210:GLN:OE1	2:B:212:ARG:NH2	2.23	0.67
3:C:245:GLU:OE1	3:C:245:GLU:CA	2.42	0.67
2:B:141:ASN:HB3	3:C:248:GLY:HA3	1.76	0.67
3:C:265:ASP:HB2	6:C:2098:HOH:O	1.95	0.67
4:D:270:ARG:HG2	4:D:286:TYR:CE1	2.30	0.67
4:D:266:VAL:HG23	6:D:2093:HOH:O	1.94	0.66
3:C:260:ARG:HD2	6:C:2093:HOH:O	1.95	0.66
2:B:57:THR:HB	2:B:58:PRO:HD2	1.76	0.66
2:B:100:ILE:CD1	2:B:105:CYS:SG	2.84	0.66
1:A:142:ASP:OD1	1:A:142:ASP:N	2.29	0.66
1:A:26:LYS:HE2	1:A:227:THR:CG2	2.26	0.66
3:C:266:VAL:HG12	3:C:289:THR:HB	1.77	0.66
1:A:26:LYS:CE	1:A:227:THR:CG2	2.74	0.65
1:A:161:GLU:OE1	1:A:168:LYS:HE2	1.97	0.65
3:C:39:TYR:N	3:C:40:PRO:CD	2.59	0.65
3:C:244:GLU:C	3:C:245:GLU:OE1	2.38	0.65
3:C:61:THR:HB	3:C:62:PRO:HD3	1.78	0.65
3:C:59:GLN:HE22	4:D:63:ARG:HH12	1.45	0.64
2:B:270:ARG:NE	2:B:289:THR:OG1	2.30	0.64
3:C:27:GLN:HE21	3:C:27:GLN:N	1.96	0.64
3:C:192:PRO:O	3:C:193:SER:O	2.15	0.64
3:C:15:THR:HG21	4:D:278:LYS:HE2	1.80	0.64
3:C:194:ALA:N	6:C:2060:HOH:O	2.31	0.63
2:B:270:ARG:CZ	2:B:289:THR:HB	2.29	0.63
4:D:150:GLU:HG2	4:D:158:ILE:CG1	2.26	0.63
4:D:111:ASP:HB2	4:D:227:THR:HG21	1.81	0.63
4:D:220:ARG:HG3	6:D:2076:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:268:GLN:HA	4:D:268:GLN:OE1	2.00	0.62
4:D:73:GLN:HG2	4:D:74:TRP:CD1	2.35	0.62
4:D:177:TYR:CE2	4:D:200:ILE:HD13	2.35	0.61
4:D:261:LYS:CE	6:D:2017:HOH:O	2.49	0.61
2:B:39:TYR:HB2	2:B:40:PRO:HD3	1.83	0.61
3:C:191:LYS:O	3:C:193:SER:N	2.26	0.61
4:D:277:ILE:HD12	6:D:2094:HOH:O	2.01	0.60
2:B:57:THR:HB	2:B:58:PRO:CD	2.31	0.60
1:A:152:ASP:HB3	1:A:154:ASN:H	1.65	0.60
4:D:164:PRO:O	4:D:167:PRO:HD3	2.02	0.60
4:D:286:TYR:HD1	6:D:2094:HOH:O	1.82	0.60
4:D:119:LEU:HB3	4:D:120:PRO:HD3	1.84	0.60
4:D:270:ARG:NE	4:D:289:THR:CG2	2.62	0.60
1:A:239:PHE:CZ	4:D:243:ILE:HD11	2.36	0.59
3:C:37:ILE:O	3:C:40:PRO:HD2	2.02	0.59
6:A:2036:HOH:O	2:B:22:MET:HE1	2.01	0.59
3:C:42:SER:OG	3:C:252:SER:HB3	2.03	0.59
3:C:57:THR:HB	3:C:58:PRO:HD2	1.84	0.59
3:C:162:GLU:OE1	3:C:201:THR:HG21	2.01	0.59
3:C:163:LYS:HZ2	3:C:195:ARG:NH2	2.00	0.59
2:B:152:ASP:C	2:B:152:ASP:OD1	2.45	0.59
4:D:286:TYR:O	4:D:289:THR:HB	2.03	0.59
1:A:117:HIS:CD2	4:D:222:TYR:CE1	2.90	0.59
2:B:157:ALA:HB2	2:B:215:VAL:HG11	1.85	0.59
2:B:152:ASP:OD1	2:B:154:ASN:N	2.33	0.58
2:B:119:LEU:HB3	2:B:120:PRO:HD3	1.84	0.58
2:B:42:SER:HG	2:B:257:ILE:CD1	2.15	0.58
2:B:61:THR:N	2:B:62:PRO:CD	2.67	0.58
2:B:270:ARG:NE	2:B:289:THR:CB	2.66	0.58
4:D:121:LYS:HZ1	4:D:124:GLU:HB3	1.68	0.58
2:B:221:GLY:N	5:C:1292:TMP:H5'1	2.19	0.58
3:C:142:ASP:CG	3:C:145:ARG:HH11	2.12	0.57
3:C:190:LEU:CD2	3:C:203:ILE:CD1	2.82	0.57
4:D:121:LYS:HE3	4:D:124:GLU:HB2	1.85	0.57
1:A:234:ILE:HD11	2:B:237:SER:HB3	1.86	0.57
2:B:3:MET:O	2:B:103:ASP:HB3	2.04	0.56
3:C:190:LEU:CD2	3:C:203:ILE:HD11	2.36	0.56
3:C:190:LEU:HD21	3:C:203:ILE:CD1	2.35	0.56
2:B:157:ALA:O	2:B:158:ILE:HD12	2.04	0.56
1:A:186:MET:HE2	6:A:2076:HOH:O	2.06	0.56
2:B:94:ILE:N	2:B:94:ILE:CD1	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LYS:NZ	1:A:227:THR:HG22	2.21	0.56
2:B:139:HIS:HD2	3:C:247:GLN:O	1.89	0.56
2:B:4:ARG:HD2	6:B:2027:HOH:O	2.04	0.55
2:B:13:SER:HB2	2:B:15:THR:HG23	1.88	0.55
2:B:180:ASP:OD1	2:B:182:ASP:HB2	2.06	0.55
4:D:289:THR:HG22	4:D:289:THR:O	2.06	0.55
1:A:62:PRO:O	1:A:66:GLN:HG3	2.06	0.55
2:B:141:ASN:HB3	3:C:248:GLY:CA	2.36	0.55
2:B:270:ARG:NH2	2:B:289:THR:OG1	2.40	0.55
1:A:152:ASP:C	1:A:153:LYS:HD3	2.26	0.55
2:B:270:ARG:NH2	2:B:289:THR:CB	2.69	0.55
3:C:17:LEU:HD11	3:C:26:LYS:HE3	1.88	0.54
3:C:163:LYS:HZ3	3:C:195:ARG:NH2	2.03	0.54
2:B:114:PHE:CZ	2:B:174:THR:HG23	2.42	0.54
3:C:163:LYS:HZ2	3:C:195:ARG:HH22	1.55	0.54
6:A:2015:HOH:O	2:B:22:MET:HE1	2.07	0.54
3:C:113:ILE:HG21	3:C:225:LEU:HD12	1.89	0.54
5:D:1292:TMP:H2'1	6:D:2100:HOH:O	2.08	0.54
1:A:50:ARG:HD2	1:A:263:PHE:CE1	2.43	0.54
2:B:27:GLN:H	2:B:27:GLN:NE2	2.06	0.54
4:D:39:TYR:HB2	4:D:40:PRO:HD3	1.90	0.54
1:A:284:TYR:O	1:A:288:MET:HG2	2.08	0.54
1:A:274:VAL:N	1:A:275:PRO:HD2	2.23	0.54
2:B:270:ARG:CZ	2:B:289:THR:CB	2.86	0.54
3:C:191:LYS:C	3:C:193:SER:H	2.15	0.54
1:A:285:LEU:O	1:A:288:MET:HG3	2.08	0.54
2:B:114:PHE:HZ	2:B:174:THR:HG23	1.73	0.53
4:D:256:GLU:HG3	4:D:288:MET:SD	2.48	0.53
2:B:137:ALA:HB3	2:B:217:LEU:HD13	1.91	0.53
3:C:31:ILE:HB	3:C:39:TYR:CE1	2.43	0.53
3:C:74:TRP:NE1	3:C:255:GLU:HG3	2.23	0.53
4:D:33:ASP:OD2	4:D:244:GLU:OE1	2.26	0.53
4:D:57:THR:HB	4:D:58:PRO:HD2	1.92	0.52
2:B:274:VAL:N	2:B:275:PRO:HD2	2.24	0.52
1:A:248:GLY:HA3	4:D:141:ASN:HB3	1.90	0.52
2:B:256:GLU:HA	2:B:288:GLN:HE22	1.74	0.52
3:C:190:LEU:HD21	3:C:203:ILE:HD13	1.92	0.52
1:A:266:VAL:HG13	1:A:289:THR:HB	1.91	0.51
1:A:119:LEU:N	1:A:120:PRO:CD	2.73	0.51
2:B:73:GLN:OE1	2:B:73:GLN:N	2.38	0.51
2:B:5:LYS:HB3	2:B:99:PHE:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1292:TMP:H2'1	6:B:2068:HOH:O	2.10	0.51
4:D:265:ASP:O	4:D:269:VAL:HG23	2.11	0.51
2:B:190:LEU:C	2:B:191:LYS:HD2	2.35	0.51
2:B:85:SER:O	2:B:87:ASP:N	2.43	0.51
2:B:104:ASP:OD1	2:B:180:ASP:HA	2.10	0.51
4:D:289:THR:CG2	4:D:289:THR:O	2.59	0.51
1:A:150:GLU:HB3	1:A:159:SER:HB3	1.91	0.51
2:B:3:MET:HE2	2:B:5:LYS:HE3	1.93	0.51
2:B:21:THR:HA	2:B:24:VAL:O	2.10	0.50
2:B:149:VAL:HB	2:B:160:LEU:HD23	1.92	0.50
3:C:266:VAL:CG1	3:C:289:THR:HB	2.41	0.50
1:A:149:VAL:HG21	1:A:151:PHE:CZ	2.46	0.50
2:B:165:LEU:N	2:B:165:LEU:CD2	2.72	0.50
2:B:163:LYS:N	2:B:164:PRO:CD	2.75	0.50
2:B:39:TYR:N	2:B:40:PRO:CD	2.73	0.50
2:B:221:GLY:HA3	5:C:1292:TMP:H5'1	1.90	0.50
3:C:127:VAL:HG23	3:C:128:ASN:CG	2.36	0.50
2:B:27:GLN:H	2:B:27:GLN:HE21	1.59	0.50
1:A:26:LYS:HE2	1:A:227:THR:HG21	1.93	0.49
3:C:194:ALA:HA	6:C:2060:HOH:O	2.12	0.49
4:D:91:GLN:O	4:D:92:ALA:C	2.55	0.49
1:A:117:HIS:CG	4:D:222:TYR:CE1	3.00	0.49
1:A:27:GLN:H	1:A:27:GLN:NE2	2.11	0.49
3:C:281:TYR:CD1	4:D:19:PRO:HD3	2.47	0.49
4:D:61:THR:HB	4:D:62:PRO:HD3	1.95	0.49
3:C:123:MET:O	3:C:127:VAL:HG13	2.12	0.49
1:A:17:LEU:HD22	1:A:230:HIS:CD2	2.48	0.49
3:C:90:ALA:HB3	3:C:198:LEU:HB3	1.94	0.49
2:B:139:HIS:CD2	3:C:247:GLN:O	2.66	0.48
2:B:136:PHE:O	2:B:174:THR:HB	2.14	0.48
3:C:270:ARG:O	3:C:274:VAL:HG23	2.12	0.48
1:A:18:TYR:CE2	1:A:19:PRO:HB3	2.48	0.48
4:D:126:ALA:HB2	4:D:134:THR:HG21	1.96	0.48
1:A:61:THR:N	1:A:62:PRO:CD	2.77	0.48
2:B:115:TYR:C	2:B:115:TYR:CD2	2.92	0.48
3:C:14:GLY:N	3:C:16:ARG:NH1	2.58	0.48
3:C:163:LYS:HZ3	3:C:195:ARG:HH22	1.56	0.48
3:C:27:GLN:NE2	3:C:27:GLN:N	2.56	0.48
3:C:162:GLU:OE1	3:C:201:THR:HG23	2.13	0.48
4:D:2:LYS:CD	4:D:77:ASN:HB2	2.35	0.48
3:C:37:ILE:C	3:C:40:PRO:HD2	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:79:GLN:C	3:C:80:TYR:CD1	2.91	0.47
1:A:274:VAL:HB	1:A:275:PRO:CD	2.40	0.47
3:C:141:ASN:C	3:C:143:PRO:HD2	2.39	0.47
4:D:121:LYS:HE3	4:D:124:GLU:CB	2.45	0.47
2:B:190:LEU:O	2:B:191:LYS:HD2	2.13	0.47
3:C:36:MET:O	3:C:40:PRO:HD3	2.13	0.47
3:C:190:LEU:HD12	3:C:190:LEU:HA	1.72	0.47
1:A:239:PHE:CE1	4:D:243:ILE:CD1	2.94	0.47
4:D:165:LEU:O	4:D:167:PRO:HD2	2.14	0.47
1:A:7:ILE:HG13	1:A:105:CYS:SG	2.53	0.47
2:B:148:VAL:O	2:B:160:LEU:HA	2.15	0.47
3:C:274:VAL:HB	3:C:275:PRO:HD3	1.97	0.47
3:C:194:ALA:CA	6:C:2060:HOH:O	2.62	0.47
4:D:166:GLU:O	4:D:167:PRO:C	2.57	0.47
4:D:168:LYS:HG3	6:D:2048:HOH:O	2.15	0.47
2:B:32:TYR:CD1	2:B:241:ALA:HB2	2.50	0.46
4:D:39:TYR:N	4:D:40:PRO:HD2	2.30	0.46
4:D:143:PRO:O	4:D:145:ARG:N	2.48	0.46
1:A:61:THR:HB	1:A:62:PRO:HD3	1.98	0.46
2:B:39:TYR:H	2:B:40:PRO:HD2	1.80	0.46
3:C:39:TYR:N	3:C:40:PRO:HD3	2.30	0.46
3:C:274:VAL:N	3:C:275:PRO:CD	2.78	0.46
4:D:261:LYS:HE3	6:D:2017:HOH:O	2.11	0.46
2:B:142:ASP:OD1	2:B:142:ASP:N	2.45	0.46
2:B:13:SER:CB	2:B:15:THR:HG23	2.46	0.46
3:C:15:THR:HG21	4:D:278:LYS:CE	2.46	0.46
3:C:88:GLY:HA2	3:C:197:GLU:HB3	1.98	0.46
1:A:111:ASP:HB2	1:A:227:THR:CG2	2.40	0.45
2:B:165:LEU:HD22	2:B:165:LEU:HA	1.59	0.45
1:A:18:TYR:CZ	1:A:19:PRO:HB3	2.51	0.45
2:B:126:ALA:HB2	2:B:134:THR:HG21	1.97	0.45
2:B:138:TYR:HD1	2:B:218:MET:HG2	1.82	0.45
2:B:152:ASP:HB3	2:B:158:ILE:HD13	1.99	0.45
4:D:270:ARG:NH2	4:D:289:THR:CG2	2.75	0.45
2:B:165:LEU:N	2:B:165:LEU:HD23	2.32	0.45
3:C:4:ARG:HD2	3:C:4:ARG:HA	1.74	0.45
1:A:27:GLN:H	1:A:27:GLN:HE21	1.65	0.45
2:B:138:TYR:CD1	2:B:218:MET:HG2	2.52	0.45
1:A:278:LYS:HD2	1:A:278:LYS:HA	1.64	0.45
2:B:33:ASP:OD2	2:B:244:GLU:OE1	2.34	0.45
3:C:192:PRO:O	3:C:193:SER:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:239:PHE:O	3:C:243:ILE:HG12	2.18	0.44
1:A:142:ASP:OD2	1:A:145:ARG:HD3	2.16	0.44
4:D:143:PRO:O	4:D:144:GLU:C	2.60	0.44
3:C:190:LEU:CD2	3:C:203:ILE:HD13	2.47	0.44
1:A:26:LYS:CE	1:A:227:THR:HG23	2.46	0.44
1:A:234:ILE:CD1	2:B:237:SER:HB3	2.47	0.44
1:A:274:VAL:N	1:A:275:PRO:CD	2.80	0.44
3:C:87:ASP:O	3:C:197:GLU:HA	2.17	0.44
3:C:163:LYS:N	3:C:164:PRO:CD	2.80	0.44
4:D:18:TYR:CZ	4:D:19:PRO:HB3	2.52	0.44
2:B:53:LEU:HD11	2:B:81:LYS:HB2	1.99	0.44
4:D:26:LYS:HZ1	4:D:227:THR:HG23	1.82	0.44
2:B:270:ARG:NH2	2:B:289:THR:HB	2.30	0.44
3:C:15:THR:CG2	4:D:278:LYS:HE2	2.47	0.44
5:C:1292:TMP:H5'2	6:C:2106:HOH:O	2.17	0.44
1:A:149:VAL:HG22	1:A:151:PHE:CE1	2.53	0.44
5:C:1293:TMP:O5'	5:C:1293:TMP:H6	2.01	0.44
4:D:177:TYR:CD2	4:D:200:ILE:HD13	2.52	0.44
1:A:136:PHE:HA	1:A:216:ALA:O	2.18	0.43
2:B:186:MET:HE1	2:B:207:TYR:CZ	2.52	0.43
4:D:243:ILE:HD13	4:D:243:ILE:N	2.31	0.43
2:B:56:SER:HB3	2:B:61:THR:OG1	2.18	0.43
4:D:26:LYS:NZ	4:D:227:THR:HG23	2.32	0.43
3:C:88:GLY:CA	3:C:197:GLU:HB3	2.48	0.43
1:A:239:PHE:HE1	4:D:243:ILE:HD11	1.76	0.43
3:C:191:LYS:HG3	3:C:192:PRO:HD2	2.00	0.43
2:B:42:SER:OG	2:B:257:ILE:HD13	2.16	0.43
1:A:59:GLN:HG3	6:A:2020:HOH:O	2.19	0.43
3:C:244:GLU:HB2	3:C:245:GLU:OE1	2.19	0.43
1:A:261:LYS:HB3	1:A:261:LYS:HE3	1.85	0.43
2:B:243:ILE:HD11	3:C:239:PHE:CE1	2.54	0.42
4:D:119:LEU:N	4:D:120:PRO:CD	2.81	0.42
2:B:217:LEU:HD13	2:B:217:LEU:HA	1.55	0.42
4:D:32:TYR:CG	4:D:33:ASP:N	2.86	0.42
1:A:174:THR:HA	1:A:224:TRP:CZ2	2.55	0.42
3:C:187:ALA:HA	3:C:190:LEU:HD22	2.01	0.42
1:A:17:LEU:O	1:A:18:TYR:C	2.61	0.42
1:A:39:TYR:N	1:A:40:PRO:HD2	2.33	0.42
1:A:84:PRO:HD2	6:A:2030:HOH:O	2.18	0.42
1:A:65:GLN:HA	1:A:80:TYR:CZ	2.55	0.42
2:B:208:LEU:HD23	2:B:213:LEU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:28:LEU:HA	4:D:28:LEU:HD23	1.39	0.42
1:A:71:GLY:HA3	1:A:78:LEU:HG	2.01	0.42
3:C:272:LEU:HD23	3:C:272:LEU:HA	1.77	0.42
4:D:80:TYR:O	4:D:81:LYS:HG3	2.20	0.42
4:D:119:LEU:CD1	4:D:123:MET:HE2	2.36	0.42
3:C:66:GLN:O	3:C:66:GLN:HG3	2.19	0.42
3:C:191:LYS:HA	3:C:192:PRO:HD3	1.63	0.42
4:D:161:GLU:O	4:D:164:PRO:HD3	2.20	0.42
2:B:152:ASP:O	2:B:153:LYS:C	2.63	0.41
3:C:265:ASP:OD1	3:C:265:ASP:C	2.63	0.41
2:B:270:ARG:CZ	2:B:289:THR:OG1	2.68	0.41
3:C:142:ASP:CG	3:C:145:ARG:HD3	2.44	0.41
4:D:266:VAL:CG1	4:D:289:THR:CG2	2.89	0.41
4:D:96:GLY:O	4:D:100:ILE:HG13	2.20	0.41
2:B:205:ARG:O	2:B:209:GLU:HG3	2.19	0.41
2:B:13:SER:OG	2:B:14:GLY:N	2.54	0.41
4:D:41:LEU:O	4:D:45:MET:HG3	2.21	0.41
1:A:28:LEU:HD21	1:A:64:PHE:CD1	2.56	0.41
2:B:25:SER:O	2:B:26:LYS:C	2.62	0.41
2:B:94:ILE:HD11	2:B:187:ALA:CB	2.51	0.41
2:B:235:GLU:HA	2:B:235:GLU:OE1	2.21	0.41
2:B:248:GLY:HA3	3:C:141:ASN:HB3	2.03	0.41
3:C:252:SER:O	3:C:254:PRO:HD3	2.21	0.41
4:D:97:GLU:HG3	4:D:184:VAL:HG11	2.03	0.41
2:B:248:GLY:CA	3:C:141:ASN:HB3	2.51	0.41
3:C:231:GLN:CD	6:C:2084:HOH:O	2.63	0.41
4:D:261:LYS:HE2	6:D:2017:HOH:O	2.20	0.40
2:B:7:ILE:HD12	2:B:105:CYS:SG	2.62	0.40
3:C:127:VAL:HG23	3:C:128:ASN:N	2.36	0.40
4:D:202:ASP:OD1	4:D:205:ARG:NH2	2.54	0.40
3:C:111:ASP:OD2	5:C:1293:TMP:O3'	2.34	0.40
3:C:113:ILE:HB	3:C:225:LEU:HB2	2.04	0.40
4:D:18:TYR:CD1	4:D:19:PRO:HA	2.57	0.40
1:A:193:SER:O	1:A:195:ARG:O	2.40	0.40
2:B:55:ILE:HA	2:B:81:LYS:O	2.20	0.40
2:B:284:TYR:O	2:B:285:LEU:C	2.63	0.40
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.80	0.40
4:D:23:ALA:C	4:D:24:VAL:CG2	2.94	0.40
2:B:182:ASP:HB3	2:B:186:MET:CE	2.52	0.40
2:B:208:LEU:HD23	2:B:208:LEU:HA	1.89	0.40
3:C:73:GLN:HG2	3:C:74:TRP:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:50:ARG:HD2	4:D:263:PHE:CE2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2048:HOH:O	6:C:2069:HOH:O[1_554]	2.12	0.08

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	288/293 (98%)	277 (96%)	11 (4%)	0	100	100
2	B	289/293 (99%)	276 (96%)	11 (4%)	2 (1%)	18	23
3	C	288/293 (98%)	276 (96%)	9 (3%)	3 (1%)	12	15
4	D	288/293 (98%)	280 (97%)	7 (2%)	1 (0%)	36	46
All	All	1153/1172 (98%)	1109 (96%)	38 (3%)	6 (0%)	24	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	290	LYS
3	C	193	SER
4	D	144	GLU
3	C	192	PRO
2	B	32	TYR
3	C	32	TYR

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	244/247 (99%)	224 (92%)	20 (8%)	10	14
2	B	243/247 (98%)	219 (90%)	24 (10%)	7	9
3	C	244/247 (99%)	219 (90%)	25 (10%)	7	8
4	D	243/247 (98%)	220 (90%)	23 (10%)	8	10
All	All	974/988 (99%)	882 (91%)	92 (9%)	8	11

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	15	THR
1	A	21	THR
1	A	25	SER
1	A	27	GLN
1	A	79	GLN
1	A	98	GLU
1	A	149	VAL
1	A	153	LYS
1	A	158	ILE
1	A	160	LEU
1	A	165	LEU
1	A	166	GLU
1	A	185	LEU
1	A	217	LEU
1	A	227	THR
1	A	278	LYS
1	A	280	ASN
1	A	288	MET
1	A	290	LYS
2	B	1	MET
2	B	4	ARG
2	B	27	GLN
2	B	41	LEU

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Mol	Chain	Res	Type
2	B	81	LYS
2	B	85	SER
2	B	89	LEU
2	B	94	ILE
2	B	105	CYS
2	B	112	ASN
2	B	130	GLU
2	B	131	SER
2	B	149	VAL
2	B	153	LYS
2	B	158	ILE
2	B	165	LEU
2	B	174	THR
2	B	200	ILE
2	B	208	LEU
2	B	215	VAL
2	B	217	LEU
2	B	243	ILE
2	B	266	VAL
2	B	290	LYS
3	C	13	SER
3	C	16	ARG
3	C	21	THR
3	C	24	VAL
3	C	27	GLN
3	C	41	LEU
3	C	66	GLN
3	C	148	VAL
3	C	149	VAL
3	C	185	GLN
3	C	190	LEU
3	C	191	LYS
3	C	193	SER
3	C	195	ARG
3	C	198	LEU
3	C	200	ILE
3	C	201	THR
3	C	245	GLU
3	C	260	ARG
3	C	264	ILE
3	C	266	VAL
3	C	267	GLU

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Mol	Chain	Res	Type
3	C	268	GLN
3	C	277	ILE
3	C	290	LYS
4	D	3	MET
4	D	15	THR
4	D	21	THR
4	D	24	VAL
4	D	41	LEU
4	D	59	GLN
4	D	79	GLN
4	D	112	ASN
4	D	119	LEU
4	D	121	LYS
4	D	124	GLU
4	D	149	VAL
4	D	150	GLU
4	D	160	LEU
4	D	165	LEU
4	D	200	ILE
4	D	215	VAL
4	D	220	ARG
4	D	227	THR
4	D	243	ILE
4	D	278	LYS
4	D	290	LYS
4	D	291	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	117	HIS
1	A	128	ASN
1	A	280	ASN
2	B	27	GLN
2	B	66	GLN
2	B	139	HIS
2	B	154	ASN
2	B	230	HIS
2	B	247	GLN
3	C	27	GLN
3	C	79	GLN

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Mol	Chain	Res	Type
3	C	185	GLN
3	C	247	GLN
3	C	268	GLN
4	D	27	GLN
4	D	181	ASN
4	D	185	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	TMP	C	1292	-	22,22,22	2.43	7 (31%)	32,33,33	3.14	18 (56%)
5	TMP	D	1292	-	22,22,22	2.25	8 (36%)	32,33,33	2.25	8 (25%)
5	TMP	A	1292	-	22,22,22	2.31	7 (31%)	32,33,33	2.09	11 (34%)
5	TMP	B	1292	-	22,22,22	2.47	8 (36%)	32,33,33	2.26	9 (28%)
5	TMP	D	1293	-	22,22,22	2.47	7 (31%)	32,33,33	2.99	14 (43%)
5	TMP	C	1293	-	22,22,22	2.37	8 (36%)	32,33,33	2.17	12 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	TMP	B	1293	-	22,22,22	2.19	7 (31%)	32,33,33	3.60	16 (50%)
5	TMP	A	1293	-	22,22,22	2.09	6 (27%)	32,33,33	2.72	11 (34%)

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
5	TMP	C	1292	-	-	2/10/22/22	0/2/2/2
5	TMP	D	1292	-	-	3/10/22/22	0/2/2/2
5	TMP	A	1292	-	-	3/10/22/22	0/2/2/2
5	TMP	B	1292	-	-	3/10/22/22	0/2/2/2
5	TMP	D	1293	-	-	0/10/22/22	0/2/2/2
5	TMP	C	1293	-	-	3/10/22/22	0/2/2/2
5	TMP	B	1293	-	-	3/10/22/22	0/2/2/2
5	TMP	A	1293	-	-	0/10/22/22	0/2/2/2

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1293	TMP	O2-C2	6.64	1.34	1.23
5	C	1293	TMP	O2-C2	6.16	1.34	1.23
5	C	1293	TMP	O4-C4	6.07	1.35	1.23
5	A	1292	TMP	O4-C4	5.96	1.34	1.23
5	C	1292	TMP	O2-C2	5.87	1.33	1.23
5	D	1293	TMP	O4-C4	5.85	1.34	1.23
5	B	1293	TMP	O4-C4	5.79	1.34	1.23
5	A	1292	TMP	O2-C2	5.69	1.33	1.23
5	B	1292	TMP	O2-C2	5.56	1.32	1.23
5	C	1292	TMP	O4-C4	5.38	1.33	1.23
5	A	1293	TMP	O2-C2	5.30	1.32	1.23
5	B	1292	TMP	O4-C4	5.23	1.33	1.23
5	B	1293	TMP	O2-C2	5.17	1.32	1.23
5	D	1292	TMP	O2-C2	4.64	1.31	1.23
5	D	1292	TMP	O4-C4	4.59	1.32	1.23
5	B	1292	TMP	C4-C5	-4.57	1.37	1.44
5	C	1292	TMP	C4-C5	-4.47	1.37	1.44
5	A	1293	TMP	O4-C4	4.11	1.31	1.23
5	D	1292	TMP	C4-C5	-4.03	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1293	TMP	C6-C5	3.87	1.40	1.34
5	B	1293	TMP	C6-C5	3.79	1.40	1.34
5	A	1293	TMP	C4-N3	-3.61	1.32	1.38
5	A	1292	TMP	C6-C5	3.52	1.40	1.34
5	D	1292	TMP	P-O5'	-3.51	1.49	1.60
5	D	1293	TMP	C4-C5	-3.38	1.39	1.44
5	A	1293	TMP	C6-C5	3.32	1.40	1.34
5	B	1292	TMP	C6-C5	3.26	1.39	1.34
5	B	1292	TMP	P-O5'	-3.18	1.50	1.60
5	C	1292	TMP	C6-C5	3.16	1.39	1.34
5	D	1293	TMP	C2-N1	-3.16	1.33	1.38
5	D	1292	TMP	C2-N3	-3.04	1.32	1.38
5	A	1292	TMP	C4-C5	-2.96	1.40	1.44
5	D	1293	TMP	C4-N3	-2.95	1.33	1.38
5	B	1292	TMP	C4-N3	-2.93	1.33	1.38
5	C	1292	TMP	C5'-C4'	2.88	1.60	1.51
5	A	1292	TMP	P-O5'	-2.88	1.51	1.60
5	B	1292	TMP	C6-N1	-2.81	1.33	1.38
5	A	1293	TMP	C4-C5	-2.68	1.40	1.44
5	D	1292	TMP	C4-N3	-2.68	1.33	1.38
5	C	1293	TMP	C4-C5	-2.64	1.40	1.44
5	D	1293	TMP	C6-N1	-2.64	1.33	1.38
5	D	1292	TMP	C2-N1	-2.56	1.34	1.38
5	C	1293	TMP	C6-N1	-2.50	1.33	1.38
5	D	1293	TMP	P-O5'	-2.48	1.52	1.60
5	A	1292	TMP	C4-N3	-2.43	1.34	1.38
5	B	1292	TMP	C2-N3	-2.42	1.33	1.38
5	C	1293	TMP	C2-N3	-2.37	1.33	1.38
5	B	1293	TMP	C4-C5	-2.37	1.41	1.44
5	B	1293	TMP	C4-N3	-2.31	1.34	1.38
5	B	1293	TMP	C2-N1	-2.24	1.34	1.38
5	C	1293	TMP	P-O5'	-2.23	1.53	1.60
5	C	1292	TMP	C4-N3	-2.21	1.34	1.38
5	D	1292	TMP	C6-N1	-2.17	1.34	1.38
5	A	1292	TMP	C6-N1	-2.13	1.34	1.38
5	A	1293	TMP	C2-N3	-2.13	1.34	1.38
5	C	1293	TMP	C4-N3	-2.08	1.35	1.38
5	C	1292	TMP	C6-N1	-2.08	1.34	1.38
5	B	1293	TMP	C6-N1	-2.02	1.34	1.38

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1293	TMP	O5'-P-O1P	-9.53	80.67	106.44
5	D	1293	TMP	O5'-P-O1P	-8.54	83.35	106.44
5	A	1293	TMP	C5-C4-N3	7.90	122.19	115.32
5	B	1293	TMP	O2P-P-O5'	-7.86	86.17	106.67
5	C	1292	TMP	O3P-P-O5'	-6.98	88.48	106.67
5	D	1293	TMP	O2P-P-O5'	-6.82	88.88	106.67
5	B	1293	TMP	O2-C2-N1	-6.53	114.29	122.80
5	C	1292	TMP	O2P-P-O5'	-6.37	90.05	106.67
5	A	1293	TMP	C4-N3-C2	-6.31	119.07	127.34
5	B	1293	TMP	C4-N3-C2	-6.17	119.25	127.34
5	B	1293	TMP	N3-C2-N1	5.94	122.63	114.89
5	D	1292	TMP	C5-C4-N3	5.53	120.13	115.32
5	C	1292	TMP	O4-C4-C5	-5.47	118.66	124.92
5	B	1292	TMP	O4-C4-C5	-5.38	118.77	124.92
5	D	1292	TMP	C4-N3-C2	-5.36	120.31	127.34
5	A	1293	TMP	C5-C6-N1	-5.31	117.55	123.31
5	A	1292	TMP	N3-C2-N1	5.22	121.69	114.89
5	C	1292	TMP	O5'-C5'-C4'	5.14	126.50	108.99
5	B	1292	TMP	N3-C2-N1	5.11	121.54	114.89
5	B	1292	TMP	C4-N3-C2	-4.94	120.86	127.34
5	C	1292	TMP	N3-C2-N1	4.91	121.28	114.89
5	D	1292	TMP	N3-C2-N1	4.86	121.22	114.89
5	B	1293	TMP	C5-C6-N1	-4.83	118.06	123.31
5	A	1293	TMP	N3-C2-N1	4.77	121.10	114.89
5	D	1293	TMP	C4-N3-C2	-4.76	121.10	127.34
5	C	1293	TMP	C4-N3-C2	-4.73	121.14	127.34
5	C	1292	TMP	C4-N3-C2	-4.69	121.19	127.34
5	D	1292	TMP	O4'-C1'-N1	4.68	116.17	107.86
5	D	1293	TMP	O4-C4-C5	-4.59	119.66	124.92
5	B	1293	TMP	C5-C4-N3	4.53	119.26	115.32
5	A	1293	TMP	O4-C4-C5	-4.50	119.77	124.92
5	B	1293	TMP	O4-C4-C5	-4.49	119.78	124.92
5	D	1293	TMP	C5-C4-N3	4.49	119.23	115.32
5	A	1292	TMP	C4-N3-C2	-4.41	121.56	127.34
5	C	1293	TMP	N3-C2-N1	4.38	120.59	114.89
5	C	1293	TMP	C5-C4-N3	4.26	119.03	115.32
5	B	1292	TMP	C5-C4-N3	4.10	118.89	115.32
5	D	1293	TMP	O3P-P-O5'	-4.04	96.13	106.67
5	B	1292	TMP	C5-C6-N1	-4.01	118.96	123.31
5	C	1292	TMP	C5-C4-N3	3.94	118.75	115.32
5	C	1292	TMP	O5'-P-O1P	-3.74	96.33	106.44
5	A	1292	TMP	C5M-C5-C6	-3.72	117.82	122.85
5	A	1293	TMP	O3P-P-O5'	3.70	116.32	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1293	TMP	N3-C2-N1	3.67	119.67	114.89
5	B	1293	TMP	O3P-P-O5'	-3.51	97.51	106.67
5	D	1292	TMP	O4-C4-C5	-3.50	120.91	124.92
5	D	1293	TMP	O2-C2-N1	-3.50	118.24	122.80
5	C	1293	TMP	C5-C6-N1	-3.43	119.59	123.31
5	D	1293	TMP	C5-C6-N1	-3.40	119.62	123.31
5	A	1292	TMP	O2-C2-N1	-3.39	118.39	122.80
5	A	1292	TMP	C5M-C5-C4	3.35	122.36	118.78
5	C	1292	TMP	C4'-O4'-C1'	3.33	117.43	109.51
5	C	1293	TMP	O4-C4-C5	-3.32	121.12	124.92
5	D	1293	TMP	O2P-P-O1P	3.30	123.69	110.83
5	D	1292	TMP	C5-C6-N1	-3.30	119.73	123.31
5	C	1292	TMP	O2P-P-O1P	3.23	123.42	110.83
5	B	1293	TMP	O2P-P-O1P	3.21	123.34	110.83
5	C	1292	TMP	O2-C2-N1	-3.19	118.64	122.80
5	A	1292	TMP	C5-C6-N1	-3.17	119.87	123.31
5	C	1293	TMP	C4'-O4'-C1'	3.13	116.94	109.51
5	C	1293	TMP	O5'-P-O1P	3.12	114.88	106.44
5	B	1293	TMP	O3P-P-O2P	3.08	119.36	107.80
5	C	1292	TMP	O3P-P-O2P	2.97	118.93	107.80
5	C	1292	TMP	O4'-C4'-C5'	2.96	118.83	109.33
5	B	1292	TMP	O2-C2-N1	-2.96	118.94	122.80
5	C	1292	TMP	C6-N1-C2	-2.87	118.44	121.30
5	A	1292	TMP	O5'-P-O1P	2.86	114.16	106.44
5	A	1292	TMP	C5-C4-N3	2.74	117.70	115.32
5	D	1292	TMP	O2-C2-N1	-2.70	119.29	122.80
5	C	1293	TMP	O4'-C1'-N1	-2.69	103.08	107.86
5	C	1292	TMP	C2'-C3'-C4'	2.69	108.26	102.80
5	C	1293	TMP	C1'-N1-C2	2.69	122.92	117.66
5	A	1293	TMP	C2'-C3'-C4'	2.69	108.25	102.80
5	B	1293	TMP	C4'-O4'-C1'	2.58	115.64	109.51
5	B	1292	TMP	C2'-C1'-N1	2.54	120.17	113.81
5	C	1292	TMP	C2'-C1'-N1	2.49	120.05	113.81
5	A	1293	TMP	O4'-C1'-N1	-2.49	103.44	107.86
5	B	1293	TMP	C5M-C5-C6	-2.48	119.50	122.85
5	A	1293	TMP	C4'-O4'-C1'	2.47	115.38	109.51
5	D	1293	TMP	O3P-P-O2P	2.44	116.94	107.80
5	C	1293	TMP	O2-C2-N3	-2.43	117.00	121.49
5	C	1293	TMP	C1'-N1-C6	-2.35	116.79	120.74
5	B	1293	TMP	O4'-C4'-C5'	2.35	116.85	109.33
5	D	1292	TMP	C4'-O4'-C1'	2.25	114.86	109.51
5	C	1292	TMP	C5-C6-N1	-2.19	120.93	123.31

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1293	TMP	O2-C2-N1	-2.19	119.95	122.80
5	D	1293	TMP	O3P-P-O1P	2.18	119.33	110.83
5	A	1292	TMP	C6-C5-C4	2.18	119.81	118.02
5	D	1293	TMP	C5M-C5-C4	2.14	121.07	118.78
5	B	1292	TMP	C4'-O4'-C1'	2.14	114.59	109.51
5	B	1293	TMP	C6-C5-C4	2.11	119.76	118.02
5	A	1293	TMP	O4'-C4'-C5'	2.09	116.04	109.33
5	B	1293	TMP	O5'-C5'-C4'	2.08	116.07	108.99
5	C	1293	TMP	C2'-C3'-C4'	2.07	106.99	102.80
5	A	1292	TMP	C6-N1-C2	-2.04	119.27	121.30
5	B	1292	TMP	O2P-P-O5'	2.03	111.97	106.67
5	D	1293	TMP	C5M-C5-C6	-2.02	120.12	122.85
5	C	1292	TMP	O4'-C4'-C3'	-2.02	101.05	105.65
5	A	1292	TMP	O4'-C1'-N1	2.00	111.42	107.86

There are no chirality outliers.

All (17) torsion outliers are listed below:

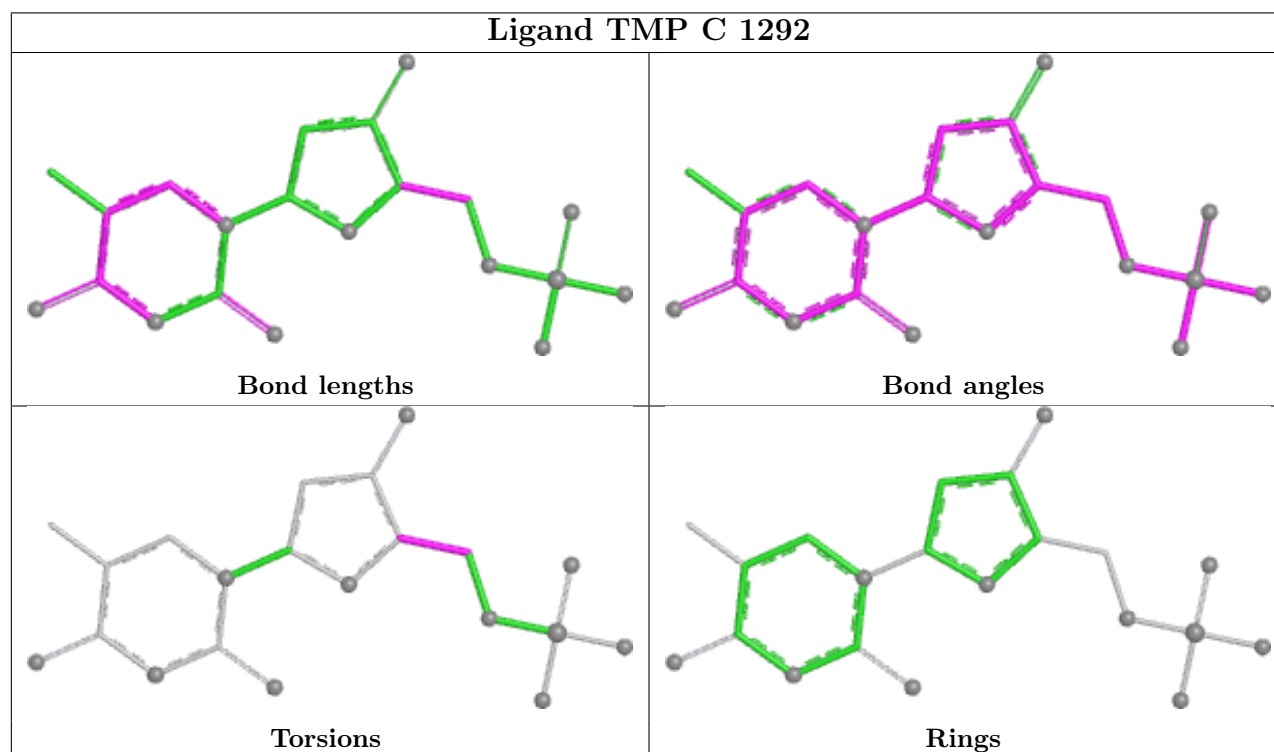
Mol	Chain	Res	Type	Atoms
5	A	1292	TMP	C5'-O5'-P-O2P
5	A	1292	TMP	C5'-O5'-P-O3P
5	B	1292	TMP	C5'-O5'-P-O2P
5	B	1292	TMP	C5'-O5'-P-O3P
5	B	1293	TMP	C5'-O5'-P-O1P
5	B	1293	TMP	C5'-O5'-P-O2P
5	B	1293	TMP	C5'-O5'-P-O3P
5	C	1292	TMP	O4'-C4'-C5'-O5'
5	C	1293	TMP	C5'-O5'-P-O1P
5	C	1293	TMP	C5'-O5'-P-O2P
5	C	1293	TMP	C5'-O5'-P-O3P
5	D	1292	TMP	C5'-O5'-P-O2P
5	D	1292	TMP	C5'-O5'-P-O3P
5	C	1292	TMP	C3'-C4'-C5'-O5'
5	A	1292	TMP	C5'-O5'-P-O1P
5	B	1292	TMP	C5'-O5'-P-O1P
5	D	1292	TMP	C5'-O5'-P-O1P

There are no ring outliers.

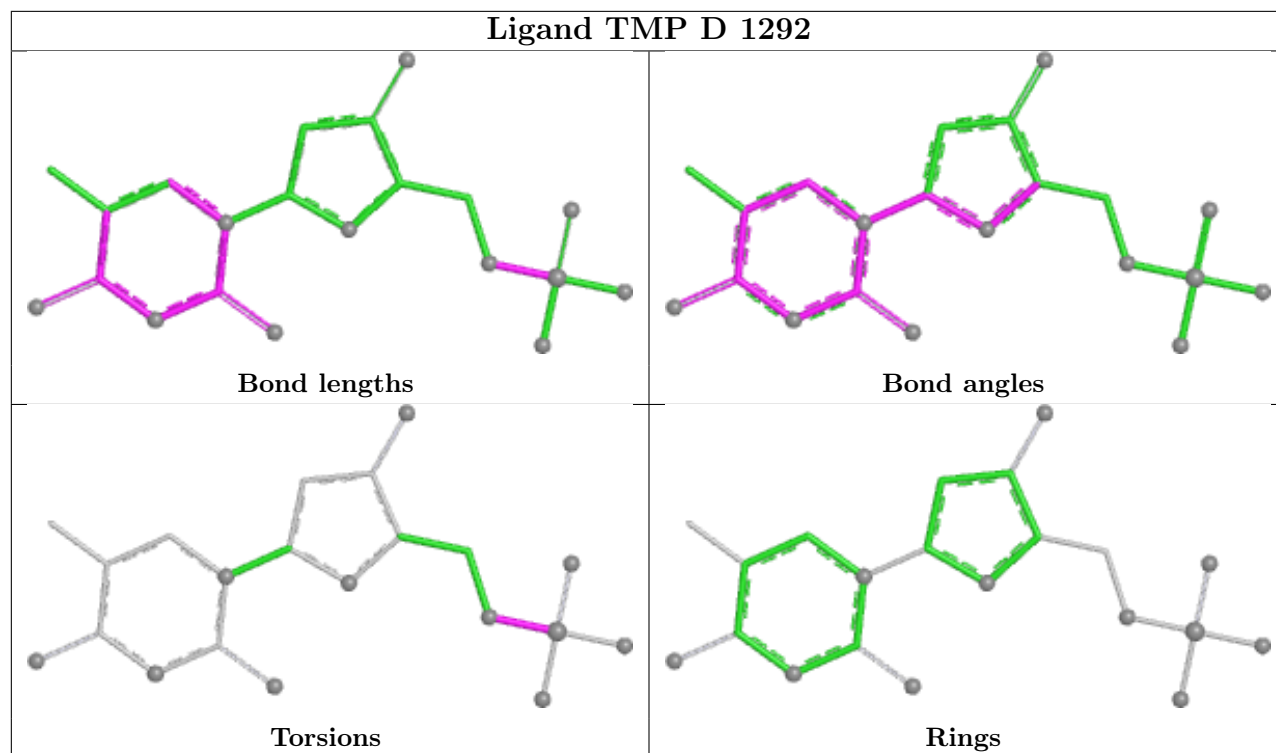
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1292	TMP	5	0
5	D	1292	TMP	1	0
5	B	1292	TMP	1	0
5	C	1293	TMP	2	0

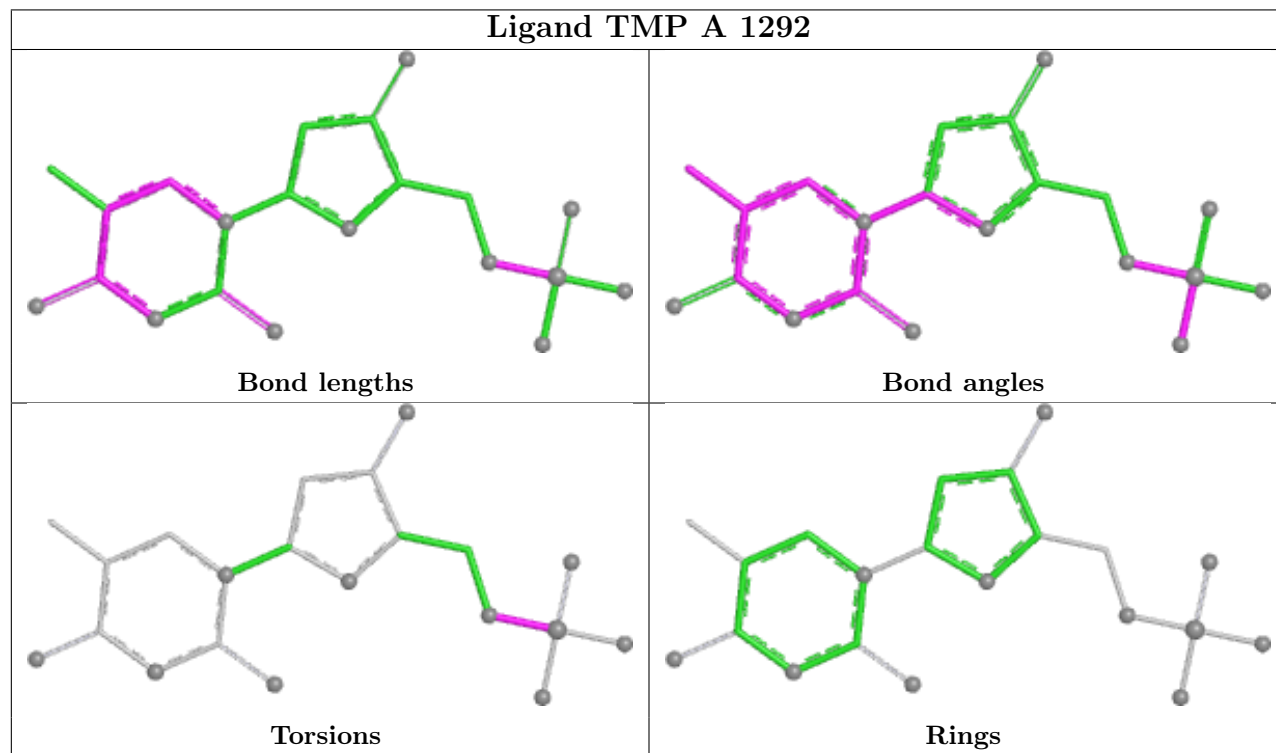
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



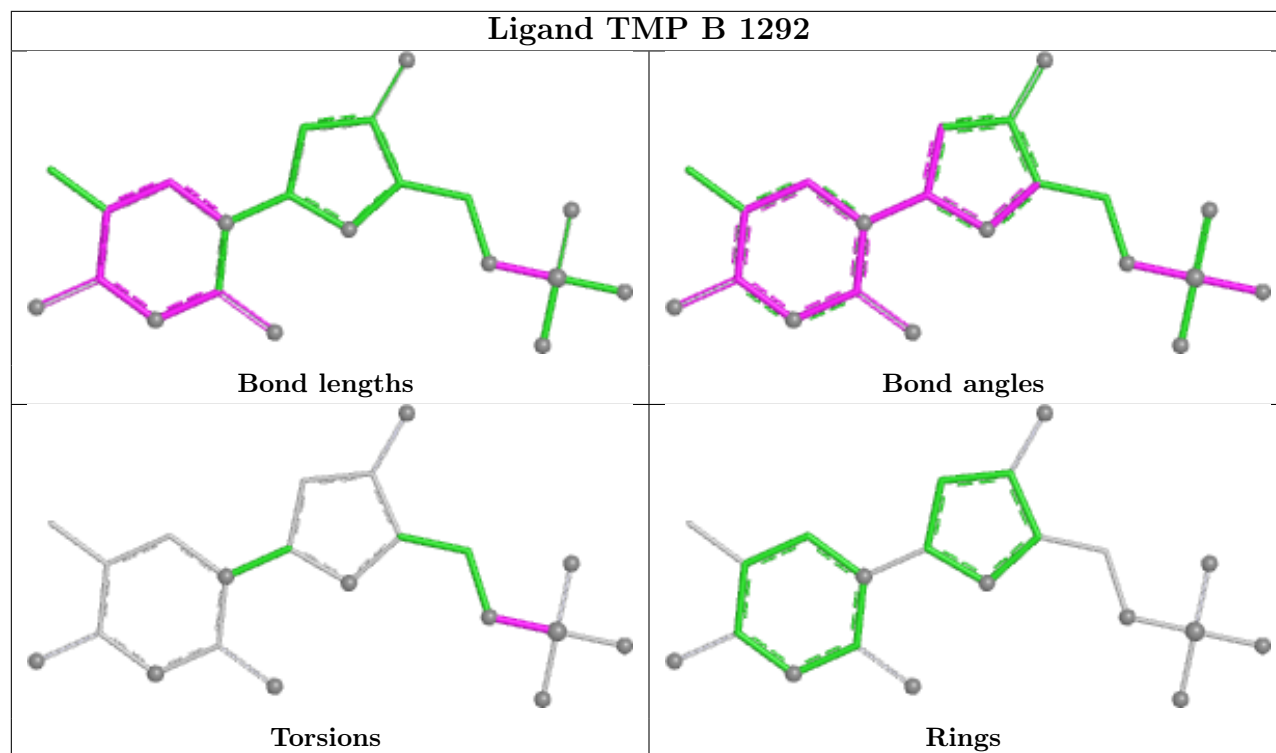
Ligand TMP D 1292



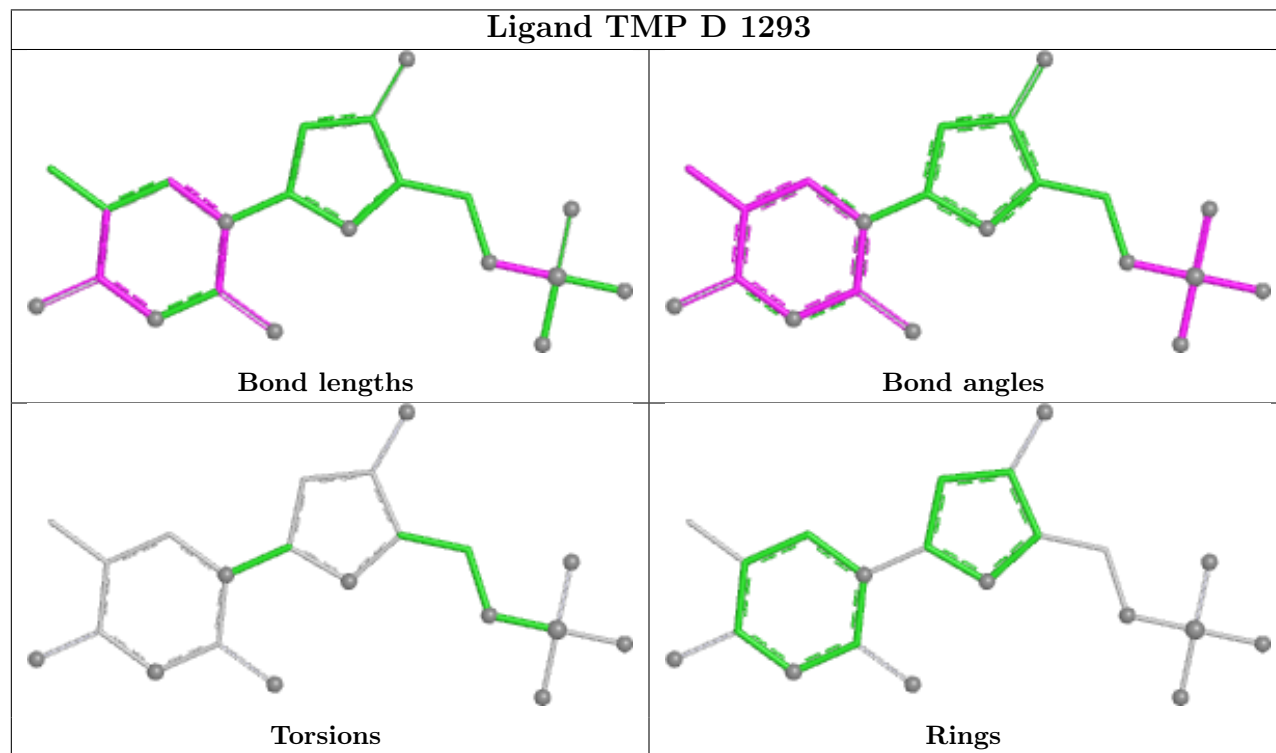
Ligand TMP A 1292



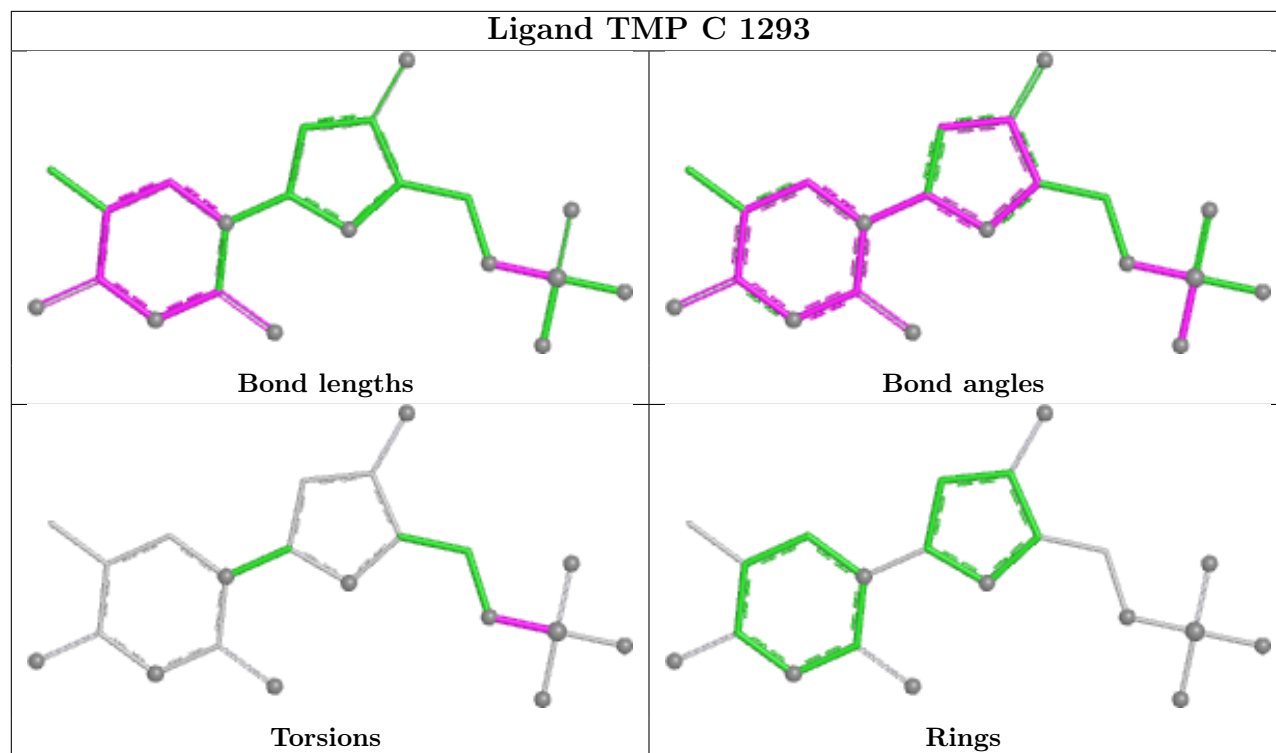
Ligand TMP B 1292



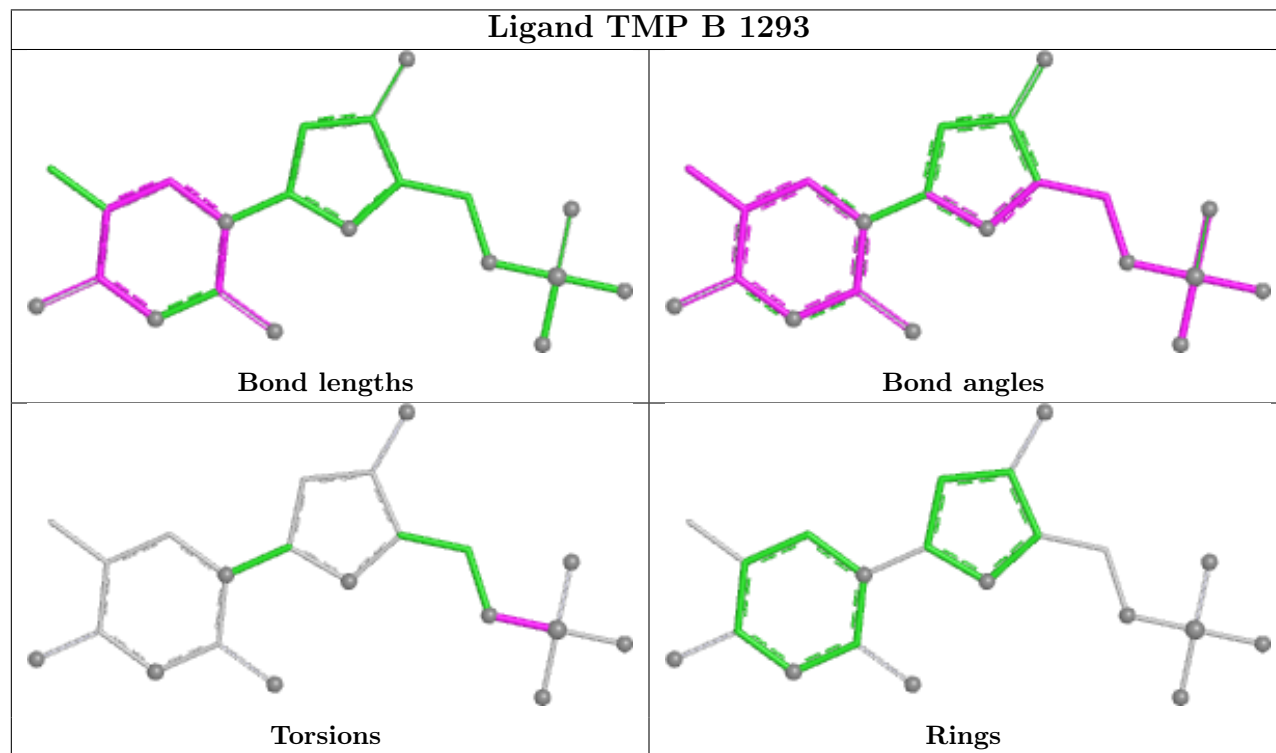
Ligand TMP D 1293

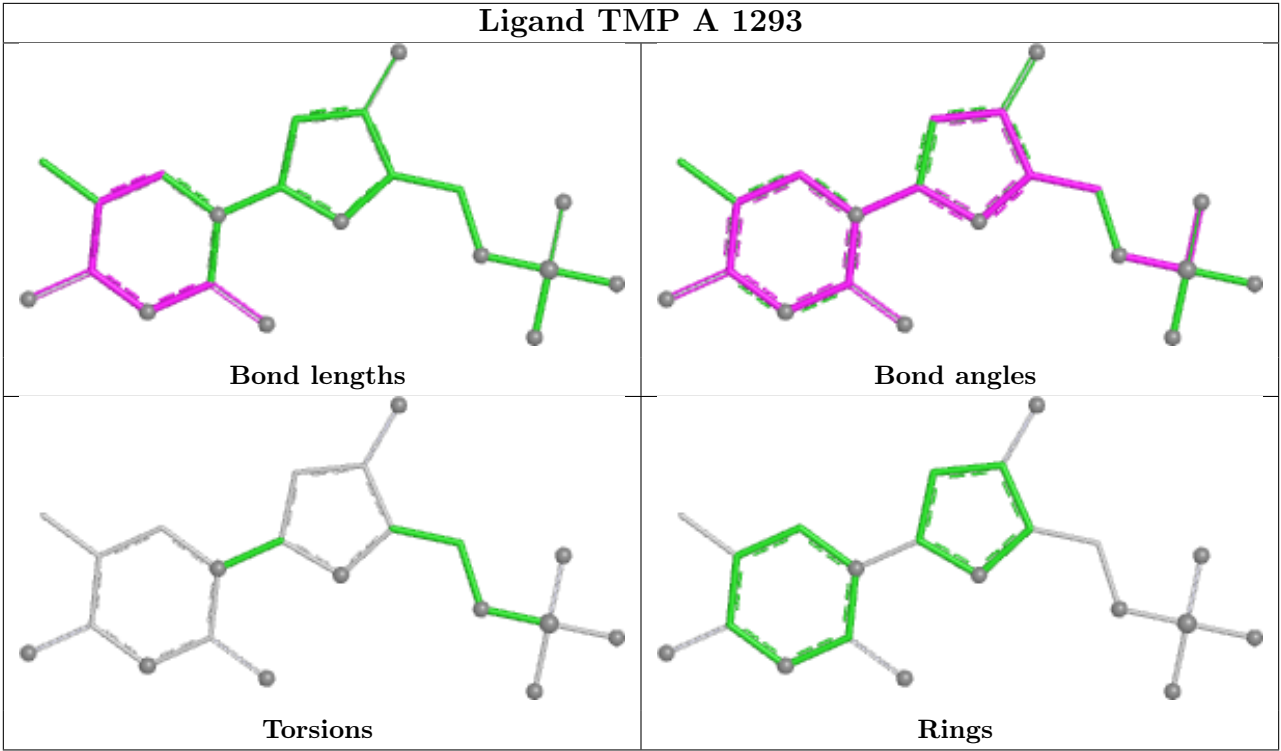


Ligand TMP C 1293



Ligand TMP B 1293





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1
4	D	1
1	A	1
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	290:LYS	C	291:ASP	N	1.98
1	D	290:LYS	C	291:ASP	N	1.89
1	A	290:LYS	C	291:ASP	N	1.70
1	B	290:LYS	C	291:ASP	N	0.88

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.