



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:34 PM EDT

PDB ID : 4BCK / pdb_00004bck
Title : Structure of CDK2 in complex with cyclin A and a 2-amino-4-heteroaryl-pyrimidine inhibitor
Authors : Hole, A.J.; Baumli, S.; Wang, S.; Endicott, J.A.; Noble, M.E.M.
Deposited on : 2012-10-02
Resolution : 2.05 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

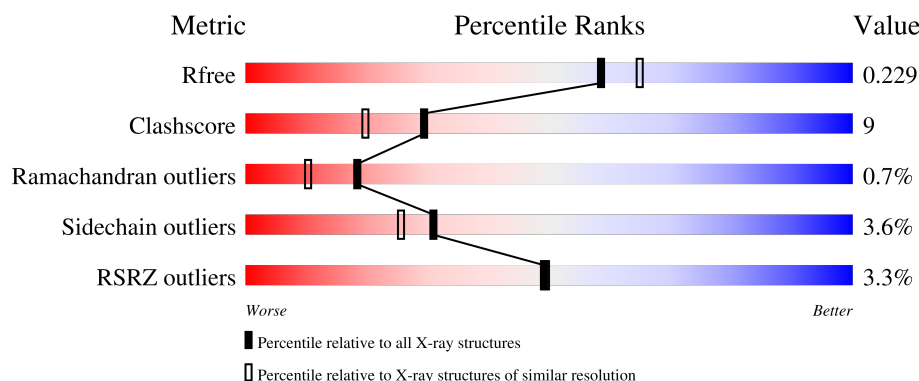
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	300	2% 78% 19% .
1	C	300	5% 77% 19% ..
2	B	262	87% 10% ..
2	D	262	5% 81% 12% ..

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
3	T3E	A	1298[C]	-	X	-	-
3	T3E	C	1295[C]	-	X	-	-
4	SGM	A	1299	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9877 atoms, of which 120 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 CYCLIN-DEPENDENT KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	P	S	0	1	0
			2410	1563	411	427	1	8			
1	C	294	Total	C	N	O	P	S	0	0	0
			2363	1534	399	421	1	8			

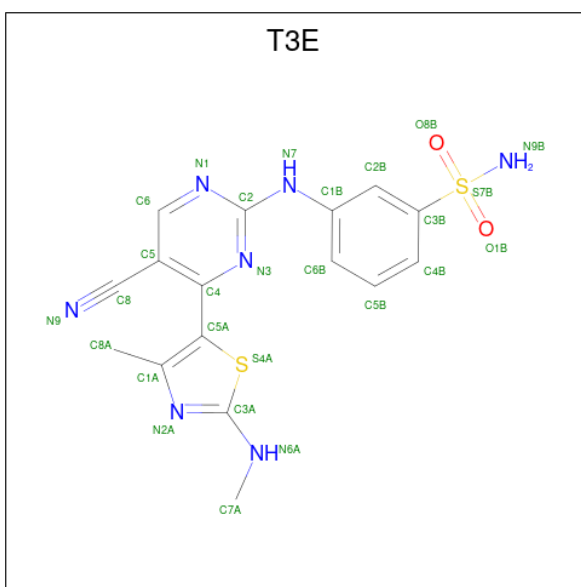
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
C	-1	GLY	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941

- Molecule 2 is a protein called CYCLIN-A2.

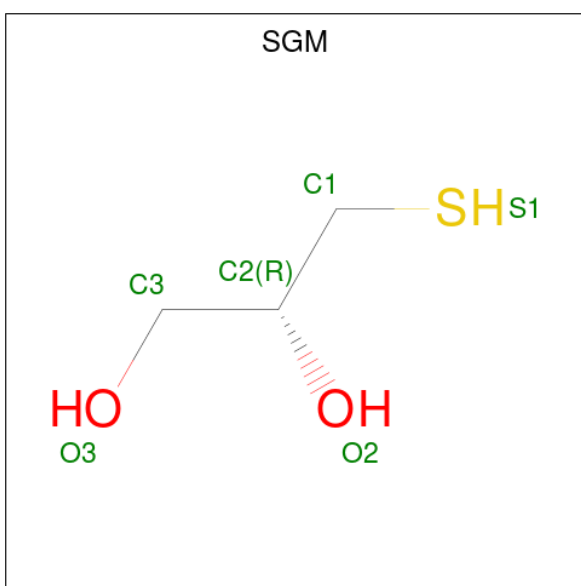
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	257	Total	C	N	O	S	0	1	0
			2082	1349	338	384	11			
2	D	253	Total	C	N	O	S	0	1	0
			2051	1330	333	377	11			

- Molecule 3 is 3-[[5-cyano-4-[4-methyl-2-(methylamino)-1,3-thiazol-5-yl]pyrimidin-2-yl]amino]benzenesulfonamide (CCD ID: T3E) (formula: C₁₆H₁₅N₇O₂S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	0	1
			168	64	60	28	8	8		
3	C	1	Total	C	H	N	O	S	0	1
			168	64	60	28	8	8		

- Molecule 4 is MONOTHIOGLYCEROL (CCD ID: SGM) (formula: $C_3H_8O_2S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			6	3	2	1		

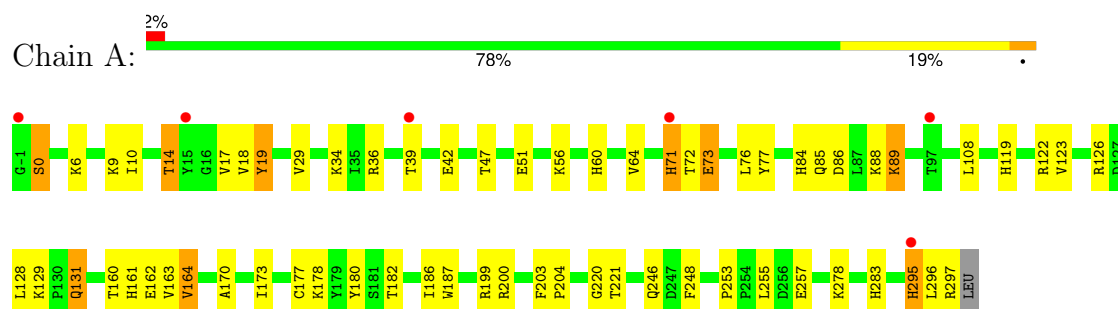
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	258	Total 258	O 258	0	0
5	B	208	Total 208	O 208	0	0
5	C	86	Total 86	O 86	0	0
5	D	77	Total 77	O 77	0	0

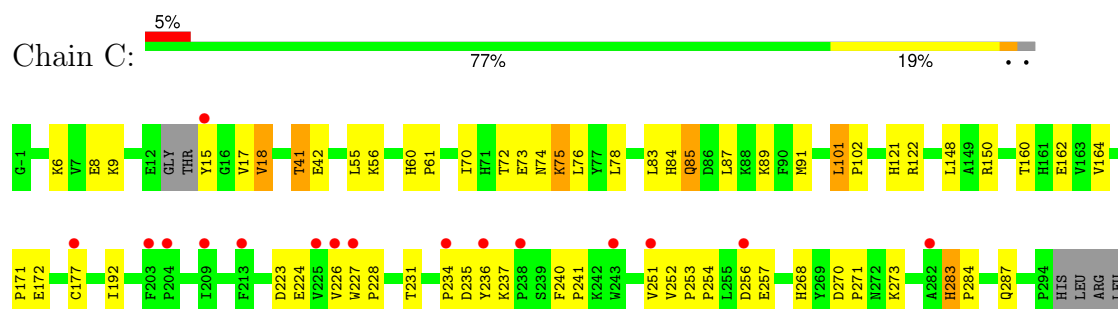
3 Residue-property plots

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.

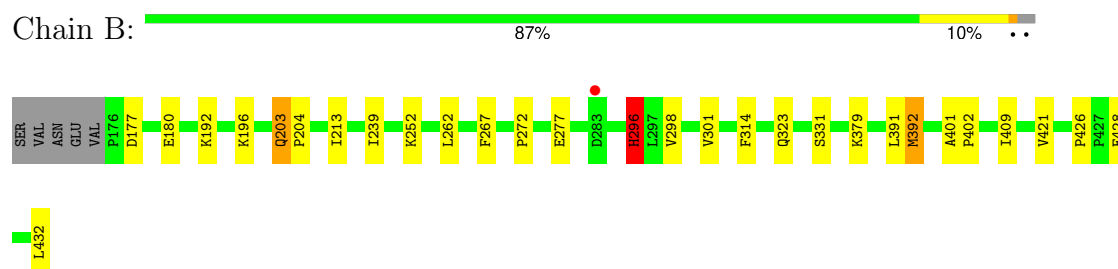
• Molecule 1: CYCLIN-DEPENDENT KINASE 2



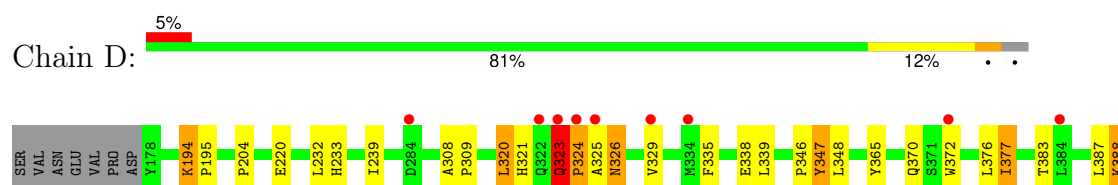
• Molecule 1: CYCLIN-DEPENDENT KINASE 2

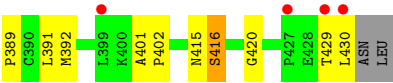


• Molecule 2: CYCLIN-A2



• Molecule 2: CYCLIN-A2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.20Å 140.37Å 155.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.86 – 2.05 29.86 – 2.05	Depositor EDS
% Data completeness (in resolution range)	96.1 (29.86-2.05) 96.0 (29.86-2.05)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.04Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.193 , 0.236 0.185 , 0.229	Depositor DCC
R_{free} test set	5083 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 86.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9877	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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: SGM, TPO, T3E

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	1.72	21/2464 (0.9%)	1.20	11/3342 (0.3%)
1	C	1.05	0/2411	1.11	8/3269 (0.2%)
2	B	1.66	12/2135 (0.6%)	1.19	8/2898 (0.3%)
2	D	0.97	0/2103	1.07	9/2854 (0.3%)
All	All	1.40	33/9113 (0.4%)	1.14	36/12363 (0.3%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	426	PRO	CA-C	7.50	1.56	1.51
1	A	204	PRO	CA-C	7.19	1.59	1.53
2	B	239	ILE	CA-CB	6.51	1.62	1.54
1	A	203	PHE	CA-C	6.06	1.59	1.52
1	A	182	THR	CA-CB	5.90	1.63	1.53
1	A	187	TRP	N-CA	5.66	1.53	1.46
1	A	180	TYR	CA-C	5.63	1.59	1.52
1	A	129	LYS	N-CA	5.51	1.51	1.46
1	A	173	ILE	CA-C	5.45	1.60	1.52
2	B	298	VAL	CA-CB	5.41	1.61	1.54
1	A	60	HIS	N-CA	5.41	1.51	1.46
1	A	119	HIS	CA-C	5.36	1.59	1.52
1	A	186	ILE	CA-C	5.34	1.59	1.52
2	B	267	PHE	N-CA	5.32	1.52	1.46
1	A	123	VAL	N-CA	5.30	1.52	1.46
2	B	262	LEU	N-CA	5.28	1.52	1.46
1	A	108	LEU	CA-C	5.27	1.59	1.52
1	A	126	ARG	CA-CB	5.26	1.61	1.53
1	A	29	VAL	CA-C	5.26	1.59	1.52
2	B	272	PRO	CA-C	5.26	1.57	1.52
1	A	51	GLU	CA-C	5.23	1.59	1.52
2	B	379	LYS	N-CA	5.22	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	314	PHE	CA-C	5.21	1.59	1.52
2	B	180	GLU	N-CA	5.11	1.52	1.46
1	A	278	LYS	CA-C	5.11	1.59	1.52
1	A	257	GLU	CA-C	5.09	1.59	1.52
1	A	221	THR	CA-C	5.09	1.58	1.52
1	A	283	HIS	N-CA	5.07	1.52	1.45
2	B	213	ILE	CA-C	5.07	1.59	1.52
1	A	128	LEU	CA-C	5.05	1.59	1.52
2	B	252	LYS	CA-C	5.05	1.59	1.52
1	A	164	VAL	CA-C	5.00	1.59	1.52
2	B	409	ILE	CA-C	5.00	1.59	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	177	ASP	N-CA-C	8.82	120.51	111.07
1	C	283	HIS	CA-C-N	8.47	129.30	119.47
1	C	283	HIS	C-N-CA	8.47	129.30	119.47
1	C	85	GLN	N-CA-C	7.45	118.39	107.88
2	D	194	LYS	CA-C-N	7.43	127.39	120.03
2	D	194	LYS	C-N-CA	7.43	127.39	120.03
2	D	347	TYR	N-CA-C	6.91	120.96	112.54
1	A	84	HIS	N-CA-C	6.81	119.72	111.82
1	A	170	ALA	N-CA-C	6.81	119.30	109.84
2	B	203	GLN	CA-C-N	6.73	126.52	119.05
2	B	203	GLN	C-N-CA	6.73	126.52	119.05
2	D	220	GLU	N-CA-C	6.37	118.22	111.28
1	A	10	ILE	CB-CA-C	-6.03	105.51	111.30
1	A	257	GLU	N-CA-C	5.81	117.28	111.07
1	C	18	VAL	N-CA-C	5.78	116.20	108.11
1	A	122	ARG	N-CA-C	5.75	119.35	111.54
1	A	123	VAL	N-CA-C	5.73	116.13	108.11
2	B	192	LYS	N-CA-C	5.63	118.36	111.82
2	D	239	ILE	N-CA-C	5.58	115.78	110.42
1	C	192	ILE	N-CA-C	5.49	116.27	110.72
2	D	372	TRP	CA-C-N	5.34	126.52	119.84
2	D	372	TRP	C-N-CA	5.34	126.52	119.84
2	D	388	LYS	CA-C-N	5.17	124.62	119.24
2	D	388	LYS	C-N-CA	5.17	124.62	119.24
2	B	421	VAL	N-CA-C	5.16	117.50	111.05
1	C	150	ARG	N-CA-C	5.16	116.91	109.07
2	B	296	HIS	N-CA-C	5.14	117.28	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	GLN	N-CA-C	5.14	118.39	110.42
2	B	331	SER	N-CA-C	5.14	116.88	111.28
1	A	73	GLU	CB-CA-C	-5.10	110.72	116.63
1	A	253	PRO	N-CA-C	5.02	116.83	110.70
1	A	220	GLY	CA-C-O	-5.01	117.88	122.24
1	A	131	GLN	N-CA-C	5.01	117.47	111.71
1	C	237	LYS	CA-C-N	5.00	124.67	119.56
1	C	237	LYS	C-N-CA	5.00	124.67	119.56
2	B	301	VAL	N-CA-C	5.00	115.72	110.62

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	2410	0	2453	52	0
1	C	2363	0	2404	53	0
2	B	2082	0	2105	14	0
2	D	2051	0	2076	33	0
3	A	108	60	60	8	0
3	C	108	60	60	12	0
4	A	6	0	8	7	0
5	A	258	0	0	6	0
5	B	208	0	0	2	0
5	C	86	0	0	2	0
5	D	77	0	0	4	0
All	All	9757	120	9166	156	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 9.

All (156) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:323:GLN:HB2	2:D:324:PRO:CD	1.71	1.16
2:D:429:THR:HG22	2:D:430:LEU:H	1.09	1.14
1:A:161[A]:HIS:CD2	1:A:162:GLU:HG3	1.82	1.14
2:D:323:GLN:CB	2:D:324:PRO:HD2	1.84	1.07
2:B:392:MET:HE2	2:B:392:MET:HA	1.47	0.95
1:A:6:LYS:HG3	5:A:2011:HOH:O	1.72	0.89
2:D:323:GLN:HB2	2:D:324:PRO:HD2	0.92	0.89
2:D:323:GLN:CB	2:D:324:PRO:CD	2.48	0.88
1:C:41:THR:HG22	1:C:42:GLU:N	1.89	0.88
1:A:0:SER:OG	1:A:72:THR:HG21	1.74	0.87
2:D:429:THR:HG22	2:D:430:LEU:N	1.90	0.86
1:A:9:LYS:HE2	1:A:17:VAL:CG2	2.09	0.83
1:C:251:VAL:HG12	1:C:252:VAL:HG23	1.61	0.81
2:D:323:GLN:H	2:D:323:GLN:CD	1.85	0.81
2:D:377:ILE:HD13	2:D:383:THR:HG22	1.63	0.81
2:D:429:THR:CG2	2:D:430:LEU:H	1.93	0.79
1:A:71:HIS:CE1	2:B:296:HIS:NE2	2.53	0.77
2:B:277[A]:GLU:OE1	5:B:2124:HOH:O	2.02	0.75
1:A:178:LYS:H	4:A:1299:SGM:H11	1.53	0.74
1:A:71:HIS:CE1	2:B:296:HIS:CD2	2.76	0.73
1:A:199:ARG:HH11	1:A:199:ARG:HG3	1.53	0.72
1:C:89:LYS:HE3	3:C:1295[A]:T3E:O1B	1.90	0.71
1:A:161[A]:HIS:NE2	1:A:162:GLU:HG3	2.05	0.71
1:A:9:LYS:CE	1:A:17:VAL:CG2	2.71	0.69
1:C:89:LYS:HE3	3:C:1295[B]:T3E:O1B	1.93	0.69
1:A:42:GLU:HG2	5:A:2035:HOH:O	1.94	0.68
1:C:85:GLN:HA	3:C:1295[B]:T3E:C5B	2.25	0.67
2:D:326:ASN:OD1	2:D:329:VAL:HG23	1.94	0.66
1:A:71:HIS:HE1	2:B:296:HIS:NE2	1.93	0.65
1:C:253:PRO:HD2	1:C:254:PRO:CD	2.28	0.64
1:C:284:PRO:O	1:C:287:GLN:HG2	1.99	0.63
1:C:60:HIS:ND1	1:C:61:PRO:HD2	2.13	0.63
1:A:19:TYR:N	1:A:19:TYR:CD1	2.67	0.62
1:A:9:LYS:CE	1:A:17:VAL:HG21	2.30	0.62
1:C:283:HIS:CG	1:C:284:PRO:HD2	2.34	0.62
1:C:253:PRO:HD2	1:C:254:PRO:HD3	1.79	0.62
1:C:60:HIS:CE1	1:C:61:PRO:HD2	2.35	0.61
1:A:9:LYS:HE3	1:A:17:VAL:HG21	1.82	0.61
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.35	0.61
2:D:326:ASN:HD21	2:D:329:VAL:CG2	2.12	0.61
2:B:392:MET:HA	2:B:392:MET:CE	2.28	0.61
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:ASP:HB3	5:C:2084:HOH:O	2.00	0.61
1:A:178:LYS:HB2	4:A:1299:SGM:C1	2.30	0.61
2:D:323:GLN:O	2:D:325:ALA:N	2.33	0.61
1:C:41:THR:HG22	1:C:42:GLU:H	1.66	0.60
1:C:256:ASP:CG	1:C:257:GLU:H	2.09	0.60
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.84	0.60
1:A:71:HIS:NE2	2:B:296:HIS:CD2	2.71	0.59
1:C:101:LEU:HD13	1:C:101:LEU:O	2.01	0.59
1:C:253:PRO:CD	1:C:254:PRO:HD3	2.32	0.59
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.33	0.58
1:C:223:ASP:H	1:C:226:VAL:HG12	1.67	0.58
2:D:321:HIS:HD2	2:D:376:LEU:HD23	1.69	0.58
1:A:88:LYS:HD2	1:A:131:GLN:NE2	2.20	0.57
1:A:71:HIS:NE2	2:B:296:HIS:HD2	2.02	0.57
1:A:88:LYS:HD2	1:A:131:GLN:HG3	1.86	0.57
1:C:9:LYS:HE2	1:C:17:VAL:CG1	2.34	0.57
1:A:88:LYS:HD2	1:A:131:GLN:HE21	1.71	0.56
2:D:338:GLU:N	5:D:2062:HOH:O	2.38	0.56
1:C:162:GLU:N	1:C:162:GLU:OE1	2.39	0.56
1:A:161[A]:HIS:NE2	1:A:162:GLU:CG	2.69	0.56
1:C:85:GLN:HA	3:C:1295[B]:T3E:H5B	1.87	0.56
1:C:72:THR:HG22	1:C:73:GLU:N	2.21	0.55
1:C:101:LEU:N	1:C:102:PRO:CD	2.70	0.55
1:C:41:THR:CG2	1:C:42:GLU:N	2.65	0.54
2:B:323:GLN:O	2:B:323:GLN:HG2	2.06	0.54
2:D:387:LEU:O	2:D:391:LEU:HB2	2.07	0.53
1:C:177:CYS:O	1:C:177:CYS:SG	2.67	0.53
1:A:178:LYS:HB2	4:A:1299:SGM:H11	1.89	0.53
3:C:1295[D]:T3E:C8A	3:C:1295[D]:T3E:C8	2.87	0.53
1:A:73:GLU:HA	1:A:73:GLU:OE1	2.09	0.53
1:C:253:PRO:CD	1:C:254:PRO:CD	2.86	0.52
2:D:365:TYR:CE2	2:D:430:LEU:HD23	2.44	0.52
1:C:42:GLU:HB3	5:C:2017:HOH:O	2.09	0.52
1:A:163:VAL:HA	5:A:2156:HOH:O	2.09	0.52
2:D:365:TYR:CE2	2:D:430:LEU:CD2	2.93	0.52
1:A:296:LEU:O	1:A:297:ARG:HB2	2.09	0.52
1:C:268:HIS:CE1	1:C:273:LYS:HB2	2.45	0.52
1:A:85:GLN:HG2	1:A:89:LYS:HZ3	1.75	0.51
1:A:177:CYS:HB3	4:A:1299:SGM:H32	1.91	0.51
1:A:71:HIS:CE1	1:A:76:LEU:HD13	2.45	0.51
1:A:178:LYS:N	4:A:1299:SGM:H11	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:HIS:CG	1:C:61:PRO:CD	2.94	0.51
1:A:9:LYS:HE2	1:A:17:VAL:HG22	1.91	0.51
2:D:401:ALA:HB3	2:D:402:PRO:HD3	1.93	0.50
1:C:85:GLN:HA	3:C:1295[A]:T3E:C5B	2.43	0.49
1:C:87:LEU:O	1:C:87:LEU:HG	2.12	0.49
1:A:34:LYS:HG3	1:A:77:TYR:CE1	2.48	0.49
3:A:1298[D]:T3E:C8A	3:A:1298[D]:T3E:C8	2.91	0.49
1:C:72:THR:HG22	1:C:74:ASN:H	1.78	0.48
1:C:121:HIS:O	1:C:122:ARG:HG3	2.13	0.48
1:C:171:PRO:HD2	1:C:172:GLU:OE1	2.13	0.48
1:C:172:GLU:O	1:C:177:CYS:HB3	2.13	0.48
2:D:321:HIS:CD2	2:D:376:LEU:HD23	2.48	0.48
1:C:83:LEU:O	3:C:1295[B]:T3E:H6B	2.13	0.48
2:D:233:HIS:HE1	5:D:2035:HOH:O	1.96	0.48
1:A:178:LYS:H	4:A:1299:SGM:C1	2.25	0.47
1:C:84:HIS:O	1:C:85:GLN:HB3	2.14	0.47
1:C:256:ASP:CG	1:C:257:GLU:N	2.72	0.47
2:D:338:GLU:HB2	5:D:2062:HOH:O	2.14	0.47
1:A:199:ARG:HG3	1:A:199:ARG:NH1	2.25	0.47
1:C:18:VAL:HG21	3:C:1295[D]:T3E:N2A	2.30	0.47
3:C:1295[D]:T3E:H6B	3:C:1295[D]:T3E:N3	2.30	0.47
1:A:161[A]:HIS:CG	1:A:162:GLU:N	2.82	0.46
2:D:320:LEU:HD12	2:D:320:LEU:HA	1.53	0.46
2:D:323:GLN:O	2:D:324:PRO:C	2.56	0.46
1:C:253:PRO:HD2	1:C:254:PRO:HD2	1.96	0.46
3:A:1298[B]:T3E:N9	3:A:1298[B]:T3E:H8A2	2.30	0.46
1:C:224:GLU:HG2	1:C:231:THR:HG23	1.98	0.45
3:C:1295[D]:T3E:C8	3:C:1295[D]:T3E:H8A1	2.47	0.45
2:D:415:ASN:OD1	2:D:416:SER:N	2.50	0.45
1:C:121:HIS:C	1:C:122:ARG:HG3	2.42	0.45
2:D:323:GLN:CD	2:D:323:GLN:N	2.63	0.45
1:A:18:VAL:HG21	3:A:1298[D]:T3E:N2A	2.31	0.44
1:A:86:ASP:H	1:A:89:LYS:HZ2	1.65	0.44
1:A:85:GLN:CG	1:A:89:LYS:HZ3	2.30	0.44
2:B:401:ALA:N	2:B:402:PRO:CD	2.80	0.44
1:C:87:LEU:O	1:C:91:MET:HG3	2.17	0.44
1:C:234:PRO:C	1:C:236:TYR:H	2.25	0.44
3:C:1295[D]:T3E:N3	3:C:1295[D]:T3E:C6B	2.80	0.44
2:B:203:GLN:HA	2:B:204:PRO:HD3	1.84	0.44
1:C:75:LYS:HB2	1:C:75:LYS:HE2	1.69	0.44
3:A:1298[D]:T3E:H6B	3:A:1298[D]:T3E:N3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:321:HIS:HD2	2:D:376:LEU:CD2	2.31	0.43
1:A:0:SER:CB	1:A:72:THR:HG21	2.49	0.43
1:A:19:TYR:N	1:A:19:TYR:HD1	2.16	0.43
1:A:199:ARG:HH11	1:A:199:ARG:CG	2.26	0.43
3:A:1298[B]:T3E:C8A	3:A:1298[B]:T3E:C8	2.97	0.43
1:A:295:HIS:ND1	1:A:295:HIS:N	2.55	0.43
1:A:47:THR:HG23	5:A:2019:HOH:O	2.18	0.43
1:A:85:GLN:HA	3:A:1298[B]:T3E:H5B	2.00	0.43
2:B:392:MET:HE2	2:B:392:MET:CA	2.33	0.43
1:A:200:ARG:NH2	5:A:2186:HOH:O	2.52	0.42
1:C:226:VAL:HG13	1:C:227:TRP:N	2.35	0.42
2:B:391:LEU:HD23	2:B:432:LEU:HD11	2.00	0.42
1:C:240:PHE:HA	1:C:241:PRO:HD3	1.88	0.42
1:C:270:ASP:O	1:C:271:PRO:C	2.61	0.42
1:A:163:VAL:H	1:A:163:VAL:HG22	1.59	0.42
1:C:72:THR:CG2	1:C:73:GLU:N	2.82	0.42
2:B:196:LYS:HG3	5:B:2066:HOH:O	2.20	0.41
1:A:64:VAL:O	1:A:64:VAL:HG13	2.20	0.41
2:D:335:PHE:CZ	2:D:339:LEU:HD11	2.55	0.41
1:C:224:GLU:HG2	1:C:231:THR:CG2	2.51	0.41
2:D:194:LYS:HA	2:D:195:PRO:HD3	1.88	0.41
2:D:204:PRO:HD2	5:D:2019:HOH:O	2.19	0.41
1:A:88:LYS:HD2	1:A:131:GLN:CG	2.50	0.41
3:C:1295[C]:T3E:H6B	3:C:1295[C]:T3E:N3	2.34	0.41
2:D:346:PRO:HD2	2:D:347:TYR:CD2	2.55	0.41
1:A:89:LYS:HE3	3:A:1298[B]:T3E:H4B	2.03	0.41
1:A:18:VAL:HG21	3:A:1298[D]:T3E:C3A	2.51	0.41
2:D:308:ALA:HA	2:D:309:PRO:HD3	1.95	0.41
1:A:6:LYS:NZ	5:A:2011:HOH:O	2.23	0.40
1:C:234:PRO:O	1:C:236:TYR:N	2.54	0.40
2:D:326:ASN:HD21	2:D:329:VAL:HB	1.86	0.40
1:A:177:CYS:CB	4:A:1299:SGM:H32	2.50	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	297/300 (99%)	286 (96%)	9 (3%)	2 (1%)	18	10
1	C	289/300 (96%)	274 (95%)	12 (4%)	3 (1%)	12	5
2	B	256/262 (98%)	254 (99%)	2 (1%)	0	100	100
2	D	252/262 (96%)	243 (96%)	6 (2%)	3 (1%)	10	4
All	All	1094/1124 (97%)	1057 (97%)	29 (3%)	8 (1%)	18	10

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	323	GLN
1	A	14	THR
1	A	164	VAL
1	C	164	VAL
2	D	324	PRO
1	C	235	ASP
1	C	228	PRO
2	D	420	GLY

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	263/263 (100%)	252 (96%)	11 (4%)	26	20
1	C	258/263 (98%)	246 (95%)	12 (5%)	23	16
2	B	232/236 (98%)	229 (99%)	3 (1%)	61	62
2	D	228/236 (97%)	219 (96%)	9 (4%)	28	23
All	All	981/998 (98%)	946 (96%)	35 (4%)	31	25

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	14	THR
1	A	19	TYR
1	A	36	ARG
1	A	39	THR
1	A	56	LYS
1	A	71	HIS
1	A	89	LYS
1	A	248	PHE
1	A	255	LEU
1	A	295	HIS
2	B	296	HIS
2	B	392	MET
2	B	428	GLU
1	C	6	LYS
1	C	8	GLU
1	C	15	TYR
1	C	41	THR
1	C	55	LEU
1	C	56	LYS
1	C	70	ILE
1	C	75	LYS
1	C	76	LEU
1	C	78	LEU
1	C	101	LEU
1	C	148	LEU
2	D	232	LEU
2	D	320	LEU
2	D	323	GLN
2	D	326	ASN
2	D	348	LEU
2	D	370	GLN
2	D	377	ILE
2	D	392	MET
2	D	416	SER

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

Mol	Chain	Res	Type
1	A	71	HIS
2	B	208	ASN
2	B	254	GLN
1	C	3	ASN

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Mol	Chain	Res	Type
2	D	321	HIS
2	D	322	GLN
2	D	326	ASN
2	D	403	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	TPO	C	160	1	8,10,11	1.28	1 (12%)	10,14,16	1.22	1 (10%)
1	TPO	A	160	1	8,10,11	2.51	2 (25%)	10,14,16	1.36	2 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	C	160	1	-	1/9/11/13	-
1	TPO	A	160	1	-	1/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TPO	P-OG1	6.02	1.70	1.59
1	C	160	TPO	P-OG1	2.62	1.64	1.59
1	A	160	TPO	CA-N	2.17	1.54	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	TPO	O-C-CA	-2.81	117.55	124.77
1	A	160	TPO	CG2-CB-CA	-2.58	108.24	113.26
1	C	160	TPO	OG1-P-O1P	-2.03	102.08	109.33

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	160	TPO	O-C-CA-CB
1	A	160	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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
3	T3E	C	1295[D]	-	27,29,29	2.97	11 (40%)	37,42,42	4.02	15 (40%)
3	T3E	C	1295[B]	-	27,29,29	3.17	12 (44%)	37,42,42	4.47	17 (45%)
3	T3E	C	1295[A]	-	27,29,29	3.08	11 (40%)	37,42,42	4.36	17 (45%)
4	SGM	A	1299	-	5,5,5	0.99	0	5,5,5	1.47	0
3	T3E	A	1298[D]	-	27,29,29	2.94	9 (33%)	37,42,42	3.95	15 (40%)
3	T3E	A	1298[B]	-	27,29,29	3.08	12 (44%)	37,42,42	4.11	15 (40%)
3	T3E	A	1298[C]	-	27,29,29	3.08	11 (40%)	37,42,42	4.30	19 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	T3E	A	1298[A]	-	27,29,29	3.07	10 (37%)	37,42,42	4.37	17 (45%)
3	T3E	C	1295[C]	-	27,29,29	3.07	11 (40%)	37,42,42	4.40	18 (48%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	T3E	C	1295[D]	-	-	8/17/18/18	0/3/3/3
3	T3E	C	1295[B]	-	-	7/17/18/18	0/3/3/3
3	T3E	C	1295[A]	-	-	4/17/18/18	0/3/3/3
4	SGM	A	1299	-	-	2/4/4/4	-
3	T3E	A	1298[D]	-	-	7/17/18/18	0/3/3/3
3	T3E	A	1298[B]	-	-	4/17/18/18	0/3/3/3
3	T3E	A	1298[C]	-	-	9/17/18/18	0/3/3/3
3	T3E	A	1298[A]	-	-	2/17/18/18	0/3/3/3
3	T3E	C	1295[C]	-	-	9/17/18/18	0/3/3/3

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1295[B]	T3E	C3A-N6A	7.42	1.45	1.34
3	C	1295[C]	T3E	C3A-N6A	7.13	1.45	1.34
3	A	1298[A]	T3E	C3A-N6A	6.86	1.44	1.34
3	A	1298[D]	T3E	C3A-N6A	6.80	1.44	1.34
3	C	1295[A]	T3E	C3A-N6A	6.76	1.44	1.34
3	A	1298[C]	T3E	C3A-N6A	6.71	1.44	1.34
3	C	1295[D]	T3E	C3A-S4A	-6.55	1.62	1.73
3	C	1295[A]	T3E	C3A-S4A	-6.46	1.63	1.73
3	C	1295[D]	T3E	C3A-N6A	6.35	1.43	1.34
3	A	1298[A]	T3E	C3A-S4A	-6.26	1.63	1.73
3	A	1298[C]	T3E	C3A-S4A	-6.25	1.63	1.73
3	A	1298[B]	T3E	C3A-N2A	6.19	1.40	1.31
3	C	1295[B]	T3E	C3A-S4A	-6.11	1.63	1.73
3	C	1295[C]	T3E	C3A-S4A	-6.06	1.63	1.73
3	A	1298[B]	T3E	C3A-N6A	6.03	1.43	1.34
3	C	1295[B]	T3E	C3A-N2A	5.98	1.40	1.31
3	A	1298[D]	T3E	C3A-N2A	5.91	1.40	1.31
3	A	1298[C]	T3E	C3A-N2A	5.84	1.40	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1295[C]	T3E	C3A-N2A	5.81	1.40	1.31
3	A	1298[D]	T3E	C3A-S4A	-5.77	1.64	1.73
3	A	1298[A]	T3E	C3A-N2A	5.73	1.40	1.31
3	A	1298[B]	T3E	C3A-S4A	-5.70	1.64	1.73
3	C	1295[A]	T3E	C3A-N2A	5.66	1.40	1.31
3	C	1295[D]	T3E	C4-C5A	5.57	1.54	1.46
3	C	1295[B]	T3E	C1A-N2A	5.57	1.49	1.38
3	C	1295[D]	T3E	C3A-N2A	5.55	1.39	1.31
3	A	1298[C]	T3E	C5A-S4A	-5.46	1.60	1.74
3	A	1298[B]	T3E	C1A-N2A	5.46	1.49	1.38
3	C	1295[A]	T3E	C1A-N2A	5.41	1.48	1.38
3	A	1298[A]	T3E	C1A-N2A	5.36	1.48	1.38
3	A	1298[A]	T3E	C5A-S4A	-5.33	1.61	1.74
3	A	1298[C]	T3E	C1A-N2A	5.30	1.48	1.38
3	C	1295[C]	T3E	C5A-S4A	-5.27	1.61	1.74
3	C	1295[C]	T3E	C1A-N2A	5.26	1.48	1.38
3	A	1298[D]	T3E	C4-C5A	5.23	1.53	1.46
3	C	1295[B]	T3E	C5A-S4A	-5.20	1.61	1.74
3	C	1295[D]	T3E	C1A-N2A	5.07	1.48	1.38
3	C	1295[A]	T3E	C4-C5A	5.01	1.53	1.46
3	A	1298[D]	T3E	C1A-N2A	4.97	1.48	1.38
3	A	1298[B]	T3E	C5A-S4A	-4.89	1.62	1.74
3	C	1295[A]	T3E	C5A-S4A	-4.88	1.62	1.74
3	A	1298[B]	T3E	C4-C5A	4.79	1.53	1.46
3	A	1298[C]	T3E	C2-N7	4.57	1.46	1.36
3	A	1298[B]	T3E	C2-N7	4.56	1.46	1.36
3	C	1295[B]	T3E	C2-N7	4.54	1.46	1.36
3	A	1298[A]	T3E	C2-N7	4.52	1.46	1.36
3	C	1295[B]	T3E	C4-C5A	4.47	1.52	1.46
3	C	1295[C]	T3E	C2-N7	4.45	1.45	1.36
3	C	1295[A]	T3E	C2-N7	4.30	1.45	1.36
3	C	1295[C]	T3E	C4-C5A	4.26	1.52	1.46
3	A	1298[A]	T3E	C4-C5A	4.18	1.52	1.46
3	A	1298[C]	T3E	C5-C8	4.17	1.50	1.44
3	A	1298[A]	T3E	C5-C8	4.08	1.50	1.44
3	C	1295[D]	T3E	C2-N7	4.04	1.45	1.36
3	A	1298[B]	T3E	C5-C8	4.01	1.50	1.44
3	A	1298[C]	T3E	C4-C5A	3.95	1.52	1.46
3	C	1295[C]	T3E	C5-C8	3.94	1.50	1.44
3	C	1295[D]	T3E	C5A-S4A	-3.93	1.64	1.74
3	C	1295[D]	T3E	C5-C8	3.87	1.50	1.44
3	A	1298[D]	T3E	C2-N7	3.84	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1295[B]	T3E	C5-C8	3.82	1.49	1.44
3	C	1295[A]	T3E	C5-C8	3.81	1.49	1.44
3	A	1298[D]	T3E	C5-C8	3.77	1.49	1.44
3	A	1298[D]	T3E	C5A-S4A	-3.49	1.65	1.74
3	A	1298[B]	T3E	C1B-N7	2.87	1.47	1.40
3	C	1295[B]	T3E	C1B-N7	2.50	1.46	1.40
3	A	1298[D]	T3E	C1B-N7	2.49	1.46	1.40
3	A	1298[C]	T3E	C1B-N7	2.45	1.46	1.40
3	A	1298[A]	T3E	C1B-N7	2.45	1.46	1.40
3	C	1295[A]	T3E	C1B-N7	2.40	1.46	1.40
3	C	1295[B]	T3E	S7B-N9B	2.39	1.65	1.60
3	A	1298[C]	T3E	C6-C5	-2.38	1.37	1.40
3	C	1295[C]	T3E	C1B-N7	2.33	1.45	1.40
3	C	1295[A]	T3E	S7B-N9B	2.31	1.65	1.60
3	C	1295[B]	T3E	C2-N1	2.29	1.37	1.34
3	C	1295[D]	T3E	C6-C5	-2.29	1.37	1.40
3	C	1295[C]	T3E	C6-C5	-2.28	1.37	1.40
3	C	1295[B]	T3E	C6-C5	-2.25	1.37	1.40
3	A	1298[B]	T3E	S7B-N9B	2.18	1.64	1.60
3	A	1298[B]	T3E	C2B-C3B	2.18	1.42	1.39
3	A	1298[B]	T3E	C2-N1	2.16	1.37	1.34
3	A	1298[A]	T3E	S7B-N9B	2.15	1.64	1.60
3	C	1295[C]	T3E	S7B-N9B	2.11	1.64	1.60
3	C	1295[D]	T3E	C1B-N7	2.10	1.45	1.40
3	A	1298[C]	T3E	S7B-N9B	2.10	1.64	1.60
3	C	1295[A]	T3E	C6-C5	-2.09	1.37	1.40
3	C	1295[D]	T3E	S7B-N9B	2.07	1.64	1.60

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1295[B]	T3E	C3A-S4A-C5A	20.50	101.11	88.35
3	C	1295[A]	T3E	C3A-S4A-C5A	20.17	100.91	88.35
3	C	1295[C]	T3E	C3A-S4A-C5A	20.14	100.89	88.35
3	A	1298[A]	T3E	C3A-S4A-C5A	20.02	100.82	88.35
3	A	1298[C]	T3E	C3A-S4A-C5A	19.35	100.40	88.35
3	A	1298[B]	T3E	C3A-S4A-C5A	18.29	99.74	88.35
3	C	1295[D]	T3E	C3A-S4A-C5A	17.88	99.48	88.35
3	A	1298[D]	T3E	C3A-S4A-C5A	16.67	98.73	88.35
3	C	1295[B]	T3E	S4A-C3A-N2A	-8.47	108.20	115.78
3	C	1295[C]	T3E	S4A-C3A-N2A	-8.34	108.32	115.78
3	A	1298[A]	T3E	S4A-C3A-N2A	-7.95	108.67	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1295[A]	T3E	S4A-C3A-N2A	-7.91	108.71	115.78
3	C	1295[D]	T3E	C5A-C1A-N2A	-7.61	109.70	115.01
3	A	1298[C]	T3E	S4A-C3A-N2A	-7.54	109.03	115.78
3	A	1298[D]	T3E	C5A-C1A-N2A	-7.29	109.92	115.01
3	A	1298[B]	T3E	O1B-S7B-O8B	-7.25	107.65	118.80
3	A	1298[A]	T3E	N1-C2-N3	-7.18	119.48	126.42
3	A	1298[C]	T3E	N1-C2-N3	-7.06	119.59	126.42
3	C	1295[B]	T3E	N1-C2-N3	-7.05	119.60	126.42
3	C	1295[B]	T3E	C5A-C1A-N2A	-6.97	110.14	115.01
3	A	1298[A]	T3E	C5A-C1A-N2A	-6.95	110.16	115.01
3	A	1298[C]	T3E	C5A-C1A-N2A	-6.91	110.19	115.01
3	C	1295[C]	T3E	C5A-C1A-N2A	-6.86	110.22	115.01
3	C	1295[A]	T3E	C5A-C1A-N2A	-6.82	110.25	115.01
3	C	1295[C]	T3E	N1-C2-N3	-6.77	119.87	126.42
3	A	1298[B]	T3E	N1-C2-N3	-6.71	119.94	126.42
3	C	1295[D]	T3E	S4A-C3A-N2A	-6.65	109.83	115.78
3	C	1295[B]	T3E	O1B-S7B-O8B	-6.54	108.75	118.80
3	A	1298[D]	T3E	S4A-C3A-N2A	-6.52	109.94	115.78
3	A	1298[B]	T3E	S4A-C3A-N2A	-6.51	109.96	115.78
3	C	1295[A]	T3E	O1B-S7B-O8B	-6.46	108.86	118.80
3	A	1298[B]	T3E	C5A-C1A-N2A	-6.30	110.61	115.01
3	C	1295[A]	T3E	N1-C2-N3	-6.13	120.50	126.42
3	A	1298[A]	T3E	O1B-S7B-O8B	-6.08	109.44	118.80
3	A	1298[C]	T3E	O1B-S7B-O8B	-5.88	109.75	118.80
3	C	1295[C]	T3E	O1B-S7B-O8B	-5.87	109.77	118.80
3	A	1298[D]	T3E	O1B-S7B-O8B	-5.84	109.81	118.80
3	A	1298[D]	T3E	N1-C2-N3	-5.78	120.83	126.42
3	C	1295[D]	T3E	O1B-S7B-O8B	-5.52	110.30	118.80
3	C	1295[D]	T3E	N1-C2-N3	-5.00	121.59	126.42
3	C	1295[D]	T3E	C1B-N7-C2	-4.69	116.74	129.38
3	A	1298[D]	T3E	C4-N3-C2	4.22	122.53	117.26
3	A	1298[D]	T3E	C7A-N6A-C3A	-3.80	117.33	123.31
3	C	1295[D]	T3E	C7A-N6A-C3A	-3.74	117.43	123.31
3	A	1298[B]	T3E	C5A-C4-N3	3.70	120.66	114.42
3	A	1298[B]	T3E	C4-N3-C2	3.60	121.75	117.26
3	A	1298[D]	T3E	C1B-N7-C2	-3.53	119.86	129.38
3	A	1298[D]	T3E	C4-C5A-C1A	-3.51	126.96	132.23
3	A	1298[C]	T3E	C4-C5A-C1A	-3.50	126.98	132.23
3	A	1298[A]	T3E	C4-N3-C2	3.48	121.60	117.26
3	A	1298[A]	T3E	C1B-N7-C2	-3.46	120.05	129.38
3	A	1298[B]	T3E	O8B-S7B-C3B	3.45	111.24	107.35
3	A	1298[D]	T3E	S4A-C3A-N6A	3.44	127.89	121.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1298[C]	T3E	C5A-C4-N3	3.38	120.11	114.42
3	A	1298[C]	T3E	C6-N1-C2	3.37	120.43	115.81
3	C	1295[C]	T3E	C1B-N7-C2	-3.30	120.47	129.38
3	A	1298[C]	T3E	C4-C5A-S4A	3.30	123.94	118.21
3	A	1298[D]	T3E	C4-C5A-S4A	3.27	123.90	118.21
3	C	1295[C]	T3E	C4-C5A-S4A	3.23	123.81	118.21
3	C	1295[D]	T3E	C6-C5-C8	-3.21	111.84	118.87
3	C	1295[B]	T3E	C4-N3-C2	3.20	121.25	117.26
3	C	1295[A]	T3E	C4-N3-C2	3.16	121.20	117.26
3	C	1295[D]	T3E	C4-N3-C2	3.12	121.15	117.26
3	C	1295[C]	T3E	C4-C5A-C1A	-3.11	127.57	132.23
3	C	1295[D]	T3E	C3A-N2A-C1A	3.08	112.26	110.38
3	A	1298[D]	T3E	C3A-N2A-C1A	3.07	112.25	110.38
3	A	1298[C]	T3E	O8B-S7B-C3B	3.01	110.75	107.35
3	C	1295[C]	T3E	C6-N1-C2	2.99	119.91	115.81
3	A	1298[B]	T3E	O1B-S7B-N9B	2.99	111.67	107.35
3	A	1298[D]	T3E	O8B-S7B-C3B	2.96	110.70	107.35
3	C	1295[A]	T3E	C4-C5A-S4A	2.95	123.33	118.21
3	C	1295[B]	T3E	C6-N1-C2	2.92	119.82	115.81
3	C	1295[A]	T3E	C1B-N7-C2	-2.91	121.54	129.38
3	C	1295[C]	T3E	S4A-C3A-N6A	2.90	126.82	121.11
3	A	1298[A]	T3E	C6-N1-C2	2.86	119.73	115.81
3	C	1295[A]	T3E	O1B-S7B-C3B	2.83	110.55	107.35
3	A	1298[B]	T3E	C7A-N6A-C3A	-2.82	118.88	123.31
3	C	1295[B]	T3E	C4-C5A-S4A	2.80	123.07	118.21
3	C	1295[D]	T3E	C4-C5A-S4A	2.79	123.06	118.21
3	C	1295[A]	T3E	C1A-C5A-S4A	-2.74	108.24	109.91
3	C	1295[C]	T3E	C4-N3-C2	2.72	120.65	117.26
3	C	1295[B]	T3E	O1B-S7B-N9B	2.70	111.25	107.35
3	C	1295[B]	T3E	O1B-S7B-C3B	2.70	110.40	107.35
3	A	1298[D]	T3E	C1B-C2B-C3B	2.69	120.91	118.84
3	C	1295[D]	T3E	C4-C5A-C1A	-2.68	128.22	132.23
3	A	1298[A]	T3E	O8B-S7B-C3B	2.65	110.35	107.35
3	A	1298[B]	T3E	C6-N1-C2	2.64	119.43	115.81
3	C	1295[B]	T3E	C8A-C1A-N2A	2.63	124.58	119.32
3	A	1298[C]	T3E	C1B-C2B-C3B	2.62	120.86	118.84
3	C	1295[B]	T3E	C4-C5A-C1A	-2.61	128.32	132.23
3	C	1295[C]	T3E	C3A-N2A-C1A	2.59	111.96	110.38
3	C	1295[B]	T3E	C3A-N2A-C1A	2.56	111.94	110.38
3	C	1295[A]	T3E	C4-C5A-C1A	-2.54	128.42	132.23
3	A	1298[A]	T3E	O1B-S7B-C3B	2.51	110.19	107.35
3	C	1295[C]	T3E	O1B-S7B-C3B	2.51	110.18	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1295[A]	T3E	C3A-N2A-C1A	2.48	111.89	110.38
3	C	1295[D]	T3E	O1B-S7B-C3B	2.44	110.11	107.35
3	C	1295[D]	T3E	S4A-C3A-N6A	2.44	125.92	121.11
3	C	1295[A]	T3E	O1B-S7B-N9B	2.43	110.86	107.35
3	C	1295[A]	T3E	C7A-N6A-C3A	-2.40	119.54	123.31
3	C	1295[C]	T3E	O8B-S7B-C3B	2.40	110.06	107.35
3	A	1298[B]	T3E	C1B-C2B-C3B	2.40	120.69	118.84
3	A	1298[C]	T3E	O1B-S7B-C3B	2.38	110.04	107.35
3	A	1298[C]	T3E	C4-N3-C2	2.38	120.23	117.26
3	A	1298[D]	T3E	C6-C5-C8	-2.37	113.68	118.87
3	C	1295[A]	T3E	C6-N1-C2	2.35	119.03	115.81
3	A	1298[C]	T3E	C8A-C1A-N2A	2.34	124.01	119.32
3	C	1295[C]	T3E	O8B-S7B-N9B	2.30	110.67	107.35
3	C	1295[A]	T3E	S4A-C3A-N6A	2.29	125.62	121.11
3	A	1298[B]	T3E	O8B-S7B-N9B	2.29	110.65	107.35
3	A	1298[A]	T3E	C4-C5A-S4A	2.29	122.18	118.21
3	A	1298[C]	T3E	C7A-N6A-C3A	-2.28	119.72	123.31
3	A	1298[A]	T3E	S4A-C3A-N6A	2.28	125.60	121.11
3	A	1298[C]	T3E	O8B-S7B-N9B	2.28	110.64	107.35
3	A	1298[A]	T3E	O1B-S7B-N9B	2.25	110.59	107.35
3	C	1295[B]	T3E	C7A-N6A-C3A	-2.24	119.80	123.31
3	A	1298[C]	T3E	C5-C6-N1	-2.23	120.19	123.56
3	C	1295[A]	T3E	O8B-S7B-C3B	2.23	109.87	107.35
3	A	1298[C]	T3E	C1B-N7-C2	-2.23	123.37	129.38
3	C	1295[B]	T3E	S4A-C3A-N6A	2.21	125.46	121.11
3	A	1298[B]	T3E	C4-C5A-S4A	2.20	122.02	118.21
3	C	1295[D]	T3E	O8B-S7B-N9B	2.20	110.52	107.35
3	C	1295[C]	T3E	C8A-C1A-N2A	2.18	123.69	119.32
3	C	1295[B]	T3E	C1A-C5A-S4A	-2.17	108.59	109.91
3	A	1298[A]	T3E	C3A-N2A-C1A	2.15	111.69	110.38
3	C	1295[C]	T3E	C5A-C4-N3	2.14	118.03	114.42
3	C	1295[C]	T3E	C1A-C5A-S4A	-2.13	108.61	109.91
3	A	1298[B]	T3E	C4-C5A-C1A	-2.13	129.03	132.23
3	A	1298[A]	T3E	C7A-N6A-C3A	-2.13	119.96	123.31
3	A	1298[C]	T3E	S4A-C3A-N6A	2.11	125.27	121.11
3	A	1298[A]	T3E	C1A-C5A-S4A	-2.06	108.66	109.91
3	A	1298[A]	T3E	C4-C5A-C1A	-2.06	129.15	132.23
3	C	1295[B]	T3E	O8B-S7B-C3B	2.00	109.61	107.35

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1298[A]	T3E	N3-C2-N7-C1B
3	A	1298[A]	T3E	N1-C2-N7-C1B
3	A	1298[B]	T3E	C4-C5-C8-N9
3	A	1298[C]	T3E	N3-C4-C5A-C1A
3	A	1298[C]	T3E	N3-C4-C5A-S4A
3	C	1295[A]	T3E	N2A-C3A-N6A-C7A
3	C	1295[A]	T3E	S4A-C3A-N6A-C7A
3	C	1295[A]	T3E	N3-C2-N7-C1B
3	C	1295[A]	T3E	N1-C2-N7-C1B
3	C	1295[B]	T3E	N2A-C3A-N6A-C7A
3	C	1295[B]	T3E	S4A-C3A-N6A-C7A
3	C	1295[C]	T3E	S4A-C3A-N6A-C7A
3	C	1295[D]	T3E	N2A-C3A-N6A-C7A
3	C	1295[D]	T3E	S4A-C3A-N6A-C7A
3	A	1298[C]	T3E	N3-C2-N7-C1B
3	A	1298[C]	T3E	N1-C2-N7-C1B
3	C	1295[B]	T3E	N3-C2-N7-C1B
3	C	1295[D]	T3E	N3-C2-N7-C1B
3	A	1298[B]	T3E	N3-C2-N7-C1B
3	C	1295[B]	T3E	N1-C2-N7-C1B
3	C	1295[D]	T3E	N1-C2-N7-C1B
3	A	1298[B]	T3E	N1-C2-N7-C1B
3	A	1298[D]	T3E	N3-C2-N7-C1B
3	A	1298[D]	T3E	N1-C2-N7-C1B
3	C	1295[C]	T3E	N2A-C3A-N6A-C7A
3	A	1298[D]	T3E	C2B-C3B-S7B-N9B
3	A	1298[C]	T3E	C2B-C3B-S7B-N9B
3	A	1298[D]	T3E	C4B-C3B-S7B-N9B
3	C	1295[D]	T3E	C2B-C3B-S7B-N9B
3	C	1295[D]	T3E	C4B-C3B-S7B-O1B
3	C	1295[C]	T3E	C2B-C3B-S7B-O1B
3	C	1295[D]	T3E	C2B-C3B-S7B-O1B
3	A	1298[C]	T3E	C4B-C3B-S7B-N9B
3	C	1295[C]	T3E	C4B-C3B-S7B-O1B
3	C	1295[D]	T3E	C4B-C3B-S7B-N9B
3	A	1298[C]	T3E	C5-C4-C5A-S4A
3	C	1295[B]	T3E	C5-C4-C5A-S4A
3	C	1295[C]	T3E	C5-C4-C5A-S4A
4	A	1299	SGM	S1-C1-C2-O2
3	C	1295[C]	T3E	C2B-C3B-S7B-N9B
4	A	1299	SGM	O2-C2-C3-O3
3	A	1298[C]	T3E	C4B-C3B-S7B-O1B
3	C	1295[B]	T3E	N3-C4-C5A-C1A

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Mol	Chain	Res	Type	Atoms
3	C	1295[C]	T3E	N3-C4-C5A-C1A
3	C	1295[C]	T3E	C4B-C3B-S7B-N9B
3	A	1298[C]	T3E	C2B-C3B-S7B-O1B
3	A	1298[B]	T3E	C5-C4-C5A-S4A
3	C	1295[B]	T3E	N3-C4-C5A-S4A
3	C	1295[C]	T3E	N3-C4-C5A-S4A
3	A	1298[D]	T3E	C2B-C3B-S7B-O1B
3	A	1298[D]	T3E	C2B-C3B-S7B-O8B
3	A	1298[D]	T3E	C4B-C3B-S7B-O1B

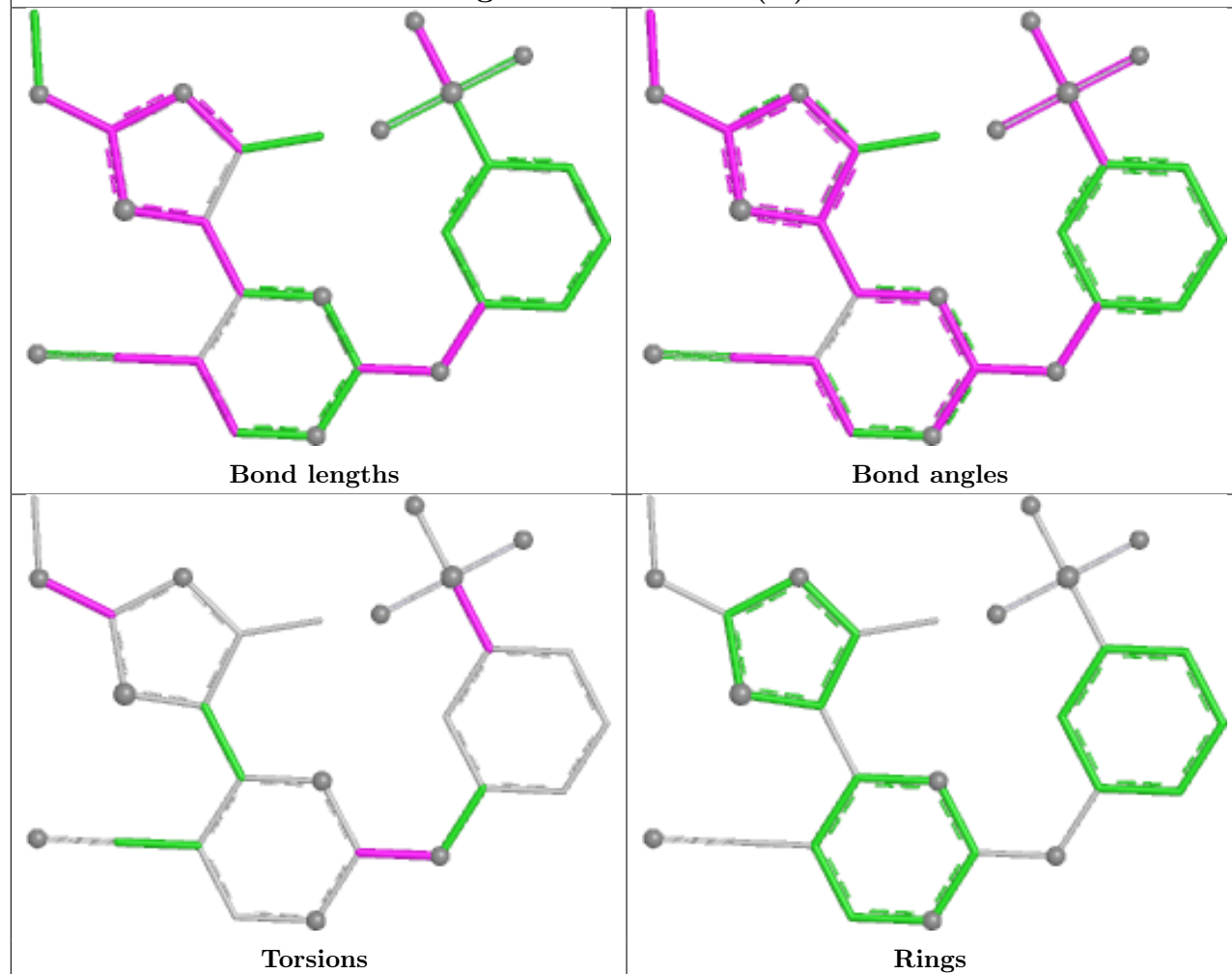
There are no ring outliers.

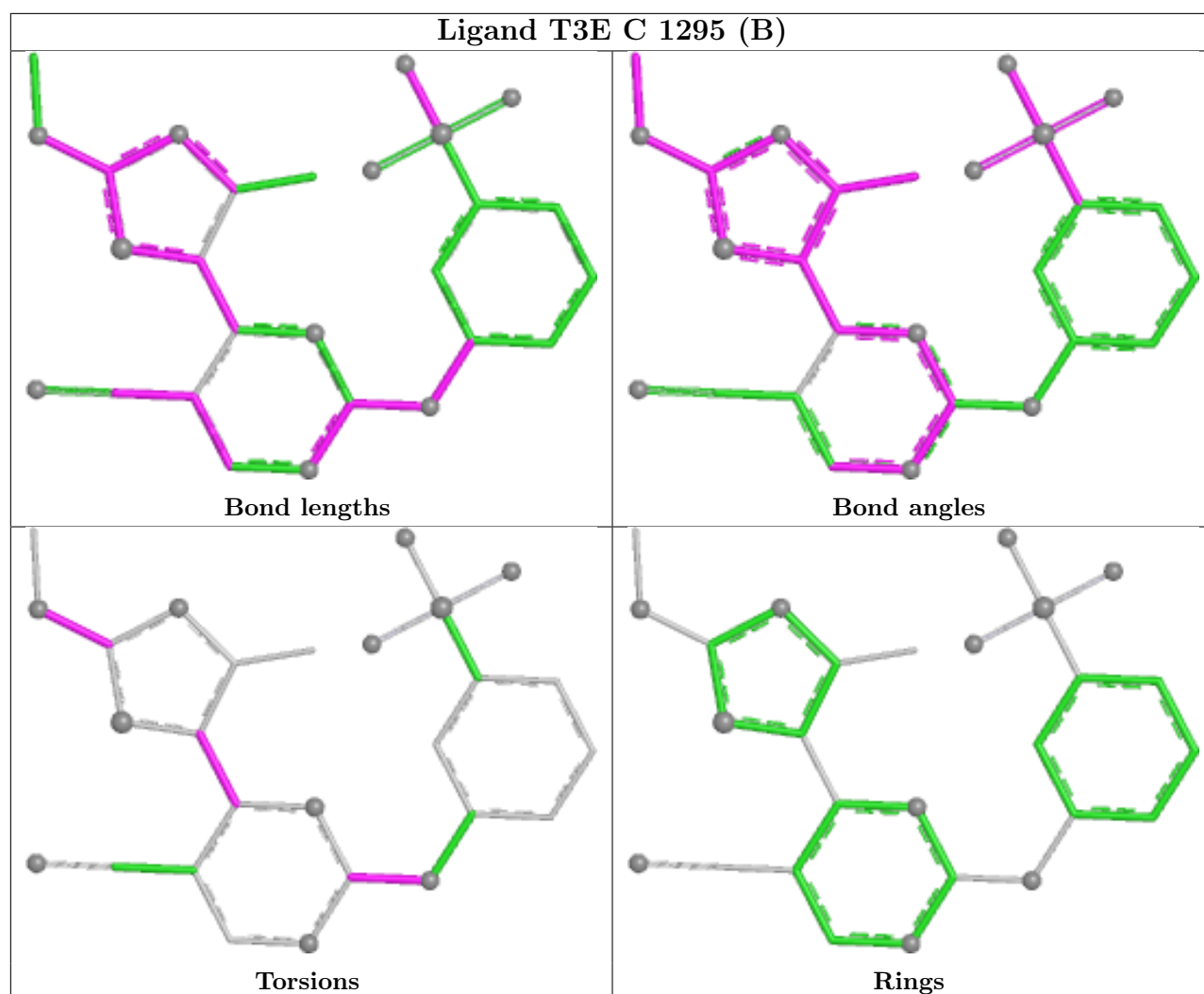
7 monomers are involved in 27 short contacts:

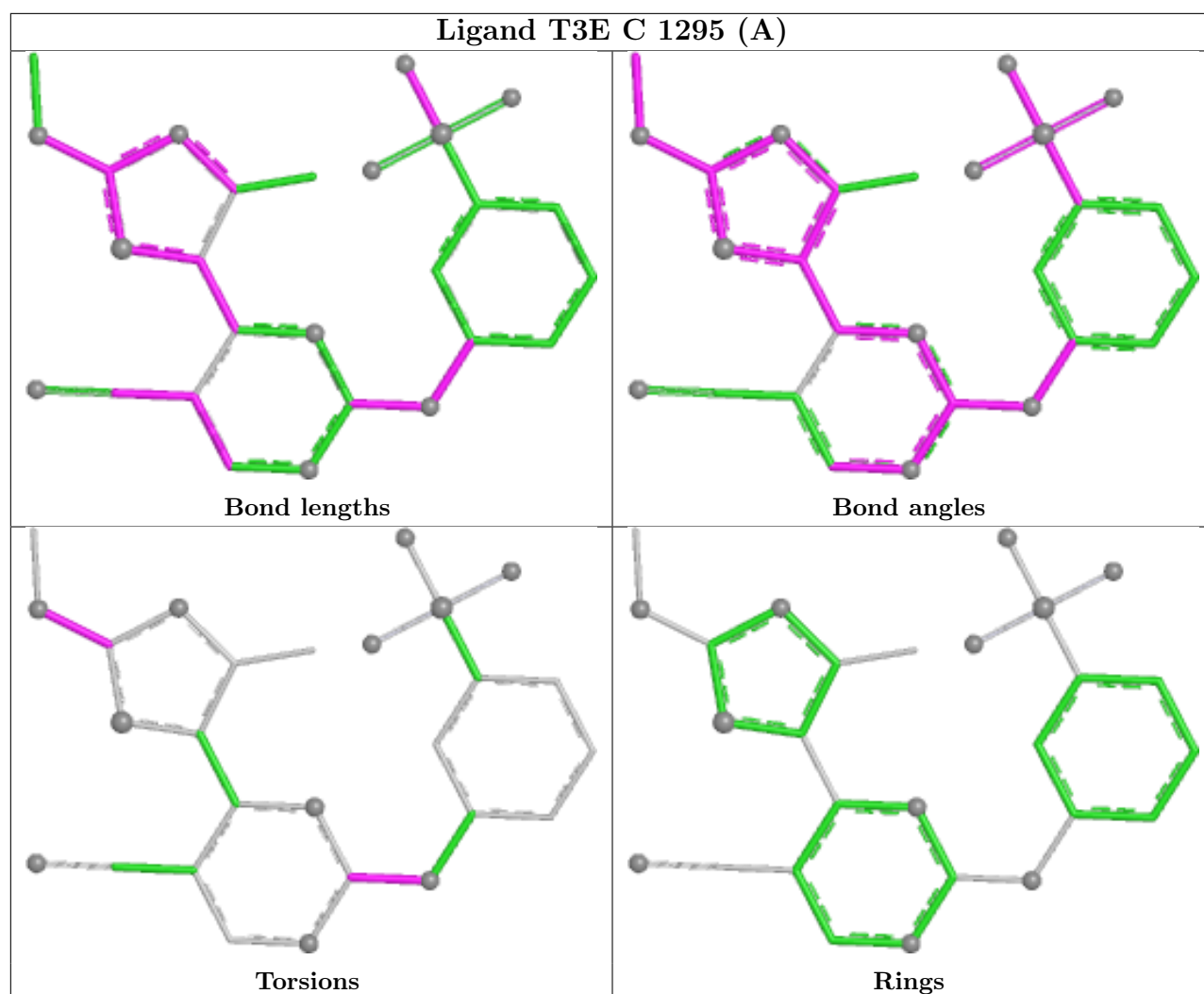
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1295[D]	T3E	5	0
3	C	1295[B]	T3E	4	0
3	C	1295[A]	T3E	2	0
4	A	1299	SGM	7	0
3	A	1298[D]	T3E	4	0
3	A	1298[B]	T3E	4	0
3	C	1295[C]	T3E	1	0

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

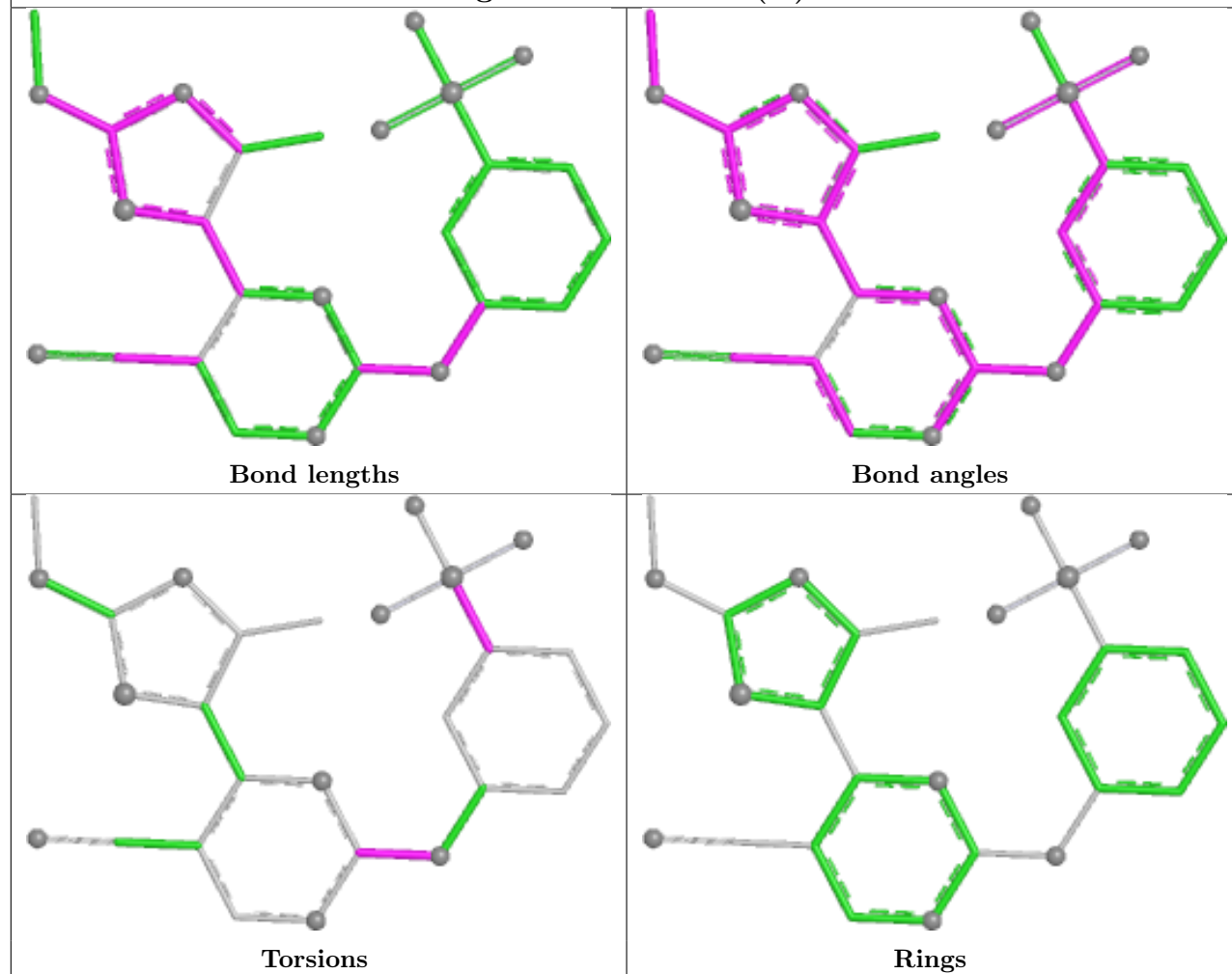
Ligand T3E C 1295 (D)

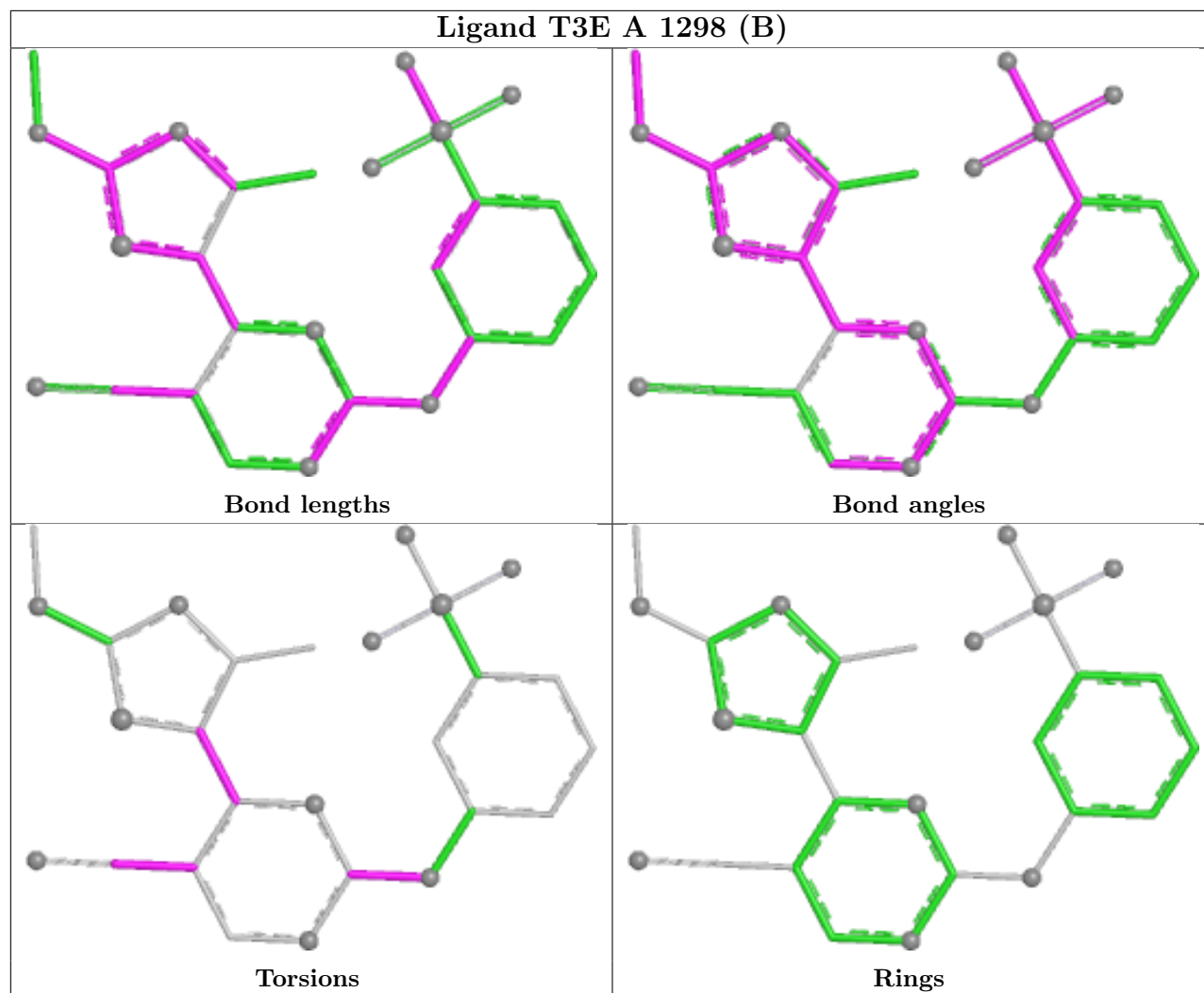


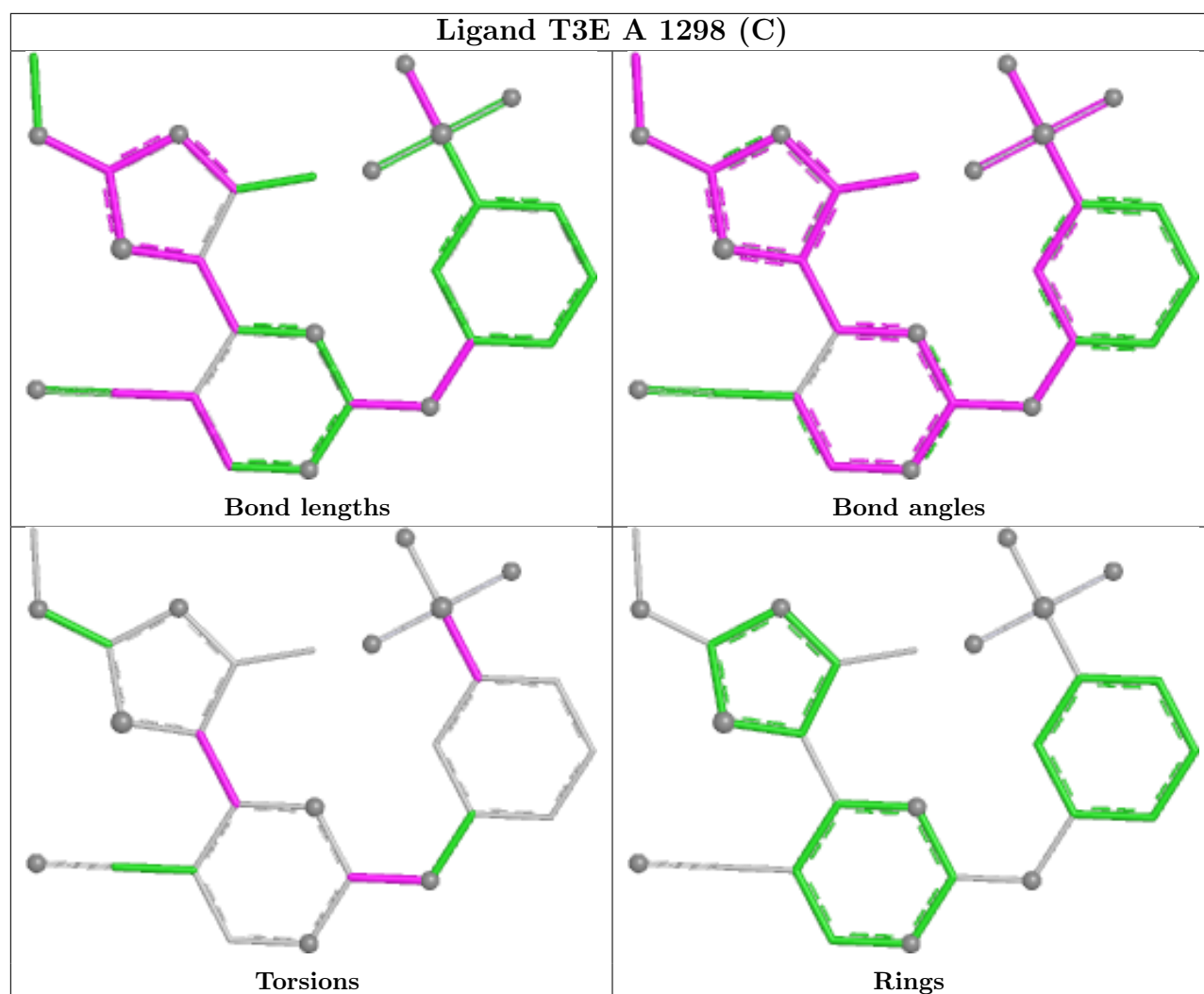




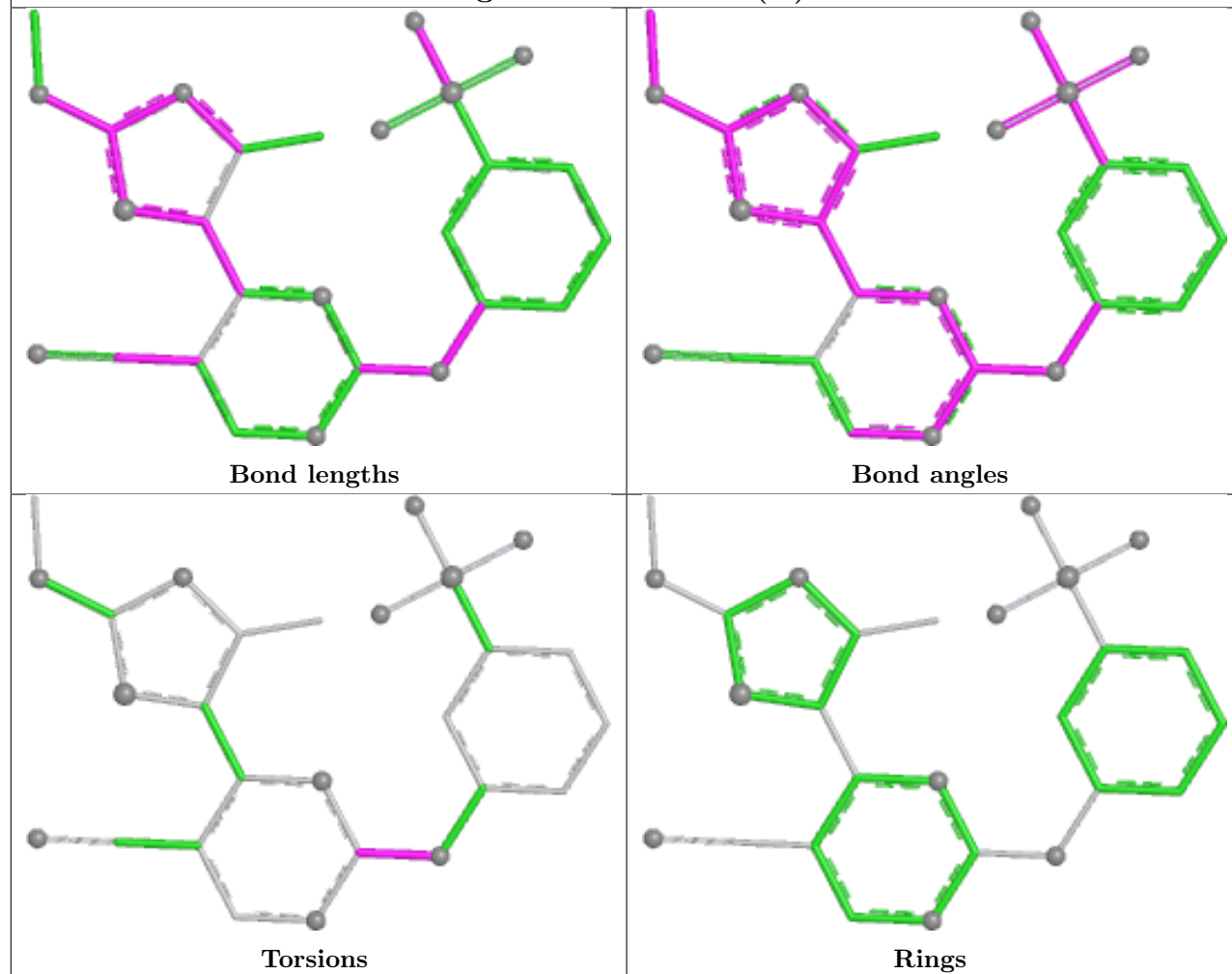
Ligand T3E A 1298 (D)

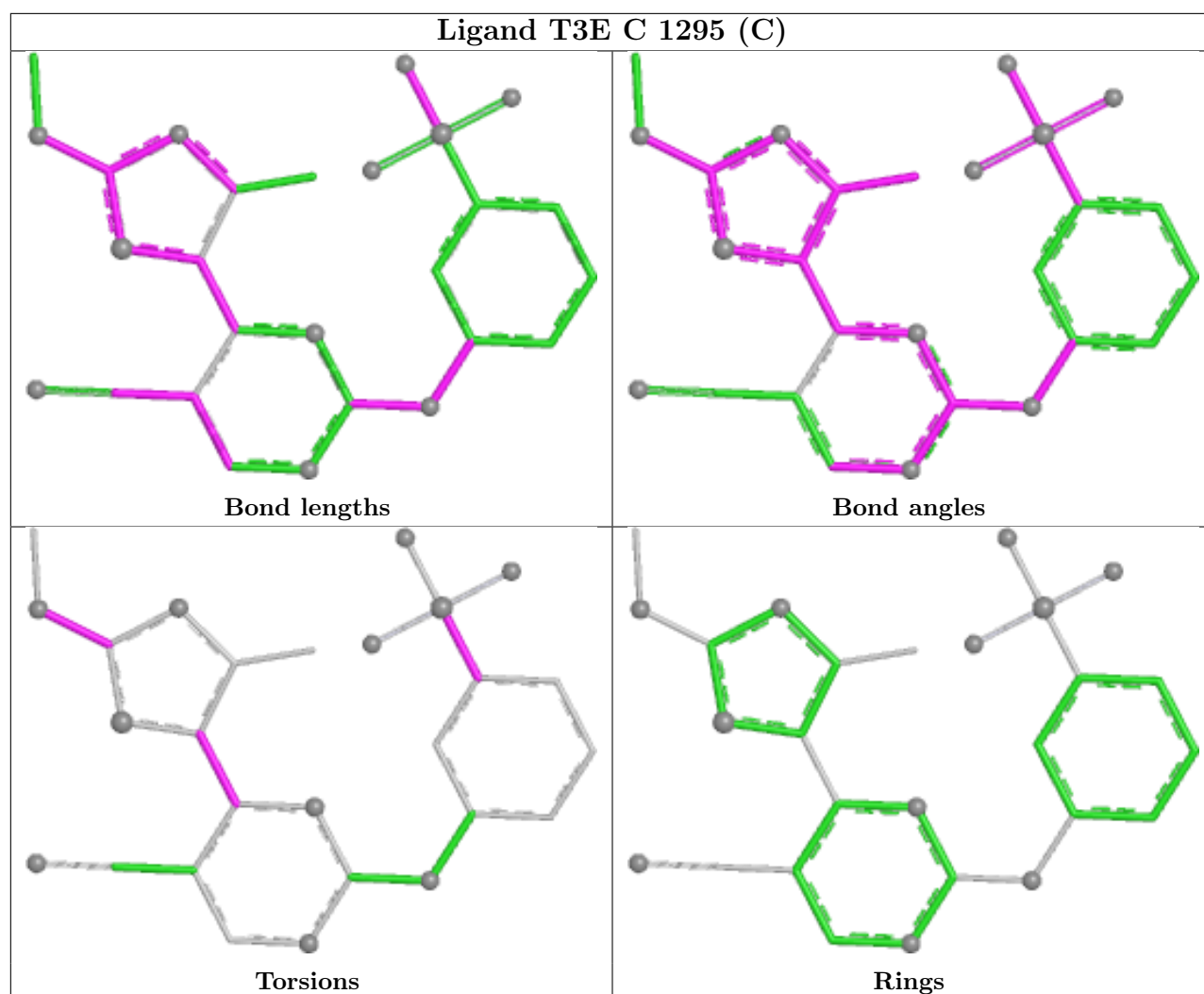






Ligand T3E A 1298 (A)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	298/300 (99%)	-0.33	6 (2%) 65 67	20, 32, 85, 121	1 (0%)
1	C	293/300 (97%)	0.45	16 (5%) 30 30	32, 61, 104, 135	0
2	B	257/262 (98%)	-0.48	1 (0%) 88 90	21, 34, 57, 89	1 (0%)
2	D	253/262 (96%)	0.34	13 (5%) 33 33	30, 60, 110, 162	1 (0%)
All	All	1101/1124 (97%)	-0.00	36 (3%) 49 49	20, 46, 98, 162	3 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	430	LEU	4.4
1	A	15	TYR	3.8
1	C	243	TRP	3.7
1	C	234	PRO	3.5
2	D	284	ASP	3.2
2	D	429	THR	3.2
2	D	334	MET	3.1
1	A	97	THR	3.0
1	C	15	TYR	2.9
2	D	322	GLN	2.8
2	D	399	LEU	2.8
1	C	251	VAL	2.6
1	C	177	CYS	2.5
1	C	238	PRO	2.5
2	D	329	VAL	2.5
1	C	256	ASP	2.5
2	B	283	ASP	2.5
1	C	225	VAL	2.4
1	C	227	TRP	2.4
1	A	71	HIS	2.4
2	D	325	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	209	ILE	2.4
2	D	323	GLN	2.3
1	C	213	PHE	2.3
1	A	295	HIS	2.3
1	C	226	VAL	2.3
2	D	384	LEU	2.2
2	D	324	PRO	2.2
1	C	236	TYR	2.2
1	A	39	THR	2.2
1	C	204	PRO	2.1
2	D	427	PRO	2.1
1	A	-1	GLY	2.1
2	D	372	TRP	2.1
1	C	282	ALA	2.1
1	C	203	PHE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPO	C	160	11/12	0.94	0.10	49,56,69,70	0
1	TPO	A	160	11/12	0.98	0.05	23,26,30,34	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	T3E	A	1298[A]	27/27	0.65	0.23	28,38,46,48	42

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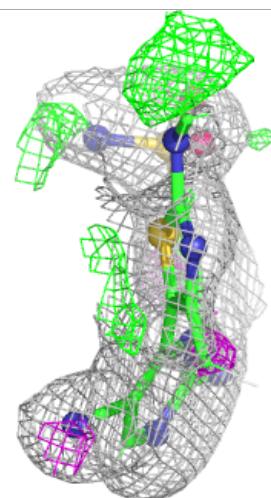
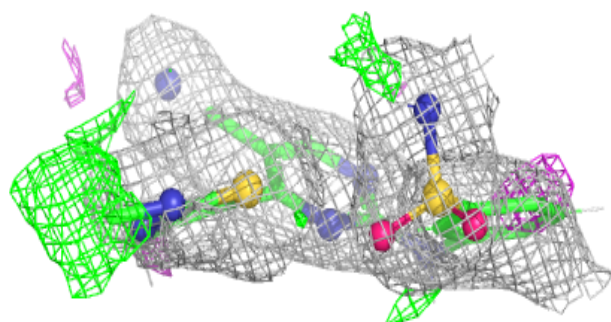
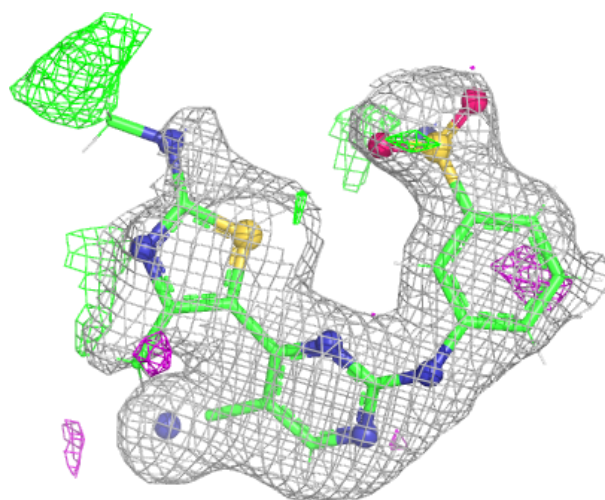
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	T3E	A	1298[B]	27/27	0.65	0.23	28,36,46,47	42
3	T3E	A	1298[C]	27/27	0.65	0.23	28,37,59,70	42
3	T3E	A	1298[D]	27/27	0.65	0.23	28,38,60,68	42
4	SGM	A	1299	6/6	0.80	0.11	60,63,69,86	0
3	T3E	C	1295[B]	27/27	0.88	0.13	39,50,61,63	42
3	T3E	C	1295[C]	27/27	0.88	0.13	39,49,64,74	42
3	T3E	C	1295[D]	27/27	0.88	0.13	32,49,64,74	42
3	T3E	C	1295[A]	27/27	0.88	0.13	39,49,61,63	42

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.

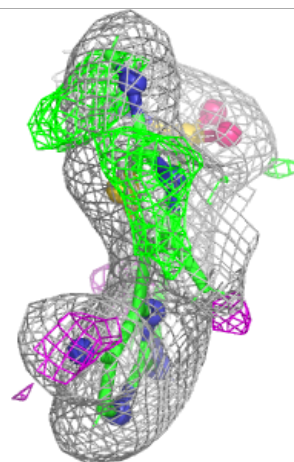
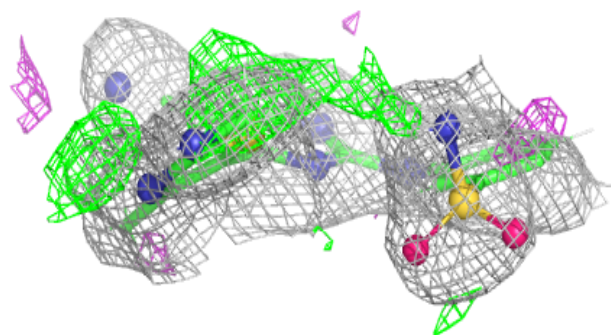
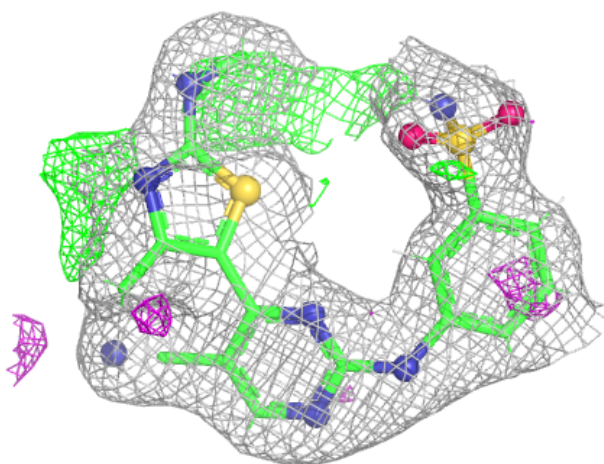
Electron density around T3E A 1298 (A):

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



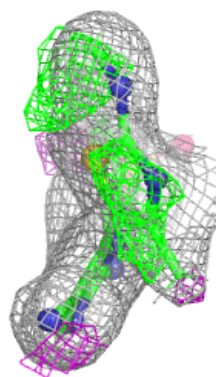
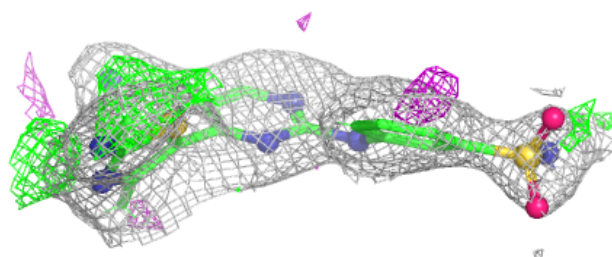
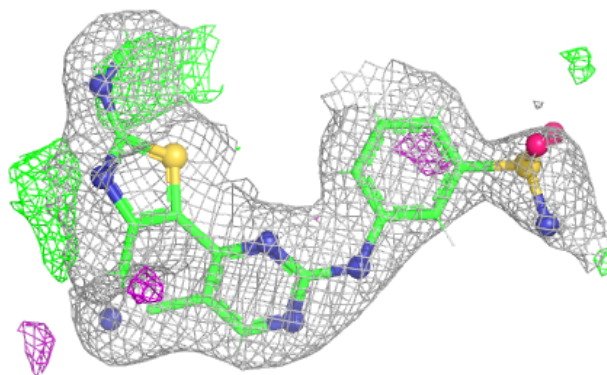
Electron density around T3E A 1298 (B):

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

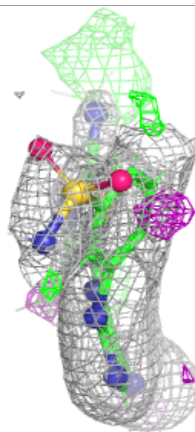
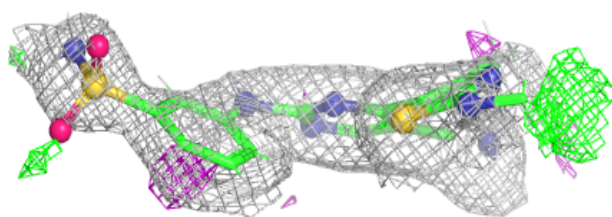
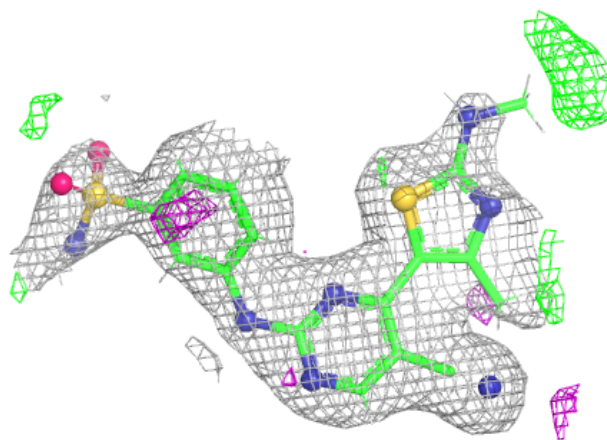


Electron density around T3E A 1298 (C):

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

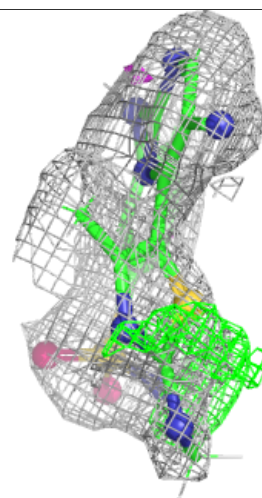
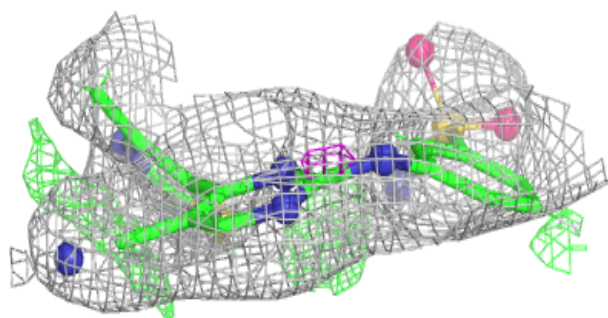
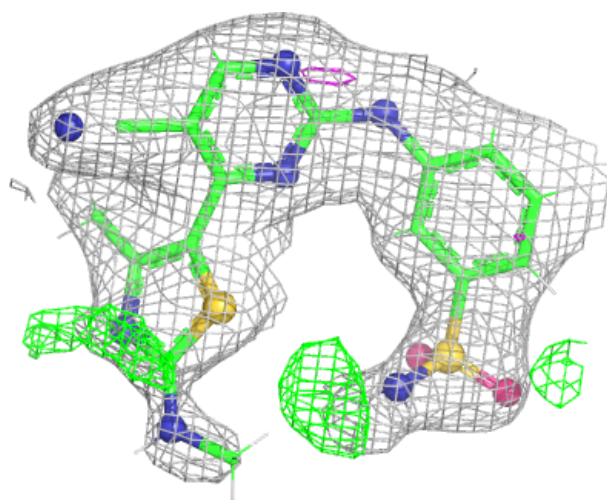
**Electron density around T3E A 1298 (D):**

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and green (positive)



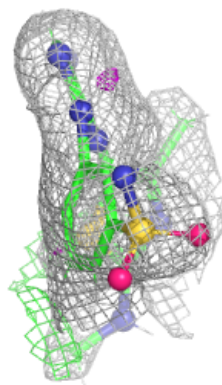
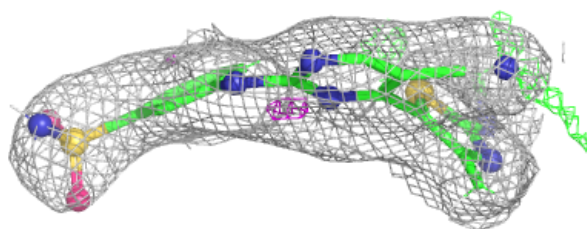
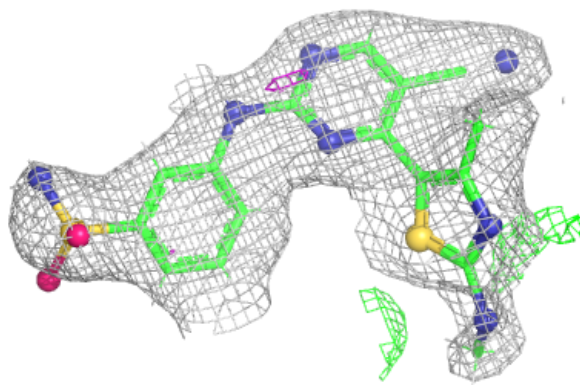
Electron density around T3E C 1295 (B):

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

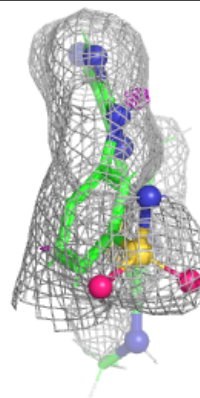
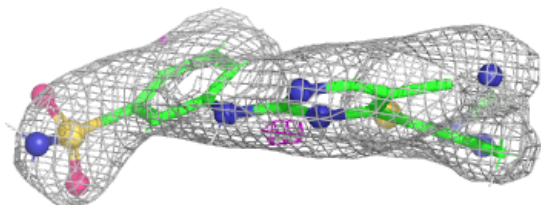
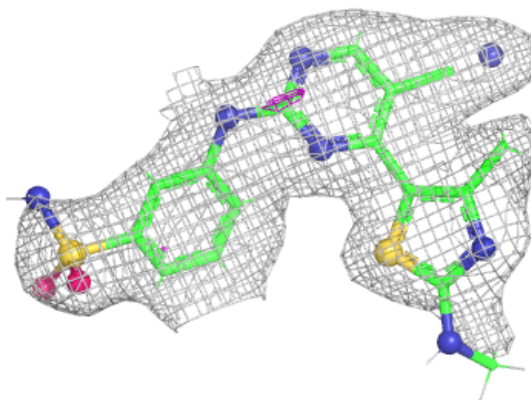


Electron density around T3E C 1295 (C):

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and green (positive)

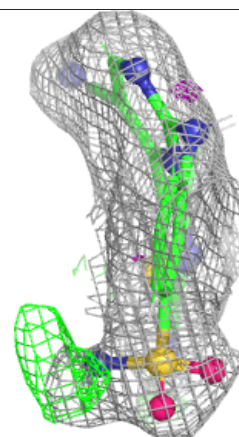
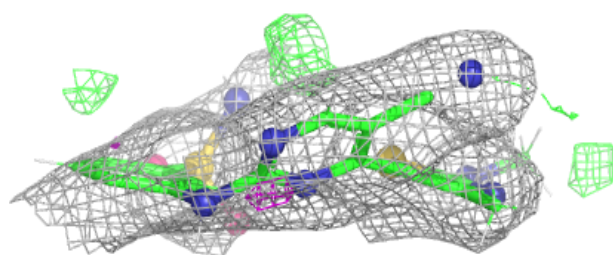
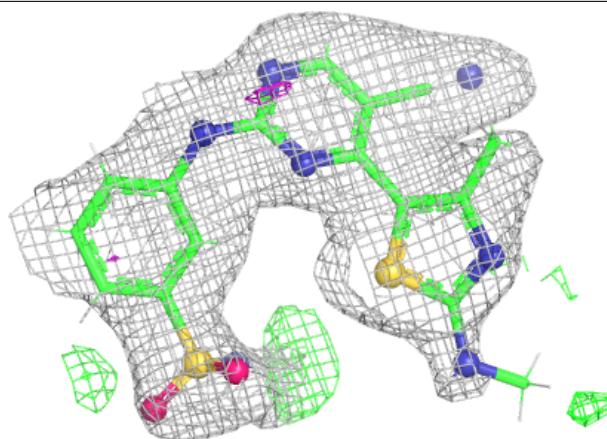
**Electron density around T3E C 1295 (D):**

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and green (positive)



Electron density around T3E C 1295 (A):

$2mF_o - DF_c$ (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.