Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 08:09 PM EDT

PDB ID	:	4BCK
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 (i) 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 (i)) were used in the production of this report:

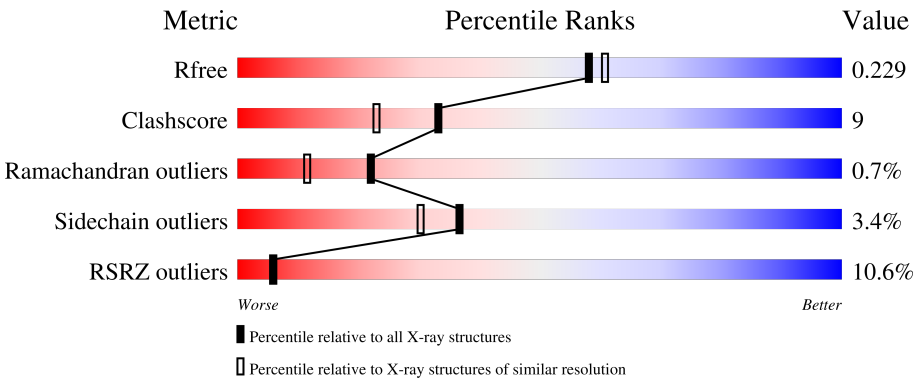
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (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 <=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	4% 84% 12% •
1	C	300	15% 78% 19% • •
2	B	262	7% 92% 6% •
2	D	262	15% 82% 13% • •

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SGM	A	1299	-	-	X	-

2 Entry composition (i)

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
			Total	C	N	O	P	S			
1	A	299	2410	1563	411	427	1	8	0	1	0
1	C	294	2363	1534	399	421	1	8	0	0	0

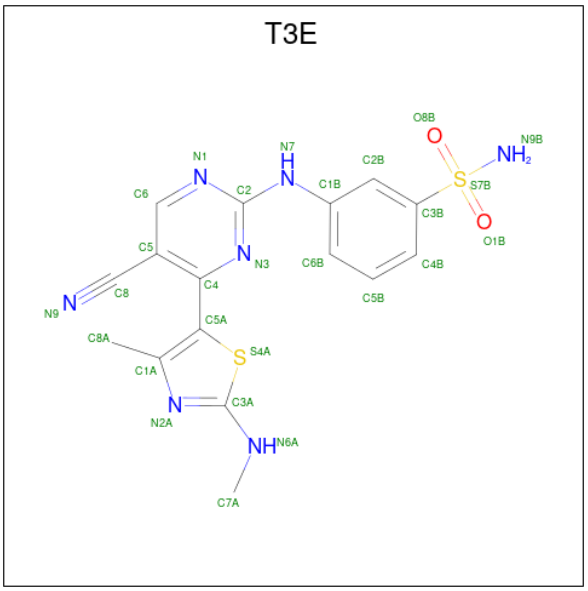
There are 4 discrepancies between the modelled and reference sequences:

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.

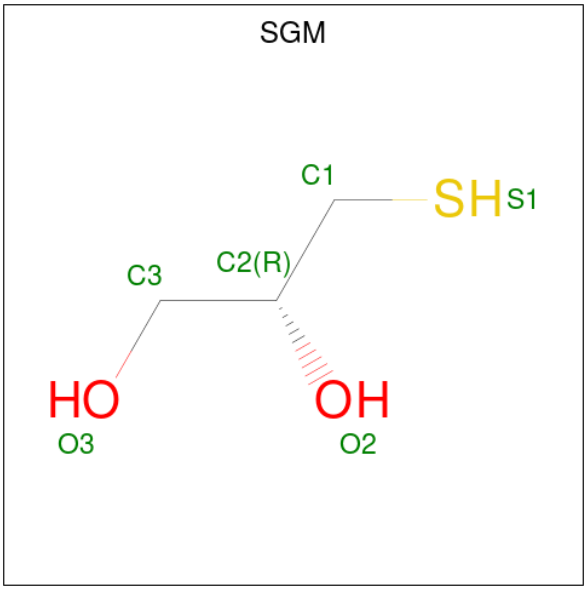
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	257	2082	1349	338	384	11	0	1	0
2	D	253	2051	1330	333	377	11	0	1	0

- Molecule 3 is 3-[[5-cyano-4-[4-methyl-2-(methylamino)-1,3-thiazol-5-yl]pyrimidin-2-yl]amino]benzenesulfonamide (three-letter code: T3E) (formula: $C_{16}H_{15}N_7O_2S_2$).



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

- Molecule 4 is MONOTHIOGLYCEROL (three-letter code: SGM) (formula: $C_3H_8O_2S$).



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

- Molecule 5 is water.

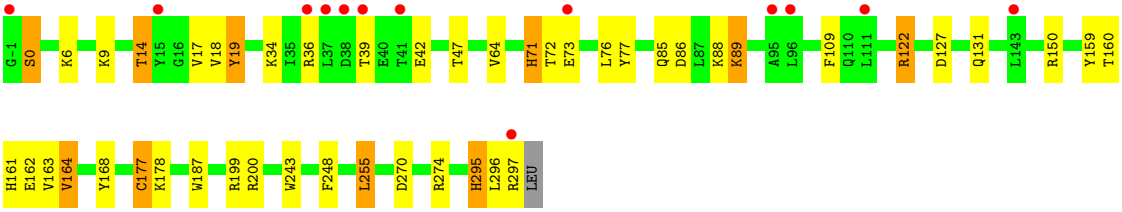
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	258	258	258	0	0
			Total	O		
5	B	208	208	208	0	0
			Total	O		
5	C	86	86	86	0	0
			Total	O		
5	D	77	77	77	0	0

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 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.

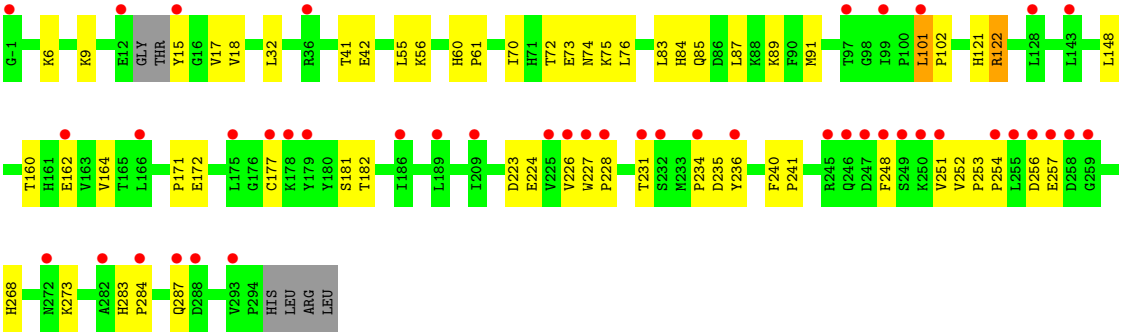
• Molecule 1: CYCLIN-DEPENDENT KINASE 2

Chain A:



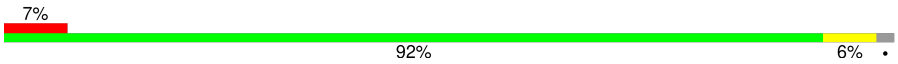
• Molecule 1: CYCLIN-DEPENDENT KINASE 2

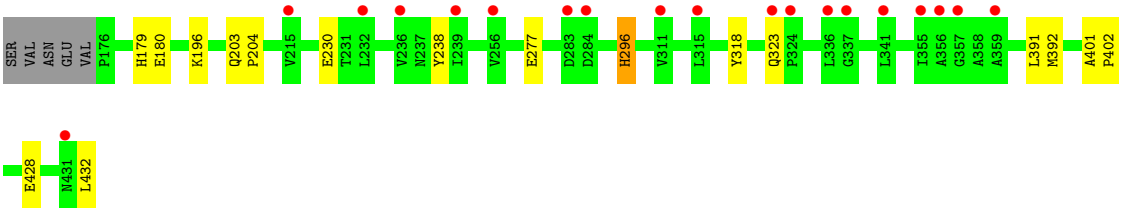
Chain C:



• Molecule 2: CYCLIN-A2

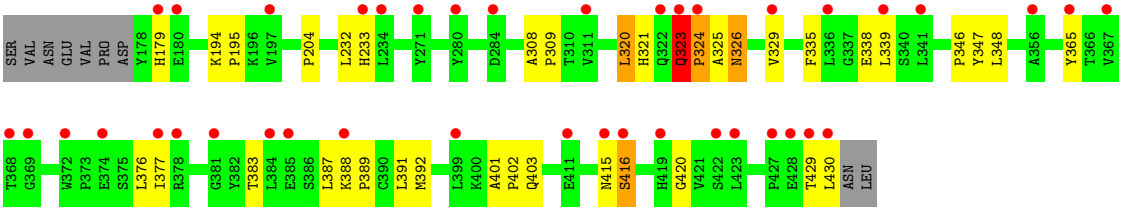
Chain B:





• Molecule 2: CYCLIN-A2

Chain D:


SER
VAL
ASN
GLU
VAL
PRO
ASP
Y178
H179
E180
K194
P195
K196
V197
P204
L232
H233
L234
Y271
Y280
D284
A308
P309
T310
V311
L320
H321
Q322
Q323
P324
A325
N326
V329
F335
L336
G337
E338
L339
S340
L341
P346
Y347
L348
A356
Y365
T366
V367
T368
G369
W372
P373
E374
S375
L376
I377
R378
G381
Y382
T383
L384
E385
S386
L387
K388
P389
C390
L391
M392
L399
K400
A401
P402
Q403
E411
N415
S416
H419
G420
V421
S422
L423
P427
E428
T429
L430
ASN
LEU

4 Data and refinement statistics (i)

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) 96.1 (29.86-2.05)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 , 83.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.34	9/2464 (0.4%)	0.92	6/3342 (0.2%)
1	C	0.75	0/2411	0.74	1/3269 (0.0%)
2	B	1.31	4/2135 (0.2%)	0.82	0/2898
2	D	0.74	0/2103	0.72	0/2854
All	All	1.08	13/9113 (0.1%)	0.81	7/12363 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	TRP	CB-CG	7.53	1.63	1.50
2	B	318	TYR	CD1-CE1	6.57	1.49	1.39
1	A	187	TRP	CB-CG	6.57	1.62	1.50
2	B	180	GLU	CB-CG	6.09	1.63	1.52
1	A	164	VAL	CB-CG2	5.86	1.65	1.52
2	B	238	TYR	CD1-CE1	5.80	1.48	1.39
1	A	168	TYR	CD2-CE2	5.70	1.48	1.39
1	A	274	ARG	CG-CD	5.67	1.66	1.51
1	A	159	TYR	CD2-CE2	5.35	1.47	1.39
1	A	127	ASP	CB-CG	5.32	1.62	1.51
1	A	177	CYS	CB-SG	5.32	1.91	1.82
1	A	109	PHE	CB-CG	5.25	1.60	1.51
2	B	230	GLU	CB-CG	5.15	1.61	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	150	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	A	150	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	A	270	ASP	CB-CG-OD1	6.72	124.35	118.30
1	C	32	LEU	CA-CB-CG	6.54	130.34	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	127	ASP	CB-CG-OD1	6.05	123.74	118.30
1	A	255	LEU	CA-CB-CG	5.83	128.72	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2410	0	2453	51	0
1	C	2363	0	2404	52	0
2	B	2082	0	2105	14	0
2	D	2051	0	2076	33	0
3	A	108	60	60	9	0
3	C	108	60	60	14	0
4	A	6	0	8	7	0
5	A	258	0	0	5	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	157	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 (157) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:1295[D]:T3E:H8A1	3:C:1295[D]:T3E:C8	2.08	0.83
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:377:ILE:HD13	2:D:383:THR:HG22	1.63	0.81
2:D:323:GLN:H	2:D:323:GLN:CD	1.85	0.79
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
3:A:1298[D]:T3E:H8A1	3:A:1298[D]:T3E:C8	2.18	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
2:B:392:MET:HA	2:B:392:MET:CE	2.28	0.64
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:D:388:LYS:HB3	2:D:389:PRO:HD3	1.81	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:256:ASP:CG	1:C:257:GLU:H	2.09	0.55
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:B:392:MET:HA	2:B:392:MET:HE2	1.90	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
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
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
3:C:1295[A]:T3E:C8	3:C:1295[A]:T3E:H8A1	2.41	0.50
2:D:401:ALA:HB3	2:D:402:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:C:1295[D]:T3E:C8	3:C:1295[D]:T3E:C8A	2.87	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
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
3:A:1298[B]:T3E:H8A1	3:A:1298[B]:T3E:C8	2.45	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
1:C:253:PRO:HD2	1:C:254:PRO:HD2	1.96	0.46
1:C:224:GLU:HG2	1:C:231:THR:HG23	1.98	0.45
3:A:1298[D]:T3E:C8	3:A:1298[D]:T3E:C8A	2.91	0.45
2:D:415:ASN:OD1	2:D:416:SER:N	2.50	0.45
1:A:18:VAL:HG21	3:A:1298[D]:T3E:N2A	2.31	0.44
2:D:323:GLN:O	2:D:324:PRO:C	2.56	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:A:86:ASP:H	1:A:89:LYS:HZ2	1.66	0.44
3:C:1295[D]:T3E:H8A1	3:C:1295[D]:T3E:N9	2.29	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
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:C8	3:A:1298[B]:T3E:C8A	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLN:HA	3:A:1298[B]:T3E:H5B	2.00	0.43
1:A:85:GLN:CG	1:A:89:LYS:HZ3	2.31	0.42
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
1:C:256:ASP:CG	1:C:257:GLU:N	2.72	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: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:HG13	1:A:64:VAL:O	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:C:181:SER:OG	1:C:182:THR:N	2.50	0.41
2:D:323:GLN:CD	2:D:323:GLN:N	2.63	0.41
2:B:392:MET:HA	2:B:392:MET:HE3	2.01	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: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
1:C:121:HIS:C	1:C:122:ARG:HG3	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	297/300 (99%)	286 (96%)	9 (3%)	2 (1%)	22	11
1	C	289/300 (96%)	274 (95%)	12 (4%)	3 (1%)	15	6
2	B	256/262 (98%)	254 (99%)	2 (1%)	0	100	100
2	D	252/262 (96%)	243 (96%)	6 (2%)	3 (1%)	13	4
All	All	1094/1124 (97%)	1057 (97%)	29 (3%)	8 (1%)	22	11

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/263 (100%)	252 (96%)	11 (4%)	30	23
1	C	258/263 (98%)	248 (96%)	10 (4%)	32	25
2	B	232/236 (98%)	229 (99%)	3 (1%)	69	67
2	D	228/236 (97%)	219 (96%)	9 (4%)	32	25
All	All	981/998 (98%)	948 (97%)	33 (3%)	37	30

All (33) 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

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Mol	Chain	Res	Type
1	A	36	ARG
1	A	39	THR
1	A	71	HIS
1	A	89	LYS
1	A	122	ARG
1	A	248	PHE
1	A	255	LEU
1	A	295	HIS
2	B	179	HIS
2	B	296	HIS
2	B	428	GLU
1	C	6	LYS
1	C	15	TYR
1	C	55	LEU
1	C	56	LYS
1	C	70	ILE
1	C	76	LEU
1	C	101	LEU
1	C	122	ARG
1	C	148	LEU
1	C	248	PHE
2	D	179	HIS
2	D	232	LEU
2	D	320	LEU
2	D	323	GLN
2	D	326	ASN
2	D	348	LEU
2	D	392	MET
2	D	403	GLN
2	D	416	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
2	D	321	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	A	160	1	8,10,11	2.51	2 (25%)	10,14,16	1.36	2 (20%)
1	TPO	C	160	1	8,10,11	1.28	1 (12%)	10,14,16	1.22	1 (10%)

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	A	160	1	-	1/9/11/13	-
1	TPO	C	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(^{o})	Ideal(^{o})
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 monosaccharides 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	A	1298[A]	-	22,29,29	1.70	4 (18%)	27,42,42	2.41	8 (29%)
3	T3E	A	1298[B]	-	22,29,29	1.87	6 (27%)	27,42,42	2.66	9 (33%)
3	T3E	C	1295[D]	-	22,29,29	1.63	6 (27%)	27,42,42	2.41	8 (29%)
3	T3E	C	1295[C]	-	22,29,29	1.70	5 (22%)	27,42,42	2.31	8 (29%)
3	T3E	C	1295[A]	-	22,29,29	1.70	6 (27%)	27,42,42	2.31	8 (29%)
3	T3E	C	1295[B]	-	22,29,29	1.78	6 (27%)	27,42,42	2.38	7 (25%)
3	T3E	A	1298[D]	-	22,29,29	1.65	4 (18%)	27,42,42	2.46	8 (29%)
4	SGM	A	1299	-	5,5,5	0.99	0	5,5,5	1.47	0
3	T3E	A	1298[C]	-	22,29,29	1.75	5 (22%)	27,42,42	2.53	11 (40%)

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	A	1298[A]	-	-	2/12/18/18	0/3/3/3
3	T3E	A	1298[B]	-	-	3/12/18/18	0/3/3/3
3	T3E	C	1295[D]	-	-	6/12/18/18	0/3/3/3
3	T3E	C	1295[C]	-	-	4/12/18/18	0/3/3/3
3	T3E	C	1295[A]	-	-	2/12/18/18	0/3/3/3
3	T3E	C	1295[B]	-	-	2/12/18/18	0/3/3/3
3	T3E	A	1298[D]	-	-	7/12/18/18	0/3/3/3
4	SGM	A	1299	-	-	2/4/4/4	-
3	T3E	A	1298[C]	-	-	6/12/18/18	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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[C]	T3E	C2-N7	4.45	1.45	1.36
3	C	1295[A]	T3E	C2-N7	4.30	1.45	1.36
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	C	1295[C]	T3E	C5-C8	3.94	1.50	1.44
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
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[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[D]	T3E	C4-C5A	2.36	1.54	1.49
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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[D]	T3E	C4-C5A	2.16	1.53	1.49
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
3	C	1295[A]	T3E	C4-C5A	2.02	1.53	1.49

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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[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[B]	T3E	O1B-S7B-O8B	-6.54	108.75	118.80
3	C	1295[A]	T3E	O1B-S7B-O8B	-6.46	108.86	118.80
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[D]	T3E	C7A-N6A-C3A	-5.95	117.33	122.85
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	C	1295[D]	T3E	C7A-N6A-C3A	-5.84	117.43	122.85
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[B]	T3E	C7A-N6A-C3A	-4.28	118.88	122.85
3	A	1298[B]	T3E	C5A-C4-N3	4.05	120.66	115.10
3	A	1298[C]	T3E	C5A-C4-N3	3.65	120.11	115.10
3	C	1295[A]	T3E	C7A-N6A-C3A	-3.57	119.54	122.85
3	A	1298[D]	T3E	C1B-N7-C2	-3.53	119.86	129.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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[C]	T3E	C7A-N6A-C3A	-3.37	119.72	122.85
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	C	1295[B]	T3E	C7A-N6A-C3A	-3.29	119.80	122.85
3	C	1295[D]	T3E	C6-C5-C8	-3.21	111.84	118.87
3	A	1298[A]	T3E	C7A-N6A-C3A	-3.11	119.96	122.85
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[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	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	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	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	A	1298[C]	T3E	C1B-C2B-C3B	2.62	120.86	118.84
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
3	C	1295[D]	T3E	C5-C4-C5A	2.50	127.95	123.58
3	C	1295[D]	T3E	O1B-S7B-C3B	2.44	110.11	107.35
3	C	1295[A]	T3E	O1B-S7B-N9B	2.43	110.86	107.35
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[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	C	1295[C]	T3E	O8B-S7B-N9B	2.30	110.67	107.35
3	A	1298[B]	T3E	O8B-S7B-N9B	2.29	110.65	107.35
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	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[D]	T3E	O8B-S7B-N9B	2.20	110.52	107.35
3	A	1298[D]	T3E	C5-C4-C5A	2.16	127.36	123.58
3	C	1295[C]	T3E	C5A-C4-N3	2.13	118.03	115.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1295[B]	T3E	O8B-S7B-C3B	2.00	109.61	107.35

There are no chirality outliers.

All (34) 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	C	1295[A]	T3E	N3-C2-N7-C1B
3	C	1295[A]	T3E	N1-C2-N7-C1B
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	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
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[C]	T3E	C4B-C3B-S7B-N9B
3	A	1298[C]	T3E	C2B-C3B-S7B-O1B
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

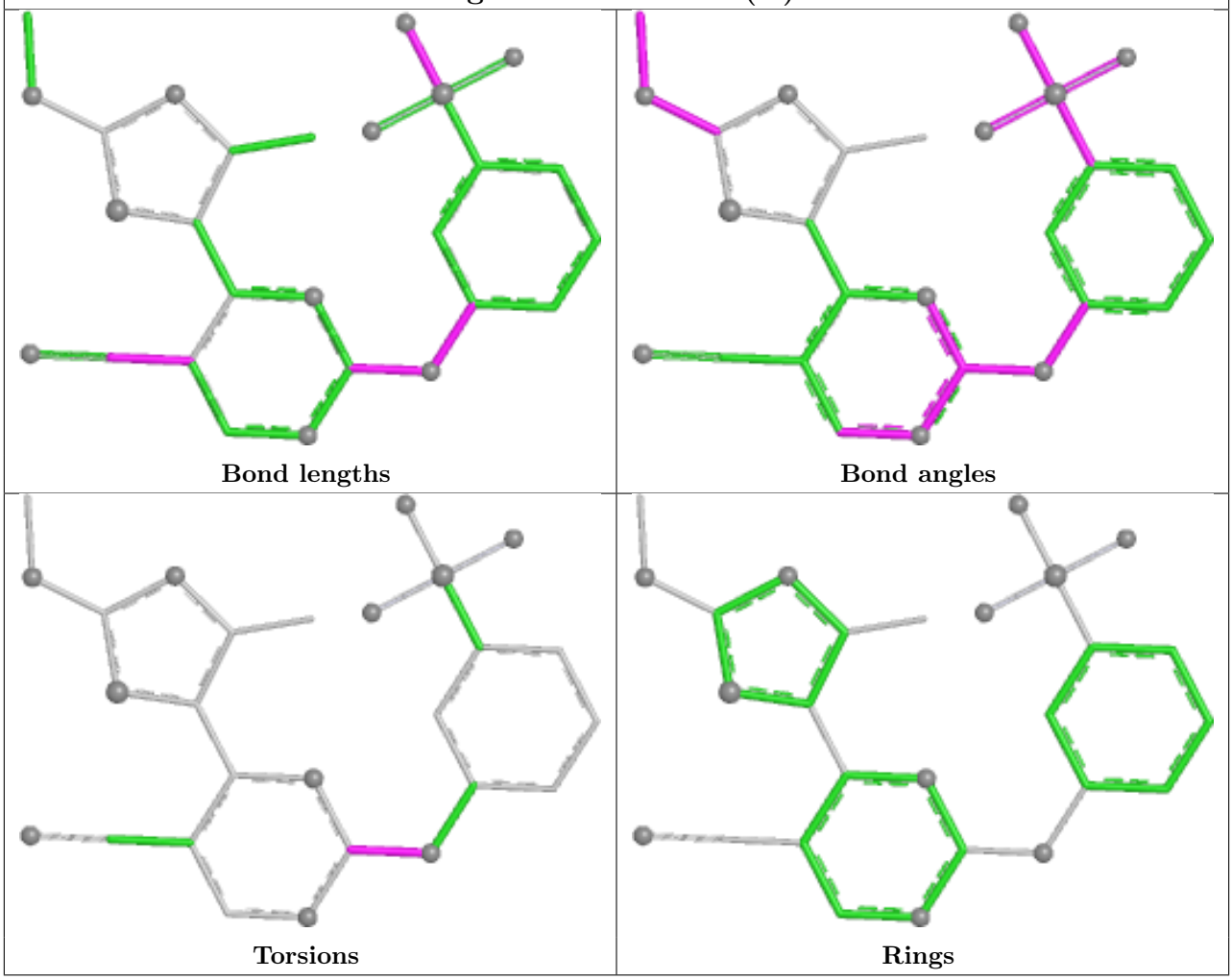
There are no ring outliers.

7 monomers are involved in 30 short contacts:

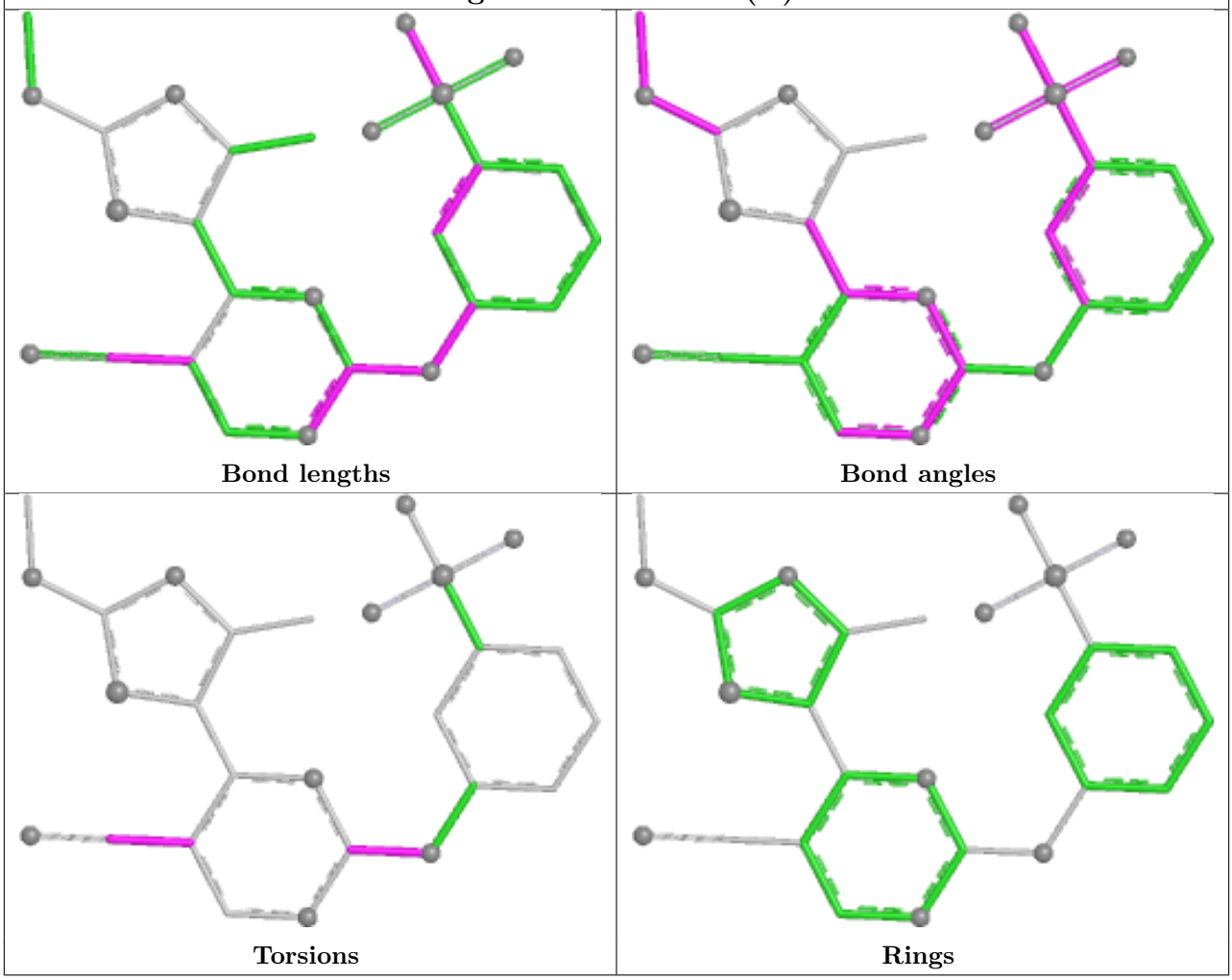
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1298[B]	T3E	4	0
3	C	1295[D]	T3E	6	0
3	C	1295[C]	T3E	1	0
3	C	1295[A]	T3E	3	0
3	C	1295[B]	T3E	4	0
3	A	1298[D]	T3E	5	0
4	A	1299	SGM	7	0

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 then 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.

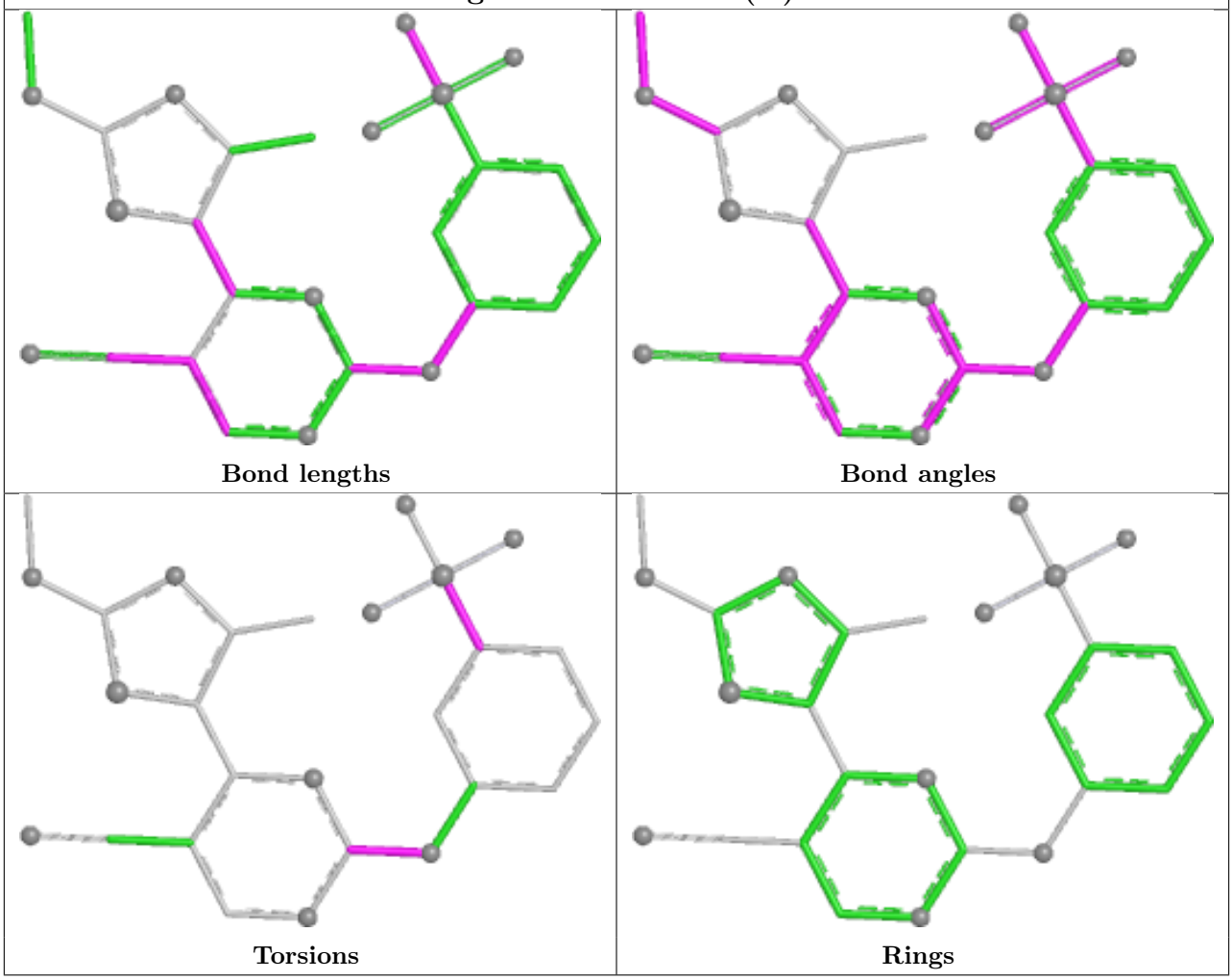
Ligand T3E A 1298 (A)



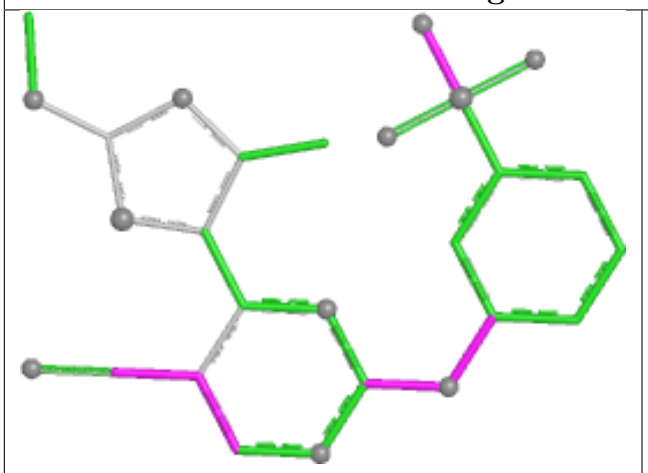
Ligand T3E A 1298 (B)



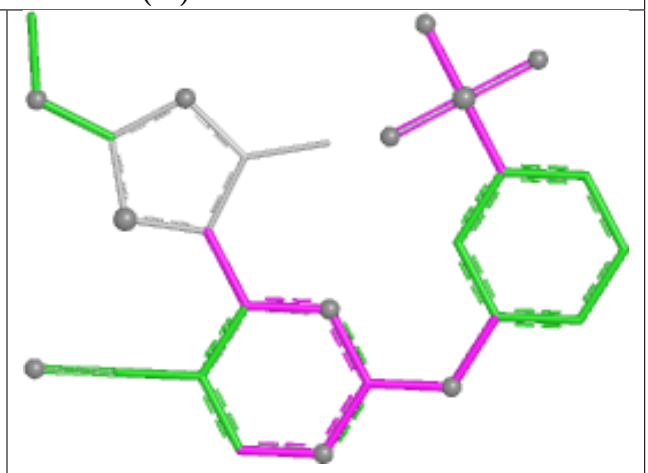
Ligand T3E C 1295 (D)



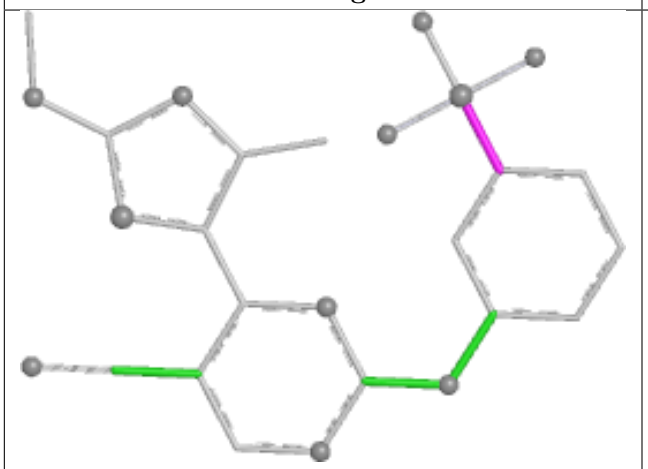
Ligand T3E C 1295 (C)



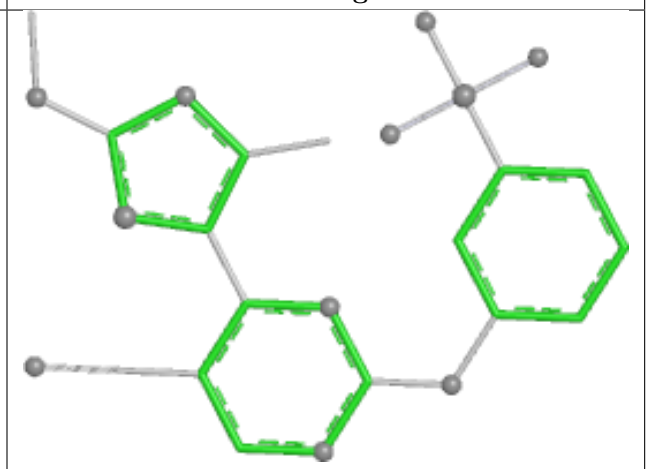
Bond lengths



Bond angles

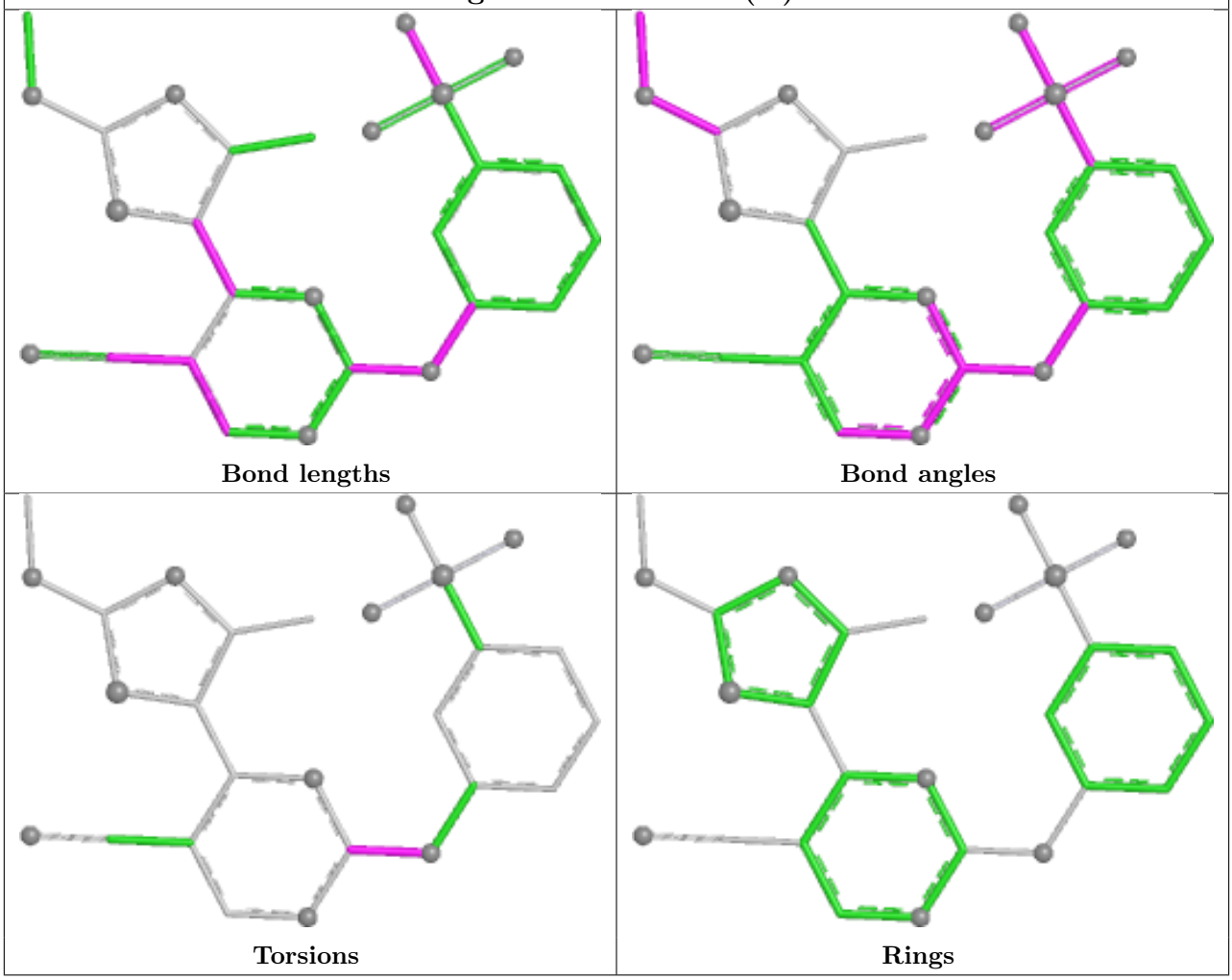


Torsions

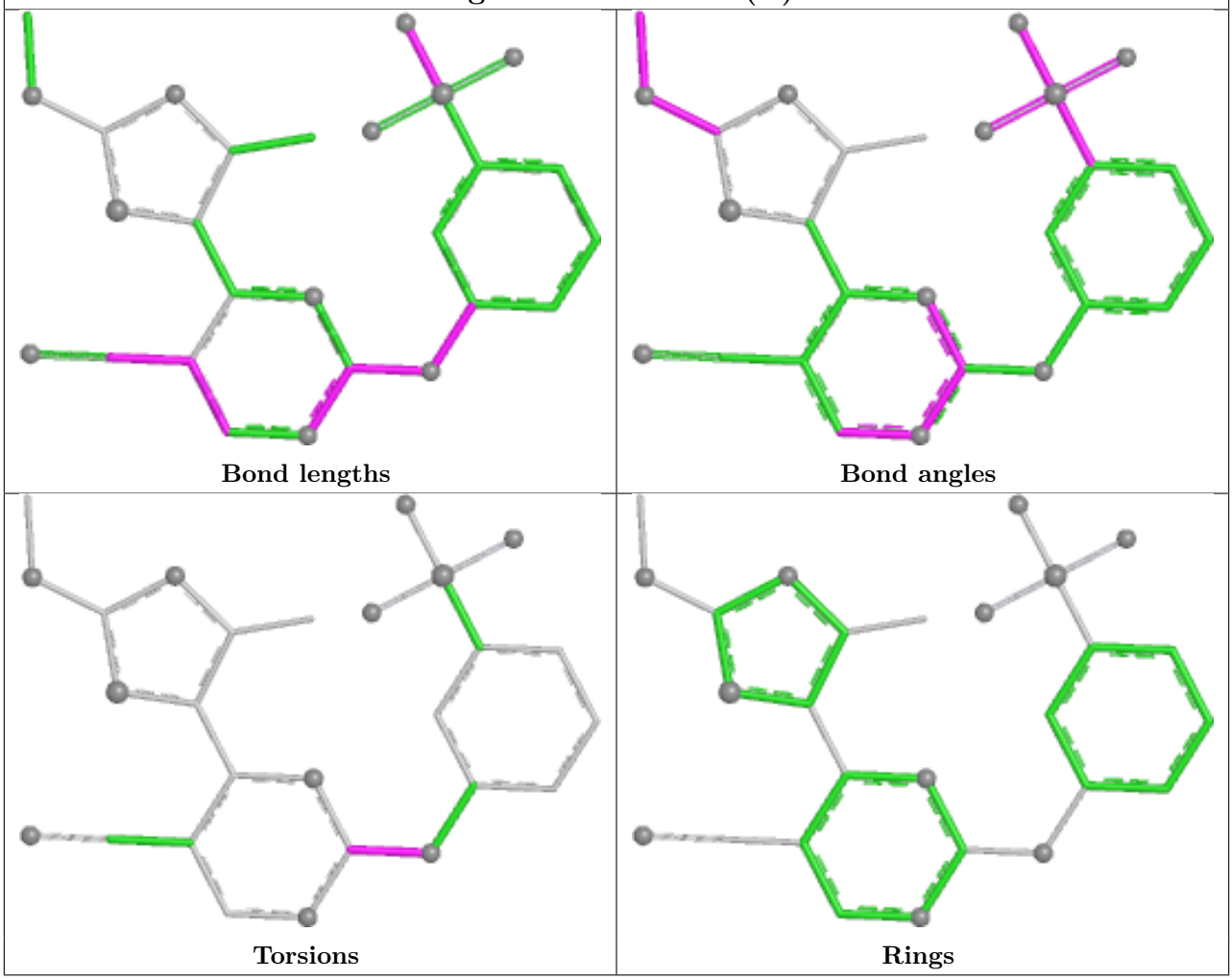


Rings

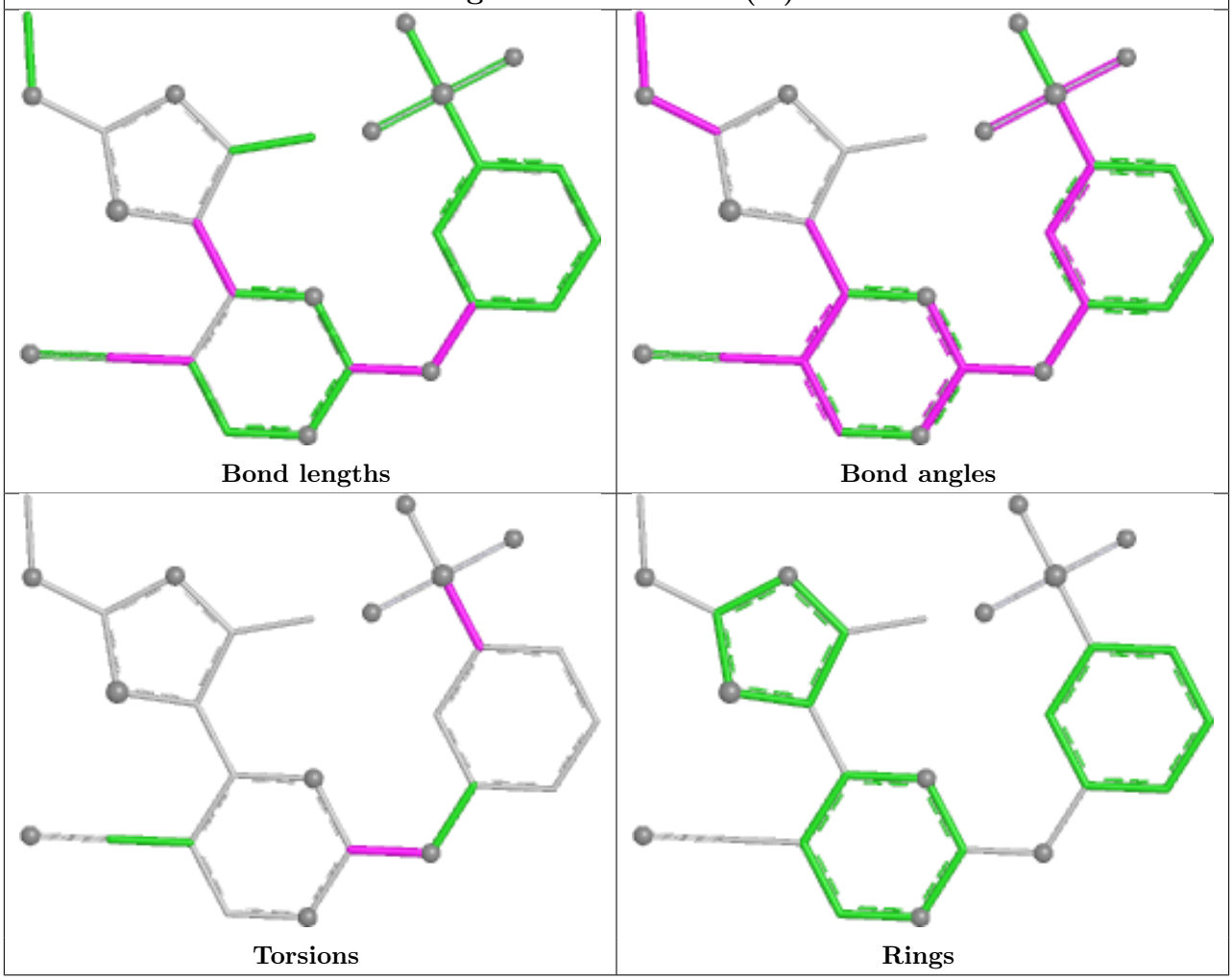
Ligand T3E C 1295 (A)



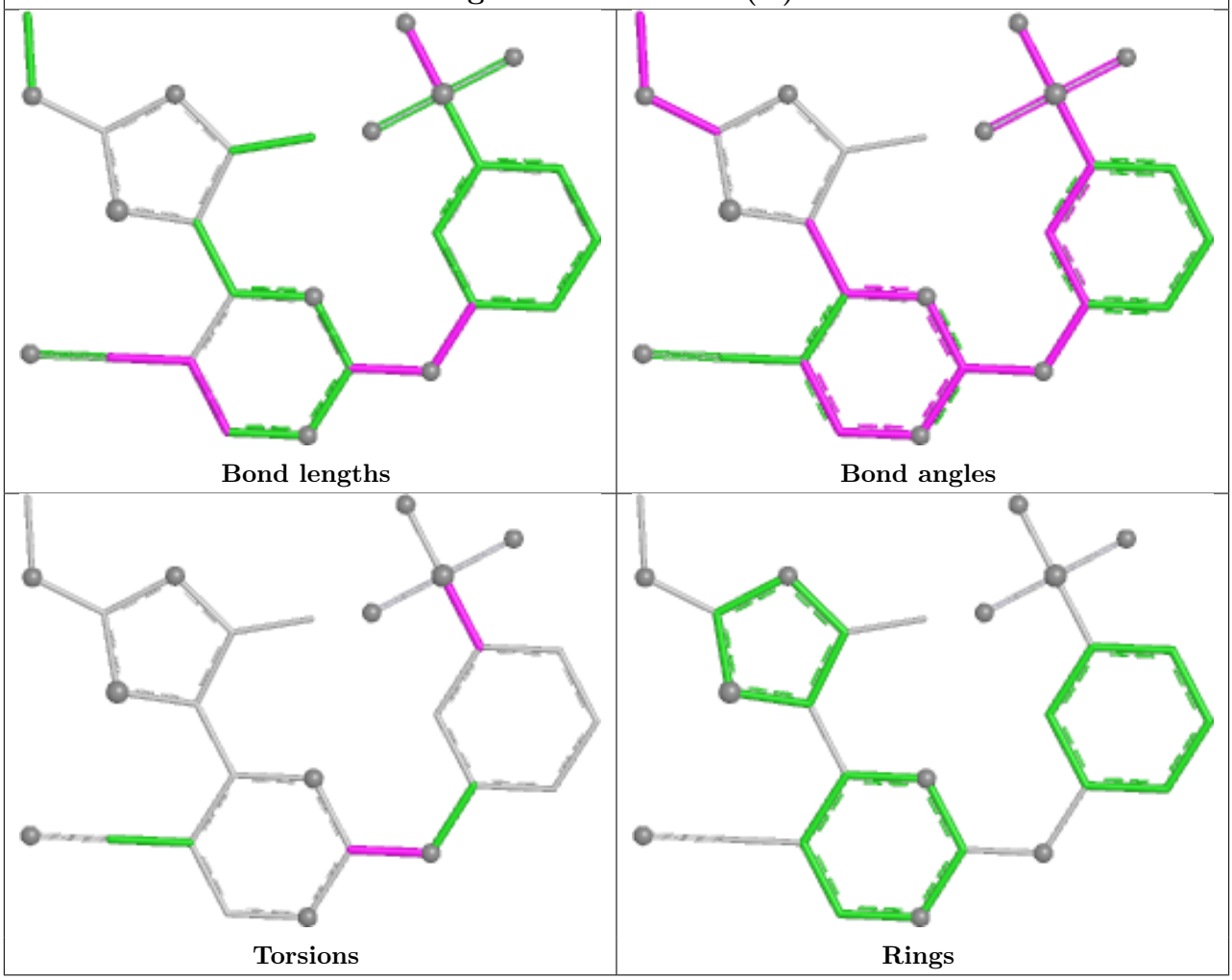
Ligand T3E C 1295 (B)



Ligand T3E A 1298 (D)



Ligand T3E A 1298 (C)



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	298/300 (99%)	0.02	13 (4%) 34 35	20, 32, 85, 121	0
1	C	293/300 (97%)	0.60	45 (15%) 2 1	32, 61, 104, 135	0
2	B	257/262 (98%)	0.05	19 (7%) 14 15	21, 34, 57, 89	0
2	D	253/262 (96%)	0.69	40 (15%) 2 1	30, 60, 110, 162	0
All	All	1101/1124 (97%)	0.34	117 (10%) 6 6	20, 46, 98, 162	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	THR	6.2
2	D	430	LEU	5.6
1	C	234	PRO	5.3
1	C	282	ALA	5.3
1	C	15	TYR	5.2
1	C	225	VAL	5.2
1	C	256	ASP	4.9
2	D	428	GLU	4.9
2	D	284	ASP	4.9
1	C	287	GLN	4.5
1	A	96	LEU	4.3
1	C	232	SER	4.2
1	A	95	ALA	4.2
2	D	429	THR	4.1
1	C	249	SER	4.1
2	D	324	PRO	4.1
2	D	416	SER	4.0
1	C	247	ASP	3.8
1	C	258	ASP	3.8
1	C	179	TYR	3.7
1	C	12	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	377	ILE	3.7
2	B	323	GLN	3.7
2	D	378	ARG	3.7
2	D	372	TRP	3.6
1	A	41	THR	3.6
2	D	388	LYS	3.5
1	A	-1	GLY	3.5
2	D	384	LEU	3.4
1	C	226	VAL	3.4
2	D	367	VAL	3.4
1	A	15	TYR	3.4
1	C	231	THR	3.4
1	A	36	ARG	3.3
2	D	323	GLN	3.3
1	A	297	ARG	3.3
2	D	385	GLU	3.3
2	D	311	VAL	3.3
2	B	355	ILE	3.3
1	C	236	TYR	3.2
2	D	415	ASN	3.2
1	C	101	LEU	3.2
2	D	197	VAL	3.2
1	A	38	ASP	3.2
1	C	255	LEU	3.2
2	B	356	ALA	3.2
2	B	311	VAL	3.1
1	C	189	LEU	3.1
2	B	284	ASP	3.0
2	D	271	TYR	3.0
2	B	236	VAL	2.9
2	B	336	LEU	2.9
1	A	73	GLU	2.9
1	C	143	LEU	2.8
2	B	324	PRO	2.8
2	B	337	GLY	2.8
2	B	431	ASN	2.8
2	D	422	SER	2.7
2	D	423	LEU	2.7
1	C	259	GLY	2.7
1	C	248	PHE	2.7
2	D	427	PRO	2.7
2	B	283	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	232	LEU	2.6
1	C	162	GLU	2.6
2	D	411	GLU	2.6
1	C	175	LEU	2.6
2	D	234	LEU	2.6
1	C	288	ASP	2.6
2	D	399	LEU	2.6
2	D	365	TYR	2.5
1	C	99	ILE	2.5
2	D	341	LEU	2.5
1	C	257	GLU	2.5
2	D	179	HIS	2.5
2	D	329	VAL	2.5
1	C	250	LYS	2.5
2	B	341	LEU	2.4
1	C	251	VAL	2.4
2	D	322	GLN	2.4
1	C	36	ARG	2.4
1	C	209	ILE	2.4
1	C	284	PRO	2.4
2	D	180	GLU	2.4
2	D	368	THR	2.4
1	C	227	TRP	2.4
2	B	315	LEU	2.3
2	B	359	ALA	2.3
2	D	336	LEU	2.3
1	C	166	LEU	2.3
1	C	-1	GLY	2.3
2	D	374	GLU	2.3
2	B	256	VAL	2.2
1	C	254	PRO	2.2
2	D	280	TYR	2.2
1	C	97	THR	2.2
1	A	111	LEU	2.2
1	C	245	ARG	2.2
1	C	246	GLN	2.1
2	B	239	ILE	2.1
2	D	339	LEU	2.1
1	C	293	VAL	2.1
2	D	369	GLY	2.1
1	C	272	ASN	2.1
2	B	357	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	143	LEU	2.1
1	C	128	LEU	2.1
2	B	215	VAL	2.1
2	D	381	GLY	2.1
2	D	419	HIS	2.0
1	C	178	LYS	2.0
1	C	228	PRO	2.0
1	A	37	LEU	2.0
2	D	233	HIS	2.0
1	C	186	ILE	2.0
1	C	177	CYS	2.0
2	D	356	ALA	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	0.14	49,56,69,70	0
1	TPO	A	160	11/12	0.99	0.06	23,26,30,34	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	T3E	A	1298[A]	27/27	0.89	0.18	28,38,46,48	42
3	T3E	A	1298[B]	27/27	0.89	0.18	28,36,46,47	42
3	T3E	A	1298[C]	27/27	0.89	0.18	28,37,59,70	42
3	T3E	A	1298[D]	27/27	0.89	0.18	28,38,60,68	42

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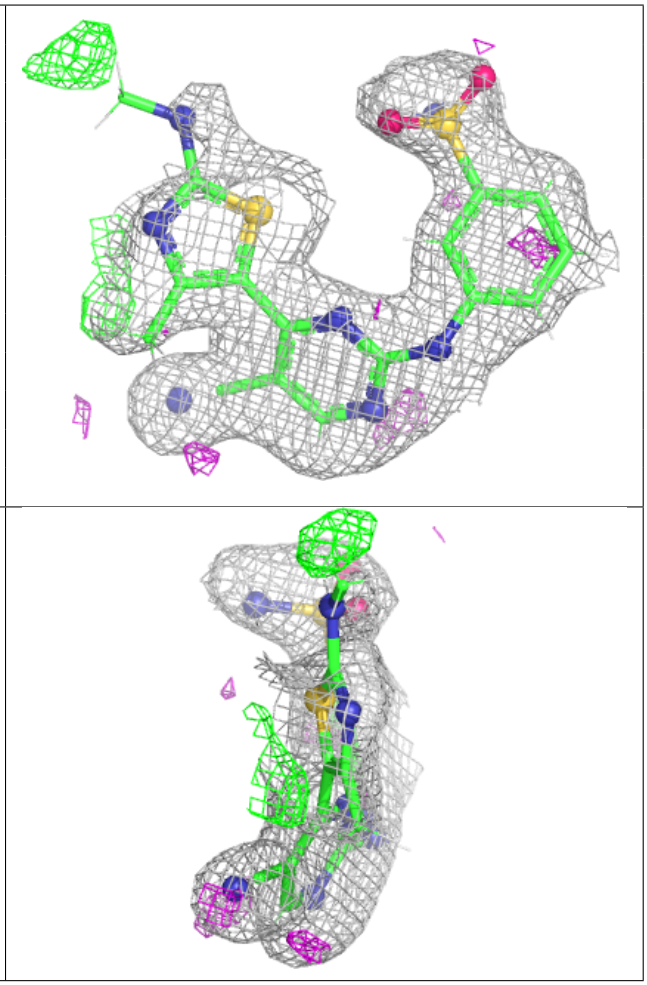
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SGM	A	1299	6/6	0.89	0.57	60,63,69,86	0
3	T3E	C	1295[B]	27/27	0.91	0.16	39,50,61,63	42
3	T3E	C	1295[C]	27/27	0.91	0.16	39,49,64,74	42
3	T3E	C	1295[D]	27/27	0.91	0.16	32,49,64,74	42
3	T3E	C	1295[A]	27/27	0.91	0.16	39,49,61,63	42

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.

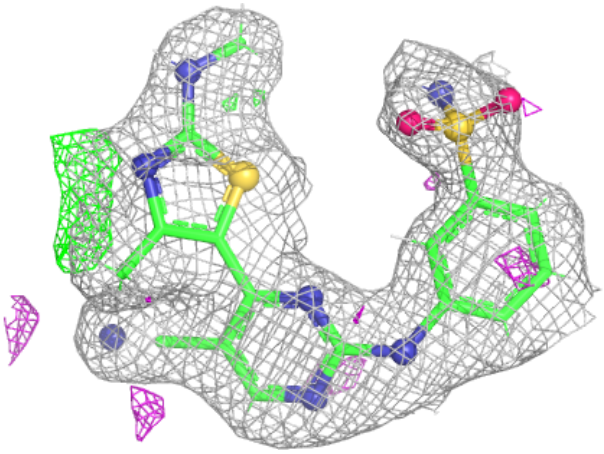
Electron density around T3E A 1298 (A):

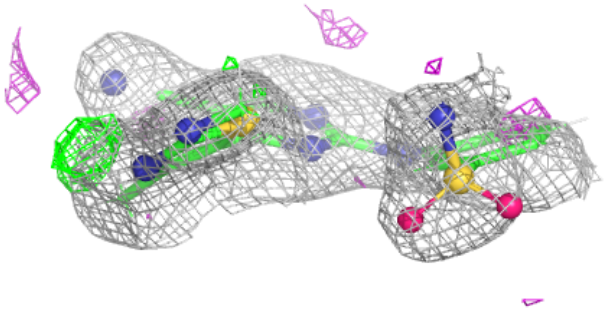
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

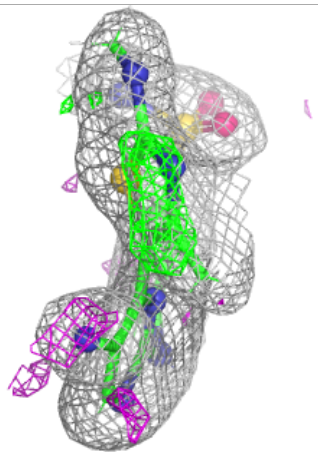


Electron density around T3E A 1298 (B):

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

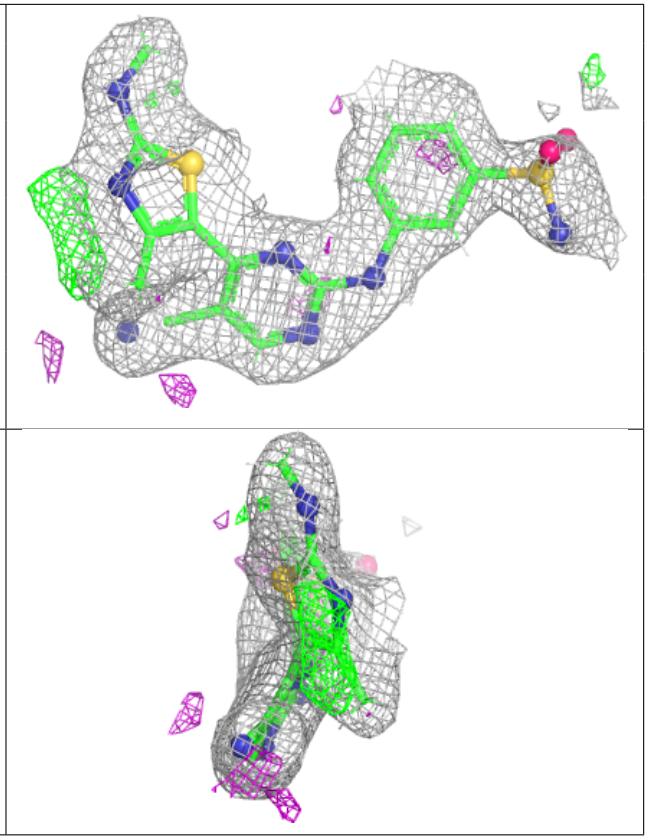






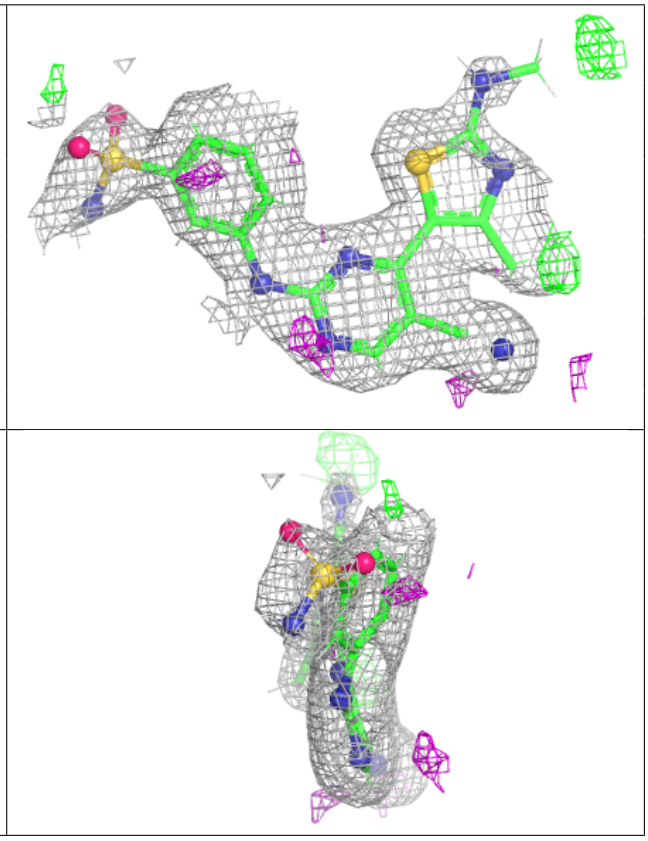
Electron density around T3E A 1298 (C):

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



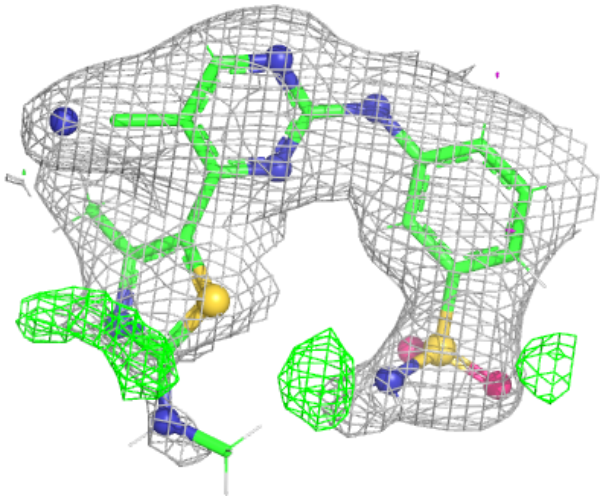
Electron density around T3E A 1298 (D):

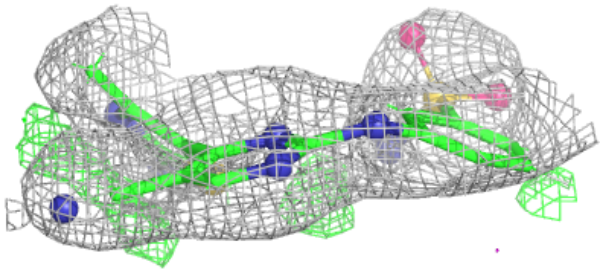
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

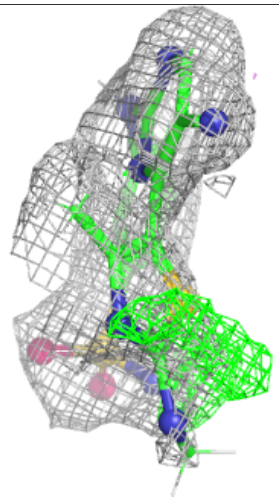


Electron density around T3E C 1295 (B):

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

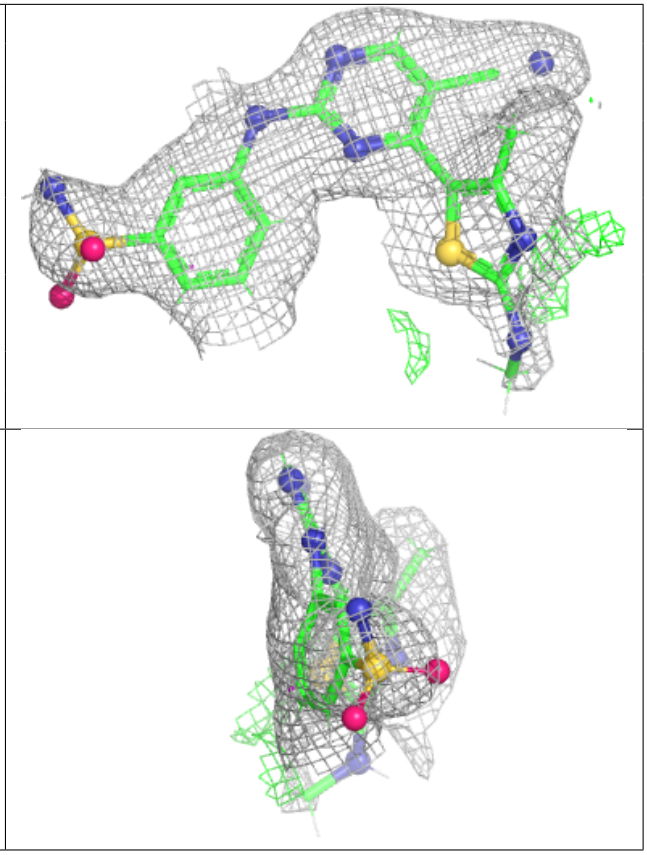






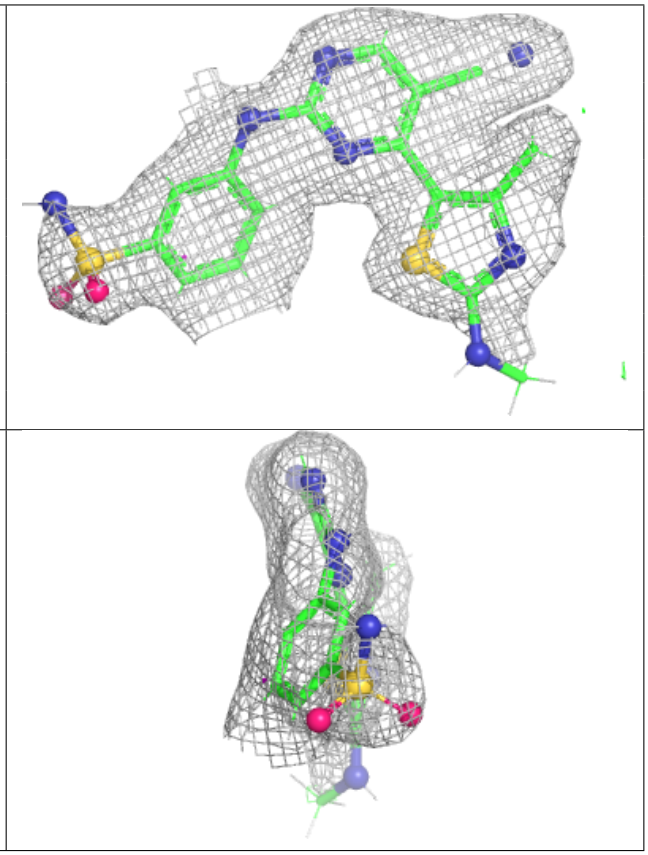
Electron density around T3E C 1295 (C):

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



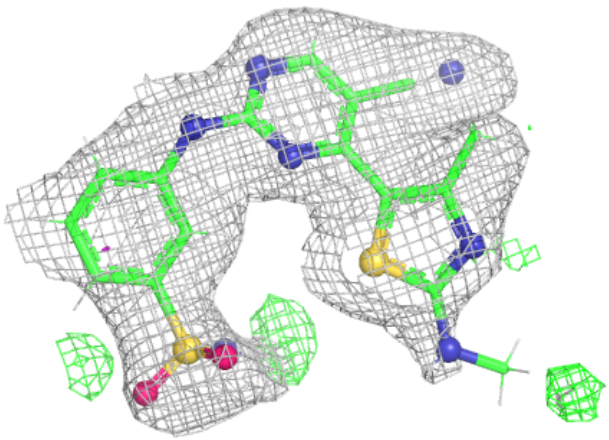
Electron density around T3E C 1295 (D):

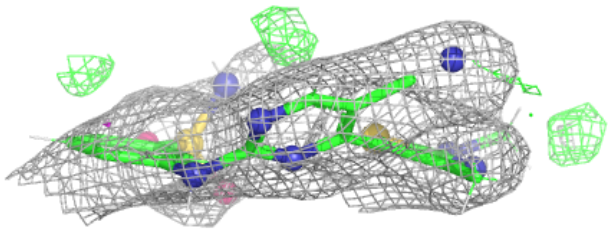
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

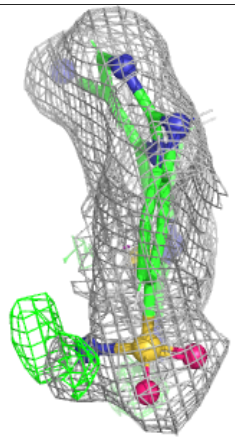


Electron density around T3E C 1295 (A):

$2mF_o$-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.