



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 04:54 am BST

PDB ID : 1OGP  
Title : The crystal structure of plant sulfite oxidase provides insight into sulfite oxidation in plants and animals  
Authors : Schrader, N.; Fischer, K.; Theis, K.; Mendel, R.R.; Schwarz, G.; Kisker, C.  
Deposited on : 2003-05-08  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

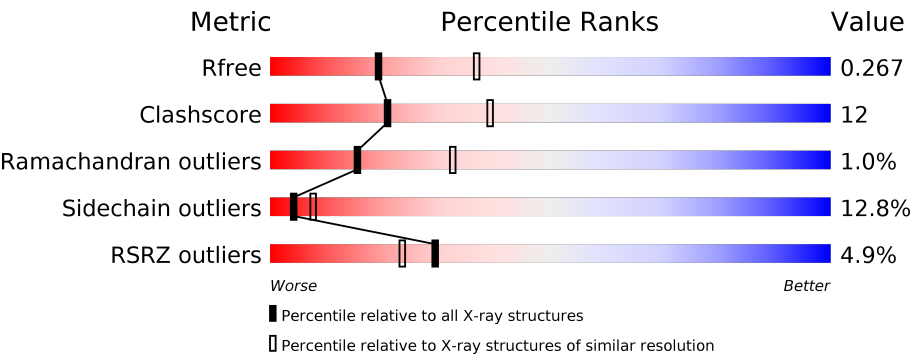
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	393	<div><div>5%</div><div><div></div><div>68%</div><div>24%</div><div>5%</div><div>..</div></div></div>
1	B	393	<div><div>3%</div><div><div></div><div>70%</div><div>22%</div><div>5%</div><div>..</div></div></div>
1	C	393	<div><div>5%</div><div><div></div><div>66%</div><div>25%</div><div>6%</div><div>..</div></div></div>
1	D	393	<div><div>9%</div><div><div></div><div>56%</div><div>30%</div><div>10%</div><div>..</div></div></div>
1	E	393	<div><div>4%</div><div><div></div><div>68%</div><div>25%</div><div>5%</div><div>..</div></div></div>
1	F	393	<div><div>3%</div><div><div></div><div>69%</div><div>23%</div><div>6%</div><div>..</div></div></div>

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	MTQ	D	1394	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18888 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SULFITE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			3014	1902	538	565	9			
1	B	388	Total	C	N	O	S	0	0	0
			3014	1902	538	565	9			
1	C	388	Total	C	N	O	S	0	0	0
			3014	1902	538	565	9			
1	D	388	Total	C	N	O	S	0	0	0
			3014	1902	538	565	9			
1	E	388	Total	C	N	O	S	0	0	0
			3014	1902	538	565	9			
1	F	388	Total	C	N	O	S	0	0	0
			3014	1902	538	565	9			

- Molecule 2 is CESIUM ION (three-letter code: CS) (formula: Cs).

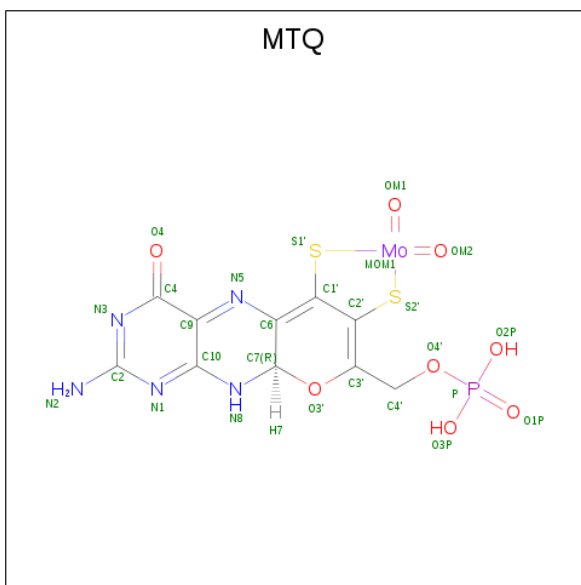
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Cs	0	0
			2	2		
2	E	2	Total	Cs	0	0
			2	2		
2	B	2	Total	Cs	0	0
			2	2		
2	C	2	Total	Cs	0	0
			2	2		
2	A	2	Total	Cs	0	0
			2	2		
2	F	2	Total	Cs	0	0
			2	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is (MOLYBDOPTERIN-S,S)-DIOXO-THIO-MOLYBDENUM(VI) (three-letter code: MTQ) (formula: C<sub>10</sub>H<sub>8</sub>MoN<sub>5</sub>O<sub>8</sub>PS<sub>2</sub>).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	A	1	Total 27	C 10	Mo 1	N 5	O 8	P 1	S 2	0	0
4	B	1	Total 27	C 10	Mo 1	N 5	O 8	P 1	S 2	0	0
4	C	1	Total 27	C 10	Mo 1	N 5	O 8	P 1	S 2	0	0
4	D	1	Total 27	C 10	Mo 1	N 5	O 8	P 1	S 2	0	0
4	E	1	Total 27	C 10	Mo 1	N 5	O 8	P 1	S 2	0	0
4	F	1	Total 27	C 10	Mo 1	N 5	O 8	P 1	S 2	0	0

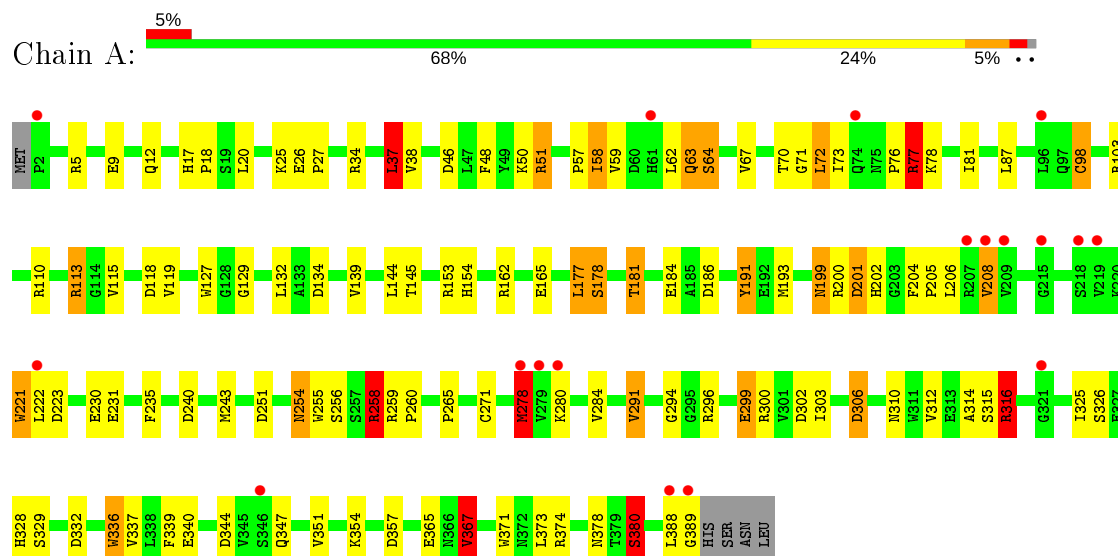
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	105	Total O 105 105	0	0
5	B	95	Total O 95 95	0	1
5	C	86	Total O 86 86	0	1
5	D	90	Total O 90 90	0	0
5	E	107	Total O 107 107	0	0
5	F	111	Total O 111 111	0	1

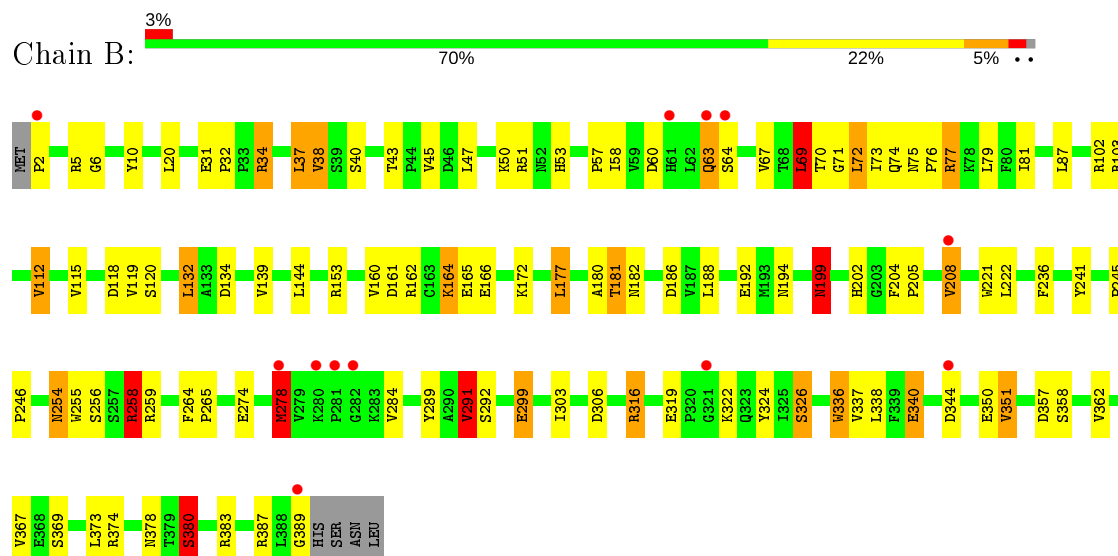
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: SULFITE OXIDASE

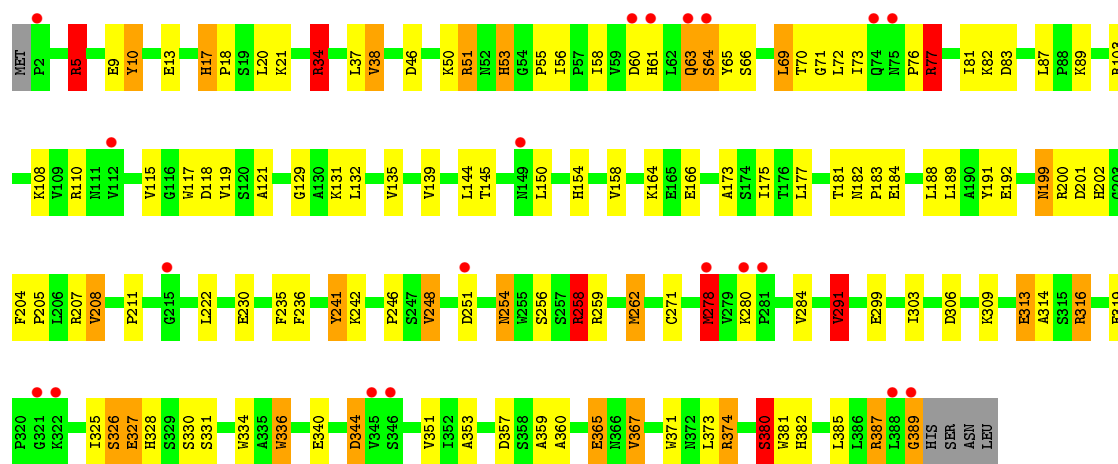


#### • Molecule 1: SULFITE OXIDASE

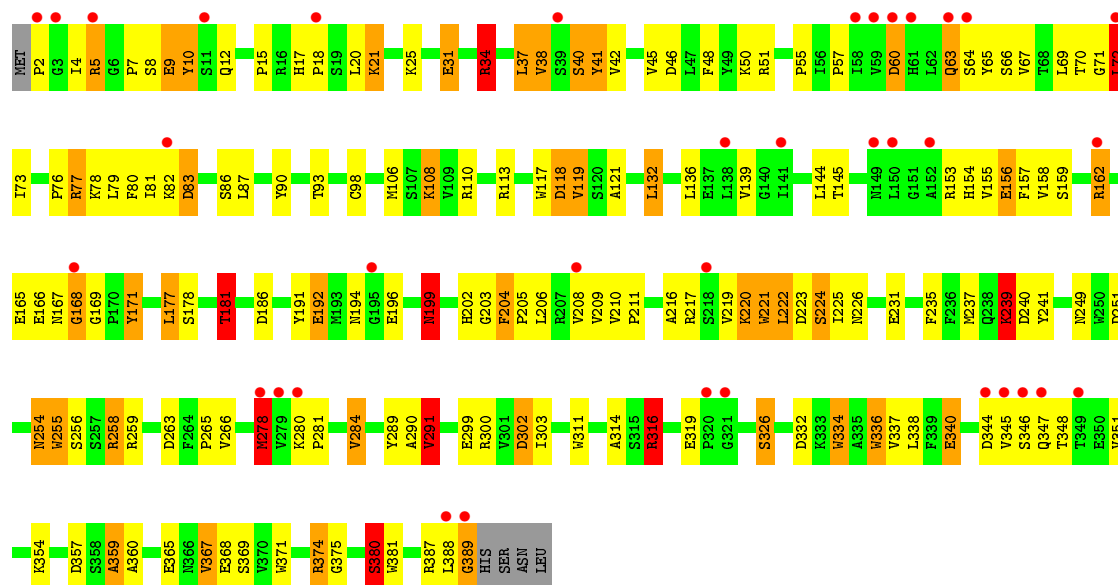


#### • Molecule 1: SULFITE OXIDASE

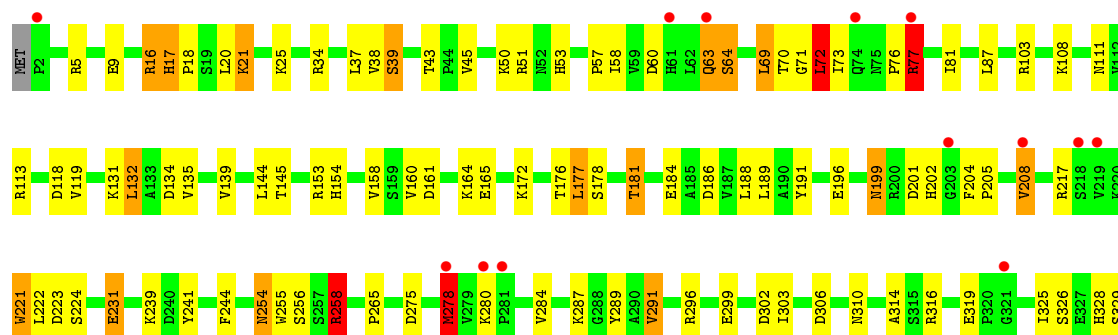




• Molecule 1: SULFITE OXIDASE



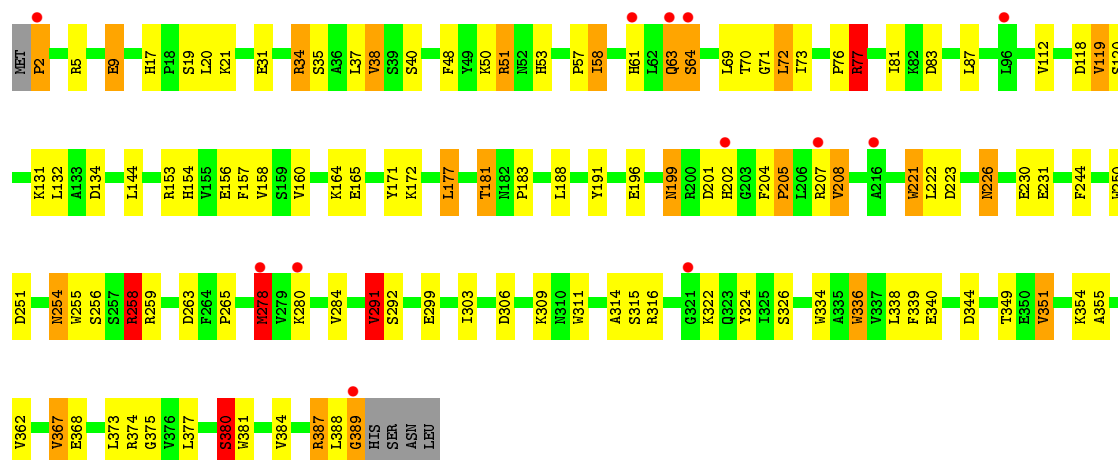
• Molecule 1: SULFITE OXIDASE







● Molecule 1: SULFITE OXIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	222.92Å 351.27Å 158.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	182.57 – 2.60 29.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (182.57-2.60) 99.0 (29.93-2.60)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.235 , 0.266 0.241 , 0.267	Depositor DCC
$R_{free}$ test set	9369 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.8	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 63.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	18888	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CS, GOL, MTQ

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	1.51	27/3085 (0.9%)	1.39	40/4196 (1.0%)
1	B	1.52	27/3085 (0.9%)	1.39	33/4196 (0.8%)
1	C	1.61	27/3085 (0.9%)	1.32	27/4196 (0.6%)
1	D	1.77	62/3085 (2.0%)	1.49	45/4196 (1.1%)
1	E	1.56	19/3085 (0.6%)	1.43	41/4196 (1.0%)
1	F	1.52	21/3085 (0.7%)	1.39	30/4196 (0.7%)
All	All	1.58	183/18510 (1.0%)	1.40	216/25176 (0.9%)

All (183) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	389	GLY	C-O	11.27	1.41	1.23
1	D	156	GLU	CD-OE1	10.77	1.37	1.25
1	A	278	MET	CG-SD	10.02	2.07	1.81
1	B	278	MET	CG-SD	9.57	2.06	1.81
1	C	241	TYR	CD2-CE2	9.55	1.53	1.39
1	D	192	GLU	CD-OE1	9.29	1.35	1.25
1	E	278	MET	SD-CE	9.19	2.29	1.77
1	D	10	TYR	CD1-CE1	-9.16	1.25	1.39
1	F	355	ALA	CA-CB	-9.10	1.33	1.52
1	B	350	GLU	CD-OE2	8.94	1.35	1.25
1	C	262	MET	CG-SD	8.63	2.03	1.81
1	E	380	SER	CB-OG	-8.52	1.31	1.42
1	D	368	GLU	CD-OE1	8.05	1.34	1.25
1	C	248	VAL	CB-CG2	8.00	1.69	1.52
1	A	371	TRP	CB-CG	8.00	1.64	1.50
1	F	278	MET	CG-SD	7.98	2.01	1.81
1	B	316	ARG	CB-CG	-7.76	1.31	1.52
1	C	327	GLU	CD-OE1	7.66	1.34	1.25
1	D	359	ALA	CA-CB	-7.55	1.36	1.52
1	B	324	TYR	CD1-CE1	-7.54	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	278	MET	CB-CG	7.53	1.75	1.51
1	C	389	GLY	C-O	7.51	1.35	1.23
1	B	45	VAL	CB-CG2	7.42	1.68	1.52
1	B	192	GLU	CD-OE1	7.42	1.33	1.25
1	A	380	SER	CB-OG	-7.38	1.32	1.42
1	B	362	VAL	CB-CG2	-7.33	1.37	1.52
1	D	278	MET	SD-CE	7.32	2.18	1.77
1	B	350	GLU	CD-OE1	7.21	1.33	1.25
1	D	221	TRP	CG-CD1	7.20	1.46	1.36
1	E	108	LYS	CD-CE	7.15	1.69	1.51
1	F	191	TYR	CD1-CE1	7.13	1.50	1.39
1	B	241	TYR	CD1-CE1	-7.07	1.28	1.39
1	D	65	TYR	CG-CD1	7.02	1.48	1.39
1	E	278	MET	CG-SD	6.98	1.99	1.81
1	E	221	TRP	CG-CD1	-6.96	1.27	1.36
1	D	10	TYR	CD2-CE2	-6.92	1.28	1.39
1	F	316	ARG	CB-CG	-6.88	1.33	1.52
1	D	380	SER	CB-OG	-6.88	1.33	1.42
1	D	21	LYS	CD-CE	6.86	1.68	1.51
1	C	353	ALA	CA-CB	-6.81	1.38	1.52
1	C	65	TYR	CD1-CE1	-6.76	1.29	1.39
1	A	316	ARG	CB-CG	-6.70	1.34	1.52
1	B	274	GLU	CD-OE1	6.69	1.33	1.25
1	C	173	ALA	CA-CB	6.67	1.66	1.52
1	D	204	PHE	CD2-CE2	6.66	1.52	1.39
1	F	244	PHE	CD2-CE2	-6.65	1.25	1.39
1	F	230	GLU	CD-OE1	6.64	1.32	1.25
1	C	66	SER	CB-OG	6.57	1.50	1.42
1	A	367	VAL	CB-CG1	-6.57	1.39	1.52
1	B	351	VAL	CB-CG1	-6.54	1.39	1.52
1	D	41	TYR	CD2-CE2	6.54	1.49	1.39
1	A	235	PHE	CE1-CZ	6.53	1.49	1.37
1	A	34	ARG	CB-CG	-6.44	1.35	1.52
1	C	166	GLU	CD-OE1	6.42	1.32	1.25
1	F	221	TRP	CB-CG	-6.42	1.38	1.50
1	E	191	TYR	CE2-CZ	6.41	1.46	1.38
1	C	200	ARG	NE-CZ	6.41	1.41	1.33
1	D	239	LYS	CD-CE	6.39	1.67	1.51
1	A	278	MET	CB-CG	6.36	1.71	1.51
1	E	39	SER	CB-OG	-6.36	1.33	1.42
1	B	199	ASN	CB-CG	-6.32	1.36	1.51
1	B	115	VAL	CA-CB	-6.30	1.41	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	365	GLU	CG-CD	6.30	1.61	1.51
1	D	191	TYR	CD2-CE2	6.28	1.48	1.39
1	D	368	GLU	CG-CD	6.24	1.61	1.51
1	F	250	TRP	CB-CG	-6.24	1.39	1.50
1	D	108	LYS	CG-CD	6.23	1.73	1.52
1	D	31	GLU	CD-OE2	6.22	1.32	1.25
1	F	165	GLU	CD-OE1	6.21	1.32	1.25
1	D	235	PHE	CD2-CE2	6.20	1.51	1.39
1	E	231	GLU	CD-OE1	-6.19	1.18	1.25
1	D	311	TRP	CB-CG	6.19	1.61	1.50
1	C	166	GLU	CD-OE2	6.18	1.32	1.25
1	C	65	TYR	CE2-CZ	-6.15	1.30	1.38
1	D	258	ARG	CD-NE	-6.14	1.36	1.46
1	C	316	ARG	CB-CG	-6.14	1.35	1.52
1	D	65	TYR	CE2-CZ	6.11	1.46	1.38
1	C	313	GLU	CD-OE2	6.09	1.32	1.25
1	D	159	SER	CB-OG	6.09	1.50	1.42
1	A	165	GLU	CD-OE2	6.09	1.32	1.25
1	E	165	GLU	CD-OE1	6.08	1.32	1.25
1	E	45	VAL	CB-CG2	6.06	1.65	1.52
1	A	365	GLU	CG-CD	6.05	1.61	1.51
1	D	354	LYS	CB-CG	-6.05	1.36	1.52
1	A	300	ARG	CB-CG	-6.04	1.36	1.52
1	C	184	GLU	CG-CD	6.02	1.60	1.51
1	D	239	LYS	CE-NZ	6.01	1.64	1.49
1	E	256	SER	CB-OG	-6.00	1.34	1.42
1	B	112	VAL	CA-CB	5.97	1.67	1.54
1	D	255	TRP	CB-CG	-5.97	1.39	1.50
1	E	111	ASN	CB-CG	-5.96	1.37	1.51
1	D	311	TRP	CG-CD1	5.93	1.45	1.36
1	A	230	GLU	CD-OE1	5.89	1.32	1.25
1	F	9	GLU	CD-OE2	5.87	1.32	1.25
1	A	178	SER	CB-OG	-5.87	1.34	1.42
1	D	93	THR	C-O	5.86	1.34	1.23
1	E	165	GLU	CG-CD	5.86	1.60	1.51
1	F	230	GLU	CG-CD	5.86	1.60	1.51
1	D	9	GLU	CD-OE2	5.85	1.32	1.25
1	D	168	GLY	C-O	5.84	1.33	1.23
1	D	108	LYS	CD-CE	5.79	1.65	1.51
1	B	40	SER	CB-OG	-5.78	1.34	1.42
1	E	241	TYR	CB-CG	-5.75	1.43	1.51
1	B	303	ILE	CA-CB	-5.73	1.41	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	TRP	CG-CD1	-5.72	1.28	1.36
1	B	166	GLU	CD-OE2	5.72	1.31	1.25
1	D	290	ALA	CA-CB	-5.72	1.40	1.52
1	D	374	ARG	CZ-NH1	5.72	1.40	1.33
1	E	184	GLU	CD-OE1	5.71	1.31	1.25
1	C	365	GLU	CD-OE1	5.68	1.31	1.25
1	A	191	TYR	CB-CG	5.68	1.60	1.51
1	C	278	MET	SD-CE	5.68	2.09	1.77
1	A	139	VAL	CB-CG2	-5.67	1.41	1.52
1	B	337	VAL	CB-CG1	-5.67	1.41	1.52
1	C	235	PHE	CD2-CE2	5.64	1.50	1.39
1	A	365	GLU	CD-OE1	5.62	1.31	1.25
1	D	220	LYS	CD-CE	5.61	1.65	1.51
1	B	6	GLY	C-O	-5.59	1.14	1.23
1	B	358	SER	C-O	-5.59	1.12	1.23
1	B	241	TYR	CB-CG	5.57	1.60	1.51
1	D	9	GLU	CD-OE1	5.57	1.31	1.25
1	D	113	ARG	CB-CG	-5.57	1.37	1.52
1	F	278	MET	CB-CG	5.56	1.69	1.51
1	B	10	TYR	CE1-CZ	5.55	1.45	1.38
1	D	340	GLU	CG-CD	5.55	1.60	1.51
1	D	204	PHE	CE1-CZ	5.55	1.47	1.37
1	D	171	TYR	CD2-CE2	5.55	1.47	1.39
1	D	5	ARG	CZ-NH1	5.49	1.40	1.33
1	D	15	PRO	CG-CD	5.47	1.68	1.50
1	D	231	GLU	CD-OE1	5.47	1.31	1.25
1	F	258	ARG	CG-CD	5.46	1.65	1.51
1	A	127	TRP	CG-CD1	-5.45	1.29	1.36
1	F	368	GLU	CD-OE1	5.45	1.31	1.25
1	D	258	ARG	NE-CZ	-5.45	1.25	1.33
1	F	324	TYR	CB-CG	5.45	1.59	1.51
1	A	299	GLU	CD-OE2	5.44	1.31	1.25
1	D	199	ASN	CB-CG	-5.43	1.38	1.51
1	D	156	GLU	CG-CD	5.40	1.60	1.51
1	C	82	LYS	CD-CE	5.39	1.64	1.51
1	D	371	TRP	CB-CG	5.39	1.59	1.50
1	D	209	VAL	CB-CG2	5.38	1.64	1.52
1	D	235	PHE	CD1-CE1	5.37	1.50	1.39
1	F	334	TRP	CB-CG	-5.37	1.40	1.50
1	C	291	VAL	CA-CB	5.37	1.66	1.54
1	A	165	GLU	CD-OE1	5.36	1.31	1.25
1	C	230	GLU	CG-CD	5.35	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	48	PHE	CD1-CE1	-5.35	1.28	1.39
1	E	21	LYS	CD-CE	5.32	1.64	1.51
1	A	294	GLY	C-O	-5.31	1.15	1.23
1	D	220	LYS	CE-NZ	5.30	1.62	1.49
1	B	289	TYR	CE1-CZ	5.29	1.45	1.38
1	E	244	PHE	CD1-CE1	-5.29	1.28	1.39
1	B	383	ARG	CD-NE	5.28	1.55	1.46
1	D	316	ARG	NE-CZ	5.28	1.40	1.33
1	F	2	PRO	CB-CG	5.28	1.76	1.50
1	A	278	MET	SD-CE	5.23	2.07	1.77
1	D	166	GLU	CD-OE2	5.22	1.31	1.25
1	F	157	PHE	CD1-CE1	-5.22	1.28	1.39
1	A	271	CYS	CB-SG	-5.21	1.73	1.81
1	D	192	GLU	CG-CD	5.19	1.59	1.51
1	D	266	VAL	CA-CB	-5.17	1.43	1.54
1	D	334	TRP	CE3-CZ3	5.15	1.47	1.38
1	C	184	GLU	CD-OE2	5.14	1.31	1.25
1	A	230	GLU	CG-CD	5.14	1.59	1.51
1	C	316	ARG	CG-CD	5.14	1.64	1.51
1	D	10	TYR	CE1-CZ	-5.13	1.31	1.38
1	D	241	TYR	CD1-CE1	-5.11	1.31	1.39
1	D	369	SER	CB-OG	5.11	1.48	1.42
1	F	384	VAL	CB-CG1	-5.10	1.42	1.52
1	E	131	LYS	CD-CE	5.10	1.64	1.51
1	C	278	MET	CB-CG	5.09	1.67	1.51
1	A	98	CYS	CB-SG	5.08	1.90	1.82
1	F	351	VAL	CB-CG2	-5.07	1.42	1.52
1	D	162	ARG	CZ-NH1	5.06	1.39	1.33
1	C	10	TYR	CD1-CE1	5.06	1.47	1.39
1	D	300	ARG	CZ-NH1	5.05	1.39	1.33
1	E	365	GLU	CG-CD	5.04	1.59	1.51
1	A	354	LYS	CD-CE	5.04	1.63	1.51
1	B	258	ARG	NE-CZ	-5.03	1.26	1.33
1	D	12	GLN	CG-CD	5.03	1.62	1.51
1	D	316	ARG	CZ-NH1	5.03	1.39	1.33
1	A	389	GLY	C-O	5.02	1.31	1.23
1	B	299	GLU	CD-OE1	5.02	1.31	1.25

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	258	ARG	NE-CZ-NH1	19.98	130.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	258	ARG	NE-CZ-NH2	-18.19	111.20	120.30
1	F	258	ARG	NE-CZ-NH2	-17.91	111.34	120.30
1	E	258	ARG	NE-CZ-NH1	15.58	128.09	120.30
1	F	259	ARG	NE-CZ-NH2	-14.73	112.93	120.30
1	D	258	ARG	NE-CZ-NH2	-13.19	113.71	120.30
1	A	258	ARG	NE-CZ-NH2	-12.91	113.84	120.30
1	B	258	ARG	NE-CZ-NH2	-12.72	113.94	120.30
1	A	258	ARG	NE-CZ-NH1	11.72	126.16	120.30
1	B	259	ARG	NE-CZ-NH2	-11.30	114.65	120.30
1	D	60	ASP	CB-CG-OD2	11.27	128.44	118.30
1	E	275	ASP	CB-CG-OD2	11.16	128.34	118.30
1	E	302	ASP	CB-CG-OD2	11.15	128.33	118.30
1	A	201	ASP	CB-CG-OD2	11.00	128.20	118.30
1	A	186	ASP	CB-CG-OD2	10.97	128.18	118.30
1	A	51	ARG	NE-CZ-NH1	10.55	125.58	120.30
1	D	34	ARG	NE-CZ-NH2	-10.31	115.15	120.30
1	B	389	GLY	CA-C-O	10.02	138.64	120.60
1	C	258	ARG	NE-CZ-NH2	-9.91	115.34	120.30
1	F	263	ASP	CB-CG-OD2	9.85	127.17	118.30
1	B	199	ASN	CB-CA-C	-9.70	91.01	110.40
1	B	278	MET	CG-SD-CE	9.39	115.22	100.20
1	C	60	ASP	CB-CG-OD2	9.34	126.70	118.30
1	A	208	VAL	CB-CA-C	-9.31	93.71	111.40
1	D	258	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	A	118	ASP	CB-CG-OD2	9.21	126.59	118.30
1	D	186	ASP	CB-CG-OD2	9.17	126.56	118.30
1	A	223	ASP	CB-CG-OD2	9.09	126.48	118.30
1	B	258	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	D	110	ARG	NE-CZ-NH1	8.93	124.76	120.30
1	D	259	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	F	118	ASP	CB-CG-OD2	8.83	126.25	118.30
1	E	374	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	D	217	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	D	223	ASP	CB-CG-OD2	8.62	126.06	118.30
1	A	316	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	F	291	VAL	CB-CA-C	-8.55	95.16	111.40
1	B	60	ASP	CB-CG-OD2	8.52	125.97	118.30
1	A	199	ASN	CB-CA-C	-8.48	93.44	110.40
1	E	316	ARG	CG-CD-NE	-8.39	94.17	111.80
1	E	296	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	B	208	VAL	CB-CA-C	-8.32	95.59	111.40
1	D	259	ARG	NE-CZ-NH1	8.25	124.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	291	VAL	CB-CA-C	-8.21	95.79	111.40
1	E	199	ASN	CB-CA-C	-8.16	94.08	110.40
1	E	380	SER	CB-CA-C	-8.12	94.68	110.10
1	A	380	SER	CB-CA-C	-8.00	94.90	110.10
1	E	275	ASP	CB-CG-OD1	-7.90	111.19	118.30
1	A	77	ARG	NE-CZ-NH1	7.89	124.24	120.30
1	B	291	VAL	CB-CA-C	-7.84	96.50	111.40
1	A	291	VAL	CB-CA-C	-7.83	96.53	111.40
1	D	291	VAL	CB-CA-C	-7.76	96.65	111.40
1	B	350	GLU	OE1-CD-OE2	7.74	132.59	123.30
1	E	316	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	E	208	VAL	CB-CA-C	-7.67	96.83	111.40
1	E	389	GLY	CA-C-O	7.62	134.33	120.60
1	B	316	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	A	302	ASP	CB-CG-OD2	7.49	125.04	118.30
1	D	199	ASN	CB-CA-C	-7.49	95.41	110.40
1	E	357	ASP	CB-CG-OD2	7.45	125.00	118.30
1	A	258	ARG	CG-CD-NE	-7.40	96.27	111.80
1	A	200	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	E	134	ASP	CB-CG-OD2	7.22	124.80	118.30
1	D	217	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	F	77	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	D	5	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	316	ARG	CG-CD-NE	-7.09	96.91	111.80
1	A	162	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	C	327	GLU	N-CA-CB	7.08	123.35	110.60
1	E	103	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	A	200	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	D	46	ASP	CB-CG-OD2	6.98	124.58	118.30
1	A	51	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	D	113	ARG	CB-CA-C	-6.92	96.56	110.40
1	F	258	ARG	CD-NE-CZ	6.90	133.26	123.60
1	F	223	ASP	CB-CG-OD2	6.89	124.50	118.30
1	C	291	VAL	CB-CA-C	-6.85	98.39	111.40
1	C	357	ASP	CB-CG-OD2	6.80	124.42	118.30
1	E	316	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	F	77	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	F	207	ARG	NE-CZ-NH2	6.72	123.66	120.30
1	D	60	ASP	CB-CG-OD1	-6.69	112.28	118.30
1	F	380	SER	CB-CA-C	-6.68	97.41	110.10
1	E	16	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	C	344	ASP	CB-CG-OD2	6.66	124.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	A	251	ASP	CB-CG-OD1	6.58	124.23	118.30
1	C	200	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	B	134	ASP	CB-CG-OD2	6.54	124.19	118.30
1	D	83	ASP	CB-CG-OD2	6.54	124.19	118.30
1	D	258	ARG	CG-CD-NE	-6.54	98.06	111.80
1	B	186	ASP	CB-CG-OD1	6.51	124.16	118.30
1	F	134	ASP	CB-CG-OD2	6.49	124.14	118.30
1	D	302	ASP	CB-CG-OD2	6.46	124.11	118.30
1	C	118	ASP	CB-CG-OD2	6.41	124.07	118.30
1	F	387	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	C	306	ASP	CB-CG-OD1	6.40	124.06	118.30
1	F	306	ASP	CB-CG-OD1	6.36	124.02	118.30
1	B	69	LEU	CA-CB-CG	-6.32	100.76	115.30
1	B	103	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	D	389	GLY	CA-C-O	6.29	131.92	120.60
1	E	161	ASP	CB-CG-OD1	6.27	123.94	118.30
1	E	34	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	D	316	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	C	83	ASP	CB-CG-OD2	6.25	123.93	118.30
1	E	153	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	D	237	MET	CG-SD-CE	-6.24	90.22	100.20
1	A	240	ASP	CB-CG-OD1	6.20	123.88	118.30
1	D	240	ASP	CB-CG-OD1	6.19	123.87	118.30
1	D	302	ASP	CB-CA-C	-6.19	98.02	110.40
1	E	217	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	F	316	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	E	69	LEU	CA-CB-CG	-6.08	101.32	115.30
1	C	158	VAL	CB-CA-C	-6.07	99.86	111.40
1	E	357	ASP	OD1-CG-OD2	-6.07	111.76	123.30
1	C	5	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	D	153	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	F	208	VAL	CB-CA-C	-6.02	99.96	111.40
1	F	278	MET	CG-SD-CE	6.00	109.80	100.20
1	E	201	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	67	VAL	CB-CA-C	-5.98	100.04	111.40
1	C	77	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	77	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	A	344	ASP	CB-CG-OD2	5.96	123.67	118.30
1	B	161	ASP	CB-CG-OD2	5.96	123.67	118.30
1	F	326	SER	C-N-CA	-5.96	106.80	121.70
1	D	110	ARG	NE-CZ-NH2	-5.95	117.32	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	118	ASP	CB-CG-OD2	5.94	123.64	118.30
1	C	326	SER	C-N-CA	-5.92	106.89	121.70
1	F	83	ASP	CB-CG-OD2	5.92	123.63	118.30
1	E	5	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	E	132	LEU	CB-CG-CD2	5.90	121.03	111.00
1	E	60	ASP	CB-CG-OD2	5.87	123.58	118.30
1	E	77	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	344	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	134	ASP	CB-CG-OD2	5.85	123.57	118.30
1	E	186	ASP	CB-CG-OD2	5.84	123.56	118.30
1	E	113	ARG	CB-CA-C	-5.82	98.76	110.40
1	C	316	ARG	CB-CA-C	5.81	122.03	110.40
1	D	374	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	C	208	VAL	CB-CA-C	-5.79	100.41	111.40
1	E	326	SER	C-N-CA	-5.75	107.32	121.70
1	D	239	LYS	CA-CB-CG	5.75	126.04	113.40
1	A	34	ARG	N-CA-CB	-5.71	100.31	110.60
1	D	8	SER	CB-CA-C	-5.70	99.27	110.10
1	E	388	LEU	CB-CG-CD1	-5.68	101.34	111.00
1	E	72	LEU	CB-CG-CD1	5.67	120.64	111.00
1	C	77	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	F	263	ASP	OD1-CG-OD2	-5.64	112.58	123.30
1	A	306	ASP	CB-CG-OD2	5.63	123.37	118.30
1	C	259	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	326	SER	C-N-CA	-5.62	107.66	121.70
1	B	102	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	278	MET	CB-CG-SD	5.57	129.12	112.40
1	B	326	SER	C-N-CA	-5.54	107.84	121.70
1	E	223	ASP	CB-CG-OD2	5.51	123.26	118.30
1	F	201	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B	387	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	E	43	THR	OG1-CB-CG2	-5.51	97.33	110.00
1	E	357	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	153	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	F	326	SER	O-C-N	-5.46	113.97	122.70
1	B	188	LEU	CB-CG-CD1	-5.45	101.74	111.00
1	F	316	ARG	CG-CD-NE	-5.44	100.37	111.80
1	C	69	LEU	CA-CB-CG	-5.44	102.80	115.30
1	B	357	ASP	CB-CG-OD1	5.43	123.18	118.30
1	B	118	ASP	CB-CG-OD2	5.38	123.14	118.30
1	C	380	SER	CB-CA-C	-5.38	99.88	110.10
1	A	113	ARG	NE-CZ-NH1	-5.37	117.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	ARG	CG-CD-NE	-5.36	100.54	111.80
1	C	258	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	46	ASP	CB-CG-OD1	5.33	123.09	118.30
1	F	389	GLY	CA-C-O	-5.33	111.01	120.60
1	D	387	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	F	251	ASP	CB-CG-OD1	5.31	123.08	118.30
1	D	118	ASP	CB-CG-OD2	5.30	123.08	118.30
1	D	326	SER	C-N-CA	-5.30	108.44	121.70
1	A	296	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	332	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	357	ASP	CB-CG-OD1	5.27	123.04	118.30
1	F	34	ARG	N-CA-CB	-5.26	101.14	110.60
1	D	108	LYS	CD-CE-NZ	5.25	123.79	111.70
1	D	181	THR	N-CA-CB	-5.25	100.33	110.30
1	C	34	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	E	258	ARG	CG-CD-NE	-5.24	100.80	111.80
1	A	326	SER	O-C-N	-5.23	114.33	122.70
1	D	162	ARG	CG-CD-NE	-5.23	100.82	111.80
1	D	357	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	34	ARG	N-CA-CB	-5.22	101.20	110.60
1	B	326	SER	O-C-N	-5.21	114.36	122.70
1	C	46	ASP	CB-CG-OD1	5.20	122.98	118.30
1	F	362	VAL	CG1-CB-CG2	-5.19	102.59	110.90
1	A	37	LEU	CA-CB-CG	5.18	127.22	115.30
1	E	258	ARG	CD-NE-CZ	5.18	130.85	123.60
1	D	263	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	243	MET	CG-SD-CE	5.15	108.44	100.20
1	C	326	SER	O-C-N	-5.14	114.48	122.70
1	A	259	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	278	MET	CB-CG-SD	5.13	127.80	112.40
1	A	258	ARG	CD-NE-CZ	5.12	130.77	123.60
1	C	199	ASN	CB-CA-C	5.12	120.64	110.40
1	C	201	ASP	CB-CG-OD2	5.11	122.90	118.30
1	D	162	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	F	316	ARG	CB-CA-C	5.10	120.60	110.40
1	C	382	HIS	CB-CA-C	-5.08	100.23	110.40
1	D	326	SER	O-C-N	-5.08	114.57	122.70
1	B	258	ARG	CD-NE-CZ	5.07	130.70	123.60
1	A	162	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	D	166	GLU	CB-CA-C	5.06	120.51	110.40
1	D	4	ILE	CB-CA-C	-5.04	101.51	111.60
1	D	110	ARG	N-CA-CB	5.03	119.66	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	306	ASP	CB-CG-OD1	5.03	122.83	118.30
1	D	316	ARG	CA-CB-CG	5.03	124.45	113.40
1	F	119	VAL	CG1-CB-CG2	5.02	118.94	110.90
1	B	316	ARG	CG-CD-NE	-5.01	101.27	111.80
1	B	162	ARG	NE-CZ-NH1	5.01	122.81	120.30

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	3014	0	2998	61	0
1	B	3014	0	2998	58	0
1	C	3014	0	2998	84	0
1	D	3014	0	2999	128	0
1	E	3014	0	2998	48	0
1	F	3014	0	2997	66	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	7	0	0
3	C	6	0	8	2	0
3	D	6	0	8	2	0
3	E	6	0	8	1	0
3	F	6	0	8	0	0
4	A	27	0	6	2	0
4	B	27	0	6	2	0
4	C	27	0	6	3	0
4	D	27	0	6	9	0
4	E	27	0	6	1	0
4	F	27	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	105	0	0	9	0
5	B	95	0	0	16	0
5	C	86	0	0	17	0
5	D	90	0	0	54	0
5	E	107	0	0	8	0
5	F	111	0	0	11	0
All	All	18888	0	18071	439	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 12.

All (439) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:MET:CB	1:B:278:MET:CG	1.75	1.59
1:B:2:PRO:CG	1:B:2:PRO:CB	1.74	1.52
1:F:2:PRO:CG	1:F:2:PRO:CB	1.76	1.50
1:F:278:MET:CG	1:F:278:MET:SD	2.01	1.48
1:F:278:MET:SD	1:F:278:MET:CE	2.03	1.47
1:C:262:MET:SD	1:C:262:MET:CG	2.03	1.46
1:B:278:MET:SD	1:B:278:MET:CG	2.06	1.44
1:A:278:MET:CE	1:A:278:MET:SD	2.07	1.43
1:A:278:MET:CG	1:A:278:MET:SD	2.07	1.42
1:C:278:MET:SD	1:C:278:MET:CE	2.09	1.40
1:D:278:MET:CE	1:D:278:MET:SD	2.18	1.30
1:E:278:MET:CE	1:E:278:MET:SD	2.29	1.20
1:D:162:ARG:HD3	5:D:2036:HOH:O	1.39	1.17
1:D:136:LEU:HA	5:D:2029:HOH:O	1.55	1.05
1:D:98:CYS:SG	4:D:1394:MTQ:OM1	2.18	1.02
1:C:144:LEU:HD11	1:D:144:LEU:HD11	1.36	1.01
1:A:98:CYS:SG	4:A:1394:MTQ:OM1	2.24	0.96
1:F:77:ARG:HG3	1:F:77:ARG:HH11	1.28	0.94
1:B:53:HIS:HE1	5:B:2053:HOH:O	1.51	0.93
1:E:17:HIS:ND1	1:E:18:PRO:HD2	1.86	0.90
1:C:17:HIS:ND1	1:C:18:PRO:HD2	1.86	0.89
1:C:77:ARG:HG3	1:C:77:ARG:HH11	1.34	0.88
1:D:17:HIS:CD2	1:D:18:PRO:HD2	2.11	0.86
1:D:80:PHE:HB2	1:D:83:ASP:OD2	1.77	0.85
1:C:144:LEU:CD1	1:D:144:LEU:HD11	2.07	0.84
1:C:73:ILE:CG1	1:C:139:VAL:HG12	2.07	0.84
1:E:154:HIS:HD2	1:E:176:THR:HA	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:ARG:HG3	1:E:77:ARG:HH11	1.41	0.84
1:D:21:LYS:HE2	5:E:2028:HOH:O	1.77	0.83
1:C:73:ILE:HG12	1:C:139:VAL:HG12	1.61	0.82
1:A:202:HIS:CE1	5:A:2061:HOH:O	2.30	0.82
1:D:157:PHE:CD1	5:D:2033:HOH:O	2.31	0.82
1:C:278:MET:HB2	5:C:2085:HOH:O	1.80	0.81
1:E:299:GLU:OE2	1:F:258:ARG:HD3	1.80	0.81
1:B:278:MET:HB3	5:B:2062:HOH:O	1.80	0.81
1:C:73:ILE:HG12	1:C:139:VAL:CG1	2.10	0.81
1:C:51:ARG:NH2	1:C:53:HIS:HE1	1.78	0.80
1:A:77:ARG:HG3	1:A:77:ARG:HH11	1.47	0.79
1:D:254:ASN:C	1:D:254:ASN:HD22	1.86	0.79
1:D:67:VAL:HG21	1:D:206:LEU:HD23	1.66	0.78
1:D:303:ILE:HD12	1:D:314:ALA:HB2	1.64	0.78
1:C:77:ARG:NH1	1:C:77:ARG:HG3	1.97	0.78
1:E:177:LEU:O	1:E:181:THR:HB	1.85	0.77
1:C:371:TRP:HA	5:C:2082:HOH:O	1.85	0.76
1:D:79:LEU:N	5:D:2013:HOH:O	2.17	0.76
1:F:50:LYS:HE3	1:F:202:HIS:CE1	2.21	0.76
1:F:199:ASN:HD22	1:F:199:ASN:C	1.88	0.75
1:D:72:LEU:HD13	5:D:2056:HOH:O	1.86	0.75
1:A:254:ASN:C	1:A:254:ASN:HD22	1.88	0.74
1:A:202:HIS:CD2	5:A:2061:HOH:O	2.39	0.74
1:A:258:ARG:HD3	1:B:299:GLU:OE2	1.87	0.74
1:C:131:LYS:NZ	1:C:183:PRO:O	2.20	0.74
1:F:389:GLY:HA3	5:F:2110:HOH:O	1.87	0.74
1:A:299:GLU:OE2	1:B:258:ARG:HD3	1.88	0.73
1:C:89:LYS:NZ	1:C:192:GLU:OE1	2.20	0.73
1:D:192:GLU:HB3	5:D:2048:HOH:O	1.89	0.73
1:D:78:LYS:HG2	5:D:2011:HOH:O	1.90	0.71
1:D:108:LYS:HD2	5:E:2005:HOH:O	1.91	0.70
1:D:98:CYS:SG	4:D:1394:MTQ:S2'	2.89	0.70
1:C:389:GLY:HA3	5:C:2085:HOH:O	1.91	0.70
1:D:177:LEU:O	1:D:181:THR:HB	1.92	0.70
1:F:77:ARG:HG3	1:F:77:ARG:NH1	1.96	0.69
1:E:63:GLN:O	1:E:64:SER:HB3	1.90	0.69
1:C:144:LEU:HD11	1:D:144:LEU:CD1	2.19	0.69
1:F:50:LYS:HE3	1:F:202:HIS:HE1	1.58	0.69
1:B:53:HIS:CE1	5:B:2053:HOH:O	2.32	0.69
1:E:144:LEU:HD11	1:F:144:LEU:HD11	1.74	0.68
1:C:51:ARG:NH2	1:C:53:HIS:CE1	2.61	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:ARG:HD3	1:D:299:GLU:OE2	1.92	0.68
1:B:340:GLU:HG3	5:B:2070:HOH:O	1.94	0.68
1:F:322:LYS:NZ	5:F:2082:HOH:O	2.26	0.68
1:D:162:ARG:HG2	1:D:168:GLY:O	1.93	0.68
1:D:157:PHE:CG	5:D:2033:HOH:O	2.47	0.68
4:C:1394:MTQ:OM2	4:C:1394:MTQ:MOM1	1.65	0.67
1:C:254:ASN:C	1:C:254:ASN:HD22	1.96	0.67
1:A:202:HIS:CG	5:A:2061:HOH:O	2.47	0.67
1:D:157:PHE:C	5:D:2034:HOH:O	2.33	0.66
1:F:50:LYS:CE	1:F:202:HIS:HE1	2.08	0.66
4:E:1394:MTQ:OM2	4:E:1394:MTQ:MOM1	1.67	0.66
1:C:371:TRP:CA	5:C:2082:HOH:O	2.43	0.66
1:F:50:LYS:NZ	1:F:202:HIS:HE1	1.94	0.66
1:C:303:ILE:HD12	1:C:314:ALA:HB2	1.77	0.65
1:C:262:MET:CG	1:C:262:MET:CE	2.74	0.65
1:E:254:ASN:HD22	1:E:254:ASN:C	1.99	0.65
1:A:202:HIS:NE2	5:A:2061:HOH:O	2.29	0.64
4:F:1394:MTQ:OM2	4:F:1394:MTQ:MOM1	1.66	0.64
1:C:154:HIS:HD2	3:C:1393:GOL:O3	1.81	0.64
1:D:90:TYR:OH	5:D:2015:HOH:O	2.15	0.64
1:A:254:ASN:ND2	1:A:256:SER:H	1.96	0.64
1:C:103:ARG:HD2	1:C:115:VAL:O	1.97	0.64
4:A:1394:MTQ:MOM1	4:A:1394:MTQ:OM1	1.69	0.64
1:A:177:LEU:O	1:A:181:THR:HB	1.98	0.63
1:D:225:ILE:C	5:D:2055:HOH:O	2.36	0.63
1:D:225:ILE:N	5:D:2055:HOH:O	2.31	0.63
1:B:73:ILE:CG1	1:B:139:VAL:HG12	2.28	0.63
1:E:63:GLN:O	1:E:64:SER:CB	2.45	0.63
1:C:365:GLU:HG3	1:C:381:TRP:CZ3	2.34	0.63
4:B:1394:MTQ:MOM1	4:B:1394:MTQ:OM2	1.70	0.63
1:B:73:ILE:HG12	1:B:139:VAL:CG1	2.29	0.63
1:F:177:LEU:O	1:F:181:THR:HB	1.99	0.62
1:C:5:ARG:HD3	5:C:2001:HOH:O	1.99	0.62
1:D:346:SER:HA	5:D:2078:HOH:O	1.98	0.62
1:F:53:HIS:HD2	1:F:171:TYR:CE1	2.17	0.62
1:A:17:HIS:CD2	1:A:18:PRO:HD2	2.34	0.62
4:D:1394:MTQ:MOM1	4:D:1394:MTQ:OM1	1.70	0.62
1:C:10:TYR:CE2	1:C:55:PRO:HG3	2.34	0.62
1:B:322:LYS:NZ	5:B:2073:HOH:O	2.32	0.62
1:E:328:HIS:HD2	1:E:329:SER:H	1.47	0.62
1:A:254:ASN:HD22	1:A:255:TRP:N	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:303:ILE:HD12	1:F:314:ALA:HB2	1.81	0.62
1:F:53:HIS:HD2	1:F:171:TYR:CD1	2.18	0.62
1:A:144:LEU:HD11	1:B:144:LEU:HD11	1.82	0.62
1:C:387:ARG:HH11	1:C:387:ARG:CG	2.12	0.62
1:C:13:GLU:OE1	1:C:56:ILE:HG12	2.00	0.62
1:C:246:PRO:HD2	5:D:2069:HOH:O	2.00	0.61
1:C:299:GLU:OE2	1:D:258:ARG:HD3	2.01	0.61
1:B:77:ARG:HG3	1:B:77:ARG:HH11	1.64	0.61
1:A:57:PRO:HD2	1:A:221:TRP:CE2	2.36	0.61
1:D:78:LYS:HE3	5:D:2011:HOH:O	2.01	0.60
1:A:254:ASN:C	1:A:254:ASN:ND2	2.51	0.60
4:D:1394:MTQ:MOM1	4:D:1394:MTQ:OM2	1.72	0.60
1:E:258:ARG:HD3	1:F:299:GLU:OE2	2.01	0.60
1:C:248:VAL:HG12	1:C:373:LEU:HD22	1.82	0.60
1:D:2:PRO:HA	5:D:2001:HOH:O	2.01	0.60
1:D:82:LYS:HD3	5:D:2014:HOH:O	2.00	0.60
1:A:48:PHE:HB3	1:A:202:HIS:HE1	1.66	0.60
1:F:254:ASN:C	1:F:254:ASN:HD22	2.02	0.60
1:F:71:GLY:O	1:F:73:ILE:N	2.33	0.60
1:D:158:VAL:N	5:D:2034:HOH:O	2.34	0.60
1:F:311:TRP:CZ2	1:F:354:LYS:HE3	2.37	0.60
1:D:21:LYS:CE	5:E:2028:HOH:O	2.42	0.59
1:A:25:LYS:HE2	1:D:239:LYS:NZ	2.17	0.59
1:E:154:HIS:CD2	1:E:176:THR:HA	2.32	0.59
1:E:77:ARG:CG	1:E:77:ARG:HH11	2.13	0.59
1:F:53:HIS:CD2	1:F:171:TYR:CE1	2.90	0.59
1:F:17:HIS:HD2	1:F:19:SER:OG	1.86	0.59
1:C:387:ARG:HH11	1:C:387:ARG:HG2	1.67	0.59
1:D:203:GLY:HA2	1:D:221:TRP:CD1	2.38	0.59
1:D:66:SER:HB2	5:D:2013:HOH:O	2.01	0.59
1:C:254:ASN:C	1:C:254:ASN:ND2	2.56	0.59
1:A:50:LYS:HE3	1:A:202:HIS:NE2	2.17	0.58
1:F:63:GLN:O	1:F:64:SER:CB	2.49	0.58
1:D:224:SER:HB2	5:D:2055:HOH:O	2.04	0.58
1:B:73:ILE:HG12	1:B:139:VAL:HG11	1.85	0.58
1:C:367:VAL:HG13	1:C:380:SER:OG	2.03	0.58
1:D:139:VAL:HB	5:D:2029:HOH:O	2.03	0.58
4:D:1394:MTQ:S1'	4:D:1394:MTQ:OM1	2.62	0.58
1:C:71:GLY:O	1:C:73:ILE:N	2.36	0.57
1:B:278:MET:HA	5:B:2062:HOH:O	2.02	0.57
1:E:328:HIS:HD2	1:E:329:SER:N	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:GLN:O	1:D:64:SER:CB	2.53	0.57
1:E:77:ARG:HG3	1:E:77:ARG:NH1	2.08	0.57
1:A:63:GLN:O	1:A:64:SER:CB	2.51	0.57
1:C:53:HIS:CD2	1:C:236:PHE:CZ	2.93	0.57
1:E:53:HIS:HE1	5:E:2066:HOH:O	1.86	0.57
1:D:77:ARG:NH1	1:D:77:ARG:HG3	2.20	0.56
1:A:25:LYS:HE2	1:D:239:LYS:HZ3	1.71	0.56
1:B:57:PRO:HD2	1:B:221:TRP:CE2	2.40	0.56
1:D:79:LEU:C	5:D:2013:HOH:O	2.43	0.56
1:E:365:GLU:HG3	1:E:381:TRP:CZ3	2.41	0.56
1:B:63:GLN:O	1:B:64:SER:CB	2.52	0.56
1:A:204:PHE:CD1	1:A:205:PRO:HA	2.41	0.56
1:D:67:VAL:HG21	1:D:206:LEU:CD2	2.36	0.56
1:B:278:MET:CB	5:B:2062:HOH:O	2.48	0.56
1:D:204:PHE:CD1	1:D:205:PRO:HA	2.40	0.56
1:D:389:GLY:C	5:D:2088:HOH:O	2.43	0.56
1:A:325:ILE:HG21	1:A:328:HIS:HD2	1.70	0.55
1:D:156:GLU:HB3	1:D:226:ASN:HB3	1.88	0.55
1:F:199:ASN:C	1:F:199:ASN:ND2	2.57	0.55
1:D:156:GLU:C	5:D:2033:HOH:O	2.44	0.55
1:F:77:ARG:CG	1:F:77:ARG:HH11	2.10	0.55
1:D:63:GLN:O	1:D:64:SER:OG	2.17	0.55
1:B:254:ASN:HD22	1:B:254:ASN:C	2.09	0.55
1:B:278:MET:CA	5:B:2062:HOH:O	2.54	0.55
1:D:254:ASN:C	1:D:254:ASN:ND2	2.55	0.55
1:D:157:PHE:CE1	5:D:2033:HOH:O	2.57	0.55
1:C:63:GLN:O	1:C:64:SER:CB	2.54	0.54
1:D:254:ASN:ND2	1:D:256:SER:H	2.06	0.54
1:D:78:LYS:C	5:D:2013:HOH:O	2.43	0.54
1:E:366:ASN:HB2	5:E:2100:HOH:O	2.06	0.54
1:F:153:ARG:C	1:F:154:HIS:ND1	2.60	0.54
1:C:145:THR:O	1:C:181:THR:HG21	2.08	0.54
1:E:254:ASN:C	1:E:254:ASN:ND2	2.61	0.54
1:F:311:TRP:CH2	1:F:354:LYS:HE3	2.43	0.54
1:D:171:TYR:CZ	5:D:2090:HOH:O	2.52	0.53
1:D:332:ASP:C	5:D:2077:HOH:O	2.46	0.53
1:F:388:LEU:C	5:F:2109:HOH:O	2.46	0.53
1:C:387:ARG:CG	1:C:387:ARG:NH1	2.70	0.53
1:D:281:PRO:HG3	5:D:2078:HOH:O	2.07	0.53
1:F:131:LYS:NZ	1:F:183:PRO:O	2.35	0.53
1:C:326:SER:HB3	5:C:2067:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:ARG:HB2	5:C:2024:HOH:O	2.07	0.53
1:B:71:GLY:O	1:B:73:ILE:N	2.41	0.53
1:D:154:HIS:HD2	3:D:1393:GOL:O3	1.91	0.53
1:B:246:PRO:HD2	5:B:2056:HOH:O	2.07	0.53
1:F:291:VAL:HG13	1:F:336:TRP:HA	1.91	0.53
1:D:203:GLY:HA2	1:D:221:TRP:NE1	2.24	0.52
1:D:34:ARG:HB2	5:D:2027:HOH:O	2.07	0.52
1:A:154:HIS:ND1	1:A:231:GLU:CA	2.72	0.52
1:D:136:LEU:CA	5:D:2029:HOH:O	2.33	0.52
1:D:117:TRP:N	5:D:2019:HOH:O	2.43	0.52
1:D:17:HIS:HD2	1:D:18:PRO:HD2	1.69	0.52
1:A:113:ARG:NH1	5:A:2039:HOH:O	2.21	0.52
1:A:77:ARG:NH1	1:A:77:ARG:HG3	2.14	0.52
1:C:328:HIS:HD2	1:C:330:SER:H	1.58	0.52
1:E:328:HIS:CD2	1:E:329:SER:N	2.77	0.52
1:D:77:ARG:HG3	1:D:77:ARG:HH11	1.74	0.51
1:B:202:HIS:ND1	4:B:1394:MTQ:O2P	2.33	0.51
1:D:73:ILE:HG13	1:D:139:VAL:HG12	1.92	0.51
1:E:357:ASP:OD1	1:E:361:ASN:HB2	2.10	0.51
1:A:12:GLN:HE21	1:D:167:ASN:ND2	2.09	0.51
1:C:77:ARG:HH11	1:C:77:ARG:CG	2.14	0.51
1:D:367:VAL:HG22	5:D:2083:HOH:O	2.10	0.51
1:A:154:HIS:ND1	1:A:231:GLU:HA	2.26	0.51
1:B:139:VAL:HG12	1:B:139:VAL:O	2.10	0.51
1:F:278:MET:HB3	5:F:2110:HOH:O	2.09	0.51
1:C:291:VAL:HG13	1:C:336:TRP:HA	1.92	0.51
4:D:1394:MTQ:C6	5:D:2090:HOH:O	2.59	0.51
1:D:71:GLY:O	1:D:73:ILE:N	2.43	0.50
1:B:278:MET:CA	1:B:278:MET:CG	2.83	0.50
1:B:69:LEU:CD1	1:B:79:LEU:HD12	2.42	0.50
1:C:73:ILE:HG12	1:C:139:VAL:HG11	1.91	0.50
1:D:45:VAL:O	1:D:50:LYS:NZ	2.42	0.50
1:A:202:HIS:ND1	5:A:2061:HOH:O	2.40	0.50
1:B:254:ASN:ND2	1:B:254:ASN:C	2.64	0.50
1:B:53:HIS:O	5:B:2016:HOH:O	2.19	0.50
1:A:154:HIS:ND1	1:A:231:GLU:N	2.60	0.50
1:D:38:VAL:HG22	1:D:338:LEU:HD22	1.93	0.49
1:A:145:THR:O	1:A:181:THR:HG21	2.12	0.49
1:A:193:MET:CE	1:A:202:HIS:HD1	2.25	0.49
1:A:37:LEU:HD22	1:A:336:TRP:HH2	1.77	0.49
1:B:165:GLU:O	5:B:2033[A]:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:LYS:HE3	1:C:202:HIS:HE1	1.77	0.49
1:C:21:LYS:HE3	5:C:2005:HOH:O	2.12	0.49
1:F:254:ASN:C	1:F:254:ASN:ND2	2.64	0.49
1:B:278:MET:HG3	1:B:278:MET:H	1.77	0.49
1:C:38:VAL:O	1:C:38:VAL:HG13	2.11	0.49
1:D:265:PRO:HD2	5:D:2065:HOH:O	2.12	0.49
1:E:204:PHE:CD1	1:E:205:PRO:HA	2.48	0.49
1:F:349:THR:CG2	5:F:2094:HOH:O	2.61	0.49
1:F:367:VAL:HG13	1:F:380:SER:OG	2.13	0.49
1:E:135:VAL:HG21	1:E:189:LEU:HD12	1.94	0.49
1:C:181:THR:HG23	5:C:2037:HOH:O	2.12	0.49
1:D:73:ILE:CG1	1:D:139:VAL:HG12	2.43	0.49
1:D:157:PHE:HB3	5:D:2034:HOH:O	2.12	0.49
1:D:165:GLU:HA	5:D:2037:HOH:O	2.13	0.49
1:A:25:LYS:CE	1:D:239:LYS:NZ	2.75	0.48
1:C:262:MET:HE2	1:C:262:MET:CG	2.43	0.48
1:D:157:PHE:CG	1:D:208:VAL:HG21	2.47	0.48
1:A:67:VAL:HG21	1:A:206:LEU:HD23	1.95	0.48
1:C:242:LYS:NZ	5:C:2049:HOH:O	2.47	0.48
1:B:164:LYS:HD3	5:B:2003:HOH:O	2.13	0.48
1:D:281:PRO:HB3	5:D:2078:HOH:O	2.12	0.48
1:E:139:VAL:HG12	1:E:139:VAL:O	2.14	0.48
1:E:21:LYS:HE2	5:E:2005:HOH:O	2.13	0.48
1:F:374:ARG:HD2	1:F:374:ARG:HA	1.58	0.48
1:C:254:ASN:ND2	1:C:256:SER:H	2.12	0.48
1:A:153:ARG:O	1:A:154:HIS:CD2	2.66	0.48
1:D:289:TYR:C	1:D:289:TYR:CD1	2.86	0.48
1:A:303:ILE:HD12	1:A:314:ALA:HB2	1.94	0.48
1:E:154:HIS:ND1	1:E:231:GLU:HA	2.29	0.48
1:F:373:LEU:HA	1:F:373:LEU:HD12	1.56	0.48
1:E:145:THR:O	1:E:181:THR:HG21	2.14	0.47
1:F:204:PHE:CD1	1:F:205:PRO:HA	2.48	0.47
1:A:71:GLY:O	1:A:73:ILE:N	2.46	0.47
1:E:71:GLY:O	1:E:73:ILE:N	2.46	0.47
1:F:389:GLY:N	5:F:2109:HOH:O	2.47	0.47
1:B:132:LEU:HD13	1:B:180:ALA:HB1	1.96	0.47
1:B:172:LYS:HE2	5:B:2040:HOH:O	2.14	0.47
1:C:150:LEU:HD12	5:C:2014:HOH:O	2.13	0.47
5:A:2012:HOH:O	1:D:239:LYS:HG2	2.13	0.47
1:D:106:MET:SD	1:D:375:GLY:HA2	2.54	0.47
1:C:202:HIS:O	1:C:207:ARG:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:377:LEU:HA	5:F:2017:HOH:O	2.13	0.47
1:B:73:ILE:HG13	1:B:139:VAL:HG12	1.95	0.47
1:B:43:THR:O	1:B:194:ASN:ND2	2.48	0.47
1:D:136:LEU:C	5:D:2029:HOH:O	2.53	0.47
1:D:284:VAL:HG12	1:D:345:VAL:HG22	1.97	0.47
1:F:38:VAL:HG22	1:F:338:LEU:HD22	1.96	0.47
1:B:74:GLN:HB3	5:B:2018:HOH:O	2.15	0.47
1:F:156:GLU:HB3	1:F:226:ASN:HB3	1.97	0.47
1:C:182:ASN:N	5:C:2037:HOH:O	2.47	0.47
1:D:210:VAL:HB	5:D:2053:HOH:O	2.15	0.47
1:F:51:ARG:CZ	1:F:53:HIS:CE1	2.97	0.47
1:D:73:ILE:HG12	1:D:139:VAL:CG1	2.45	0.46
1:B:177:LEU:O	1:B:181:THR:HB	2.15	0.46
1:D:211:PRO:HB2	1:D:334:TRP:CD2	2.50	0.46
1:F:254:ASN:ND2	1:F:256:SER:H	2.13	0.46
1:A:78:LYS:CE	5:A:2025:HOH:O	2.63	0.46
1:B:77:ARG:HG3	1:B:77:ARG:NH1	2.29	0.46
1:C:135:VAL:HG21	1:C:189:LEU:HD12	1.97	0.46
1:C:326:SER:CB	5:C:2067:HOH:O	2.63	0.46
1:C:51:ARG:CZ	1:C:53:HIS:CE1	2.98	0.46
1:D:249:ASN:OD1	1:D:251:ASP:N	2.45	0.46
1:E:239:LYS:HA	1:E:255:TRP:CE3	2.51	0.46
1:E:303:ILE:HD12	1:E:314:ALA:HB2	1.96	0.46
1:A:25:LYS:CE	1:D:239:LYS:HZ1	2.29	0.46
1:D:64:SER:HA	1:D:80:PHE:HE2	1.81	0.46
1:F:38:VAL:HG13	1:F:38:VAL:O	2.14	0.46
1:A:367:VAL:HG13	1:A:380:SER:OG	2.14	0.46
1:D:347:GLN:HG2	1:D:348:THR:N	2.29	0.46
1:D:45:VAL:HG21	5:D:2047:HOH:O	2.16	0.46
1:D:48:PHE:CD1	1:D:202:HIS:HE1	2.34	0.46
1:D:169:GLY:C	5:D:2040:HOH:O	2.52	0.46
1:D:359:ALA:O	1:D:360:ALA:HB3	2.16	0.46
1:E:154:HIS:CE1	1:E:231:GLU:HB3	2.51	0.46
1:B:378:ASN:OD1	1:B:380:SER:HB2	2.16	0.46
1:D:119:VAL:HG13	1:D:119:VAL:O	2.16	0.46
1:B:291:VAL:HG13	1:B:336:TRP:HA	1.97	0.46
1:F:154:HIS:CD2	1:F:231:GLU:HA	2.51	0.45
1:F:51:ARG:NH2	1:F:53:HIS:HE1	2.14	0.45
1:B:326:SER:HB3	5:B:2075:HOH:O	2.15	0.45
1:C:129:GLY:HA2	1:C:191:TYR:CE2	2.51	0.45
1:B:254:ASN:ND2	1:B:256:SER:H	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:31:GLU:OE1	1:F:120:SER:HB2	2.16	0.45
1:A:77:ARG:HH11	1:A:77:ARG:CG	2.21	0.45
1:C:117:TRP:CE3	1:C:121:ALA:HB2	2.52	0.45
1:C:50:LYS:HE3	1:C:202:HIS:CE1	2.51	0.45
1:E:158:VAL:HG22	1:E:172:LYS:HD3	1.98	0.45
1:F:158:VAL:HG22	1:F:172:LYS:HD3	1.98	0.45
1:A:374:ARG:HD2	1:A:374:ARG:HA	1.75	0.45
1:A:63:GLN:O	1:A:64:SER:HB3	2.15	0.45
1:D:139:VAL:O	1:D:139:VAL:HG12	2.17	0.45
1:A:347:GLN:HA	1:A:388:LEU:HD11	1.98	0.45
1:B:32:PRO:HG3	1:B:47:LEU:O	2.16	0.45
1:A:260:PRO:HB3	5:A:2070:HOH:O	2.15	0.45
1:D:45:VAL:HG23	1:D:194:ASN:HD22	1.81	0.44
1:D:7:PRO:HD3	1:D:57:PRO:HA	1.98	0.44
1:D:216:ALA:HA	4:D:1394:MTQ:S1'	2.58	0.44
1:D:157:PHE:CB	5:D:2034:HOH:O	2.66	0.44
1:C:110:ARG:HB3	1:C:371:TRP:CE2	2.52	0.44
3:D:1393:GOL:H12	5:D:2089:HOH:O	2.16	0.44
1:C:50:LYS:CE	1:C:202:HIS:HE1	2.31	0.44
1:D:132:LEU:HD22	1:D:132:LEU:O	2.18	0.44
1:A:103:ARG:HD2	1:A:115:VAL:O	2.18	0.44
1:B:204:PHE:CD1	1:B:205:PRO:HA	2.52	0.44
1:C:34:ARG:HG2	1:C:271:CYS:O	2.17	0.44
1:B:373:LEU:HA	1:B:373:LEU:HD12	1.64	0.44
1:C:204:PHE:CD1	1:C:205:PRO:HA	2.53	0.44
1:A:373:LEU:HD12	1:A:373:LEU:HA	1.70	0.44
1:D:18:PRO:HG2	5:D:2006:HOH:O	2.18	0.44
1:D:281:PRO:CB	5:D:2078:HOH:O	2.65	0.43
1:D:41:TYR:HA	1:D:338:LEU:HD11	1.99	0.43
1:D:37:LEU:HD22	1:D:336:TRP:HH2	1.83	0.43
1:E:325:ILE:O	1:E:331:SER:HB3	2.18	0.43
1:F:58:ILE:HD11	5:F:2004:HOH:O	2.18	0.43
1:E:154:HIS:ND1	1:E:231:GLU:CA	2.81	0.43
1:A:129:GLY:HA2	1:A:191:TYR:CE2	2.53	0.43
1:A:58:ILE:HG13	1:A:59:VAL:N	2.32	0.43
1:C:110:ARG:HB3	1:C:371:TRP:NE1	2.33	0.43
1:D:10:TYR:CZ	1:D:55:PRO:HG3	2.53	0.43
1:D:220:LYS:NZ	4:D:1394:MTQ:O1P	2.49	0.43
1:D:40:SER:OG	1:D:42:VAL:O	2.36	0.43
1:B:374:ARG:HA	1:B:374:ARG:HD2	1.66	0.43
1:F:53:HIS:CD2	1:F:171:TYR:HE1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:PRO:HD2	1:D:221:TRP:CD2	2.54	0.43
1:E:347:GLN:HG2	1:E:348:THR:N	2.34	0.43
1:F:153:ARG:O	1:F:154:HIS:ND1	2.51	0.43
1:A:153:ARG:O	1:A:154:HIS:HD2	2.02	0.43
1:C:182:ASN:CA	5:C:2037:HOH:O	2.67	0.43
1:D:222:LEU:HD12	5:D:2034:HOH:O	2.18	0.43
1:C:241:TYR:OH	4:C:1394:MTQ:OM1	2.33	0.43
1:C:359:ALA:O	1:C:360:ALA:HB3	2.19	0.43
1:D:254:ASN:HD22	1:D:256:SER:H	1.66	0.43
1:F:17:HIS:CD2	1:F:19:SER:OG	2.68	0.43
1:F:254:ASN:HD22	1:F:255:TRP:N	2.16	0.43
1:A:62:LEU:O	1:A:62:LEU:HD12	2.19	0.43
1:C:164:LYS:HG2	5:C:2031:HOH:O	2.17	0.43
1:E:231:GLU:OE2	3:E:1393:GOL:O2	2.37	0.43
1:D:365:GLU:HA	1:D:381:TRP:CE2	2.54	0.43
1:A:316:ARG:HB2	1:A:337:VAL:CG1	2.49	0.42
1:B:37:LEU:HD22	1:B:336:TRP:HH2	1.83	0.42
1:E:347:GLN:HA	1:E:388:LEU:HD11	2.01	0.42
1:F:354:LYS:HD3	1:F:381:TRP:CE2	2.54	0.42
1:B:31:GLU:OE1	1:B:120:SER:HB2	2.19	0.42
1:B:132:LEU:O	1:B:132:LEU:HD22	2.19	0.42
1:D:255:TRP:HH2	1:D:374:ARG:HD3	1.83	0.42
1:C:175:ILE:HA	3:C:1393:GOL:H31	2.01	0.42
1:C:211:PRO:HB2	1:C:334:TRP:CD2	2.54	0.42
1:E:373:LEU:HD12	1:E:373:LEU:HA	1.71	0.42
1:E:306:ASP:OD2	1:E:310:ASN:HB2	2.18	0.42
1:F:51:ARG:NH2	1:F:53:HIS:CE1	2.88	0.42
1:B:254:ASN:HD22	1:B:255:TRP:N	2.17	0.42
1:D:155:VAL:HG12	5:D:2033:HOH:O	2.20	0.42
1:D:347:GLN:HA	1:D:388:LEU:HD11	2.02	0.42
1:C:53:HIS:CD2	1:C:236:PHE:CE2	3.08	0.42
1:A:315:SER:O	1:A:339:PHE:HA	2.20	0.42
1:C:182:ASN:HB2	5:C:2037:HOH:O	2.20	0.42
1:E:154:HIS:ND1	1:E:231:GLU:N	2.68	0.42
1:A:26:GLU:HA	1:A:27:PRO:HA	1.87	0.41
1:B:53:HIS:CE1	1:B:236:PHE:CE2	3.09	0.41
1:C:291:VAL:HG13	1:C:336:TRP:CA	2.50	0.41
1:C:387:ARG:HD3	5:C:2084:HOH:O	2.19	0.41
1:E:21:LYS:CE	5:E:2005:HOH:O	2.68	0.41
1:E:73:ILE:HG12	1:E:139:VAL:HG11	2.02	0.41
1:F:349:THR:HA	5:F:2094:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:367:VAL:HG22	5:F:2101:HOH:O	2.20	0.41
1:D:77:ARG:CG	1:D:77:ARG:HH11	2.32	0.41
1:E:57:PRO:HD2	1:E:221:TRP:CE2	2.56	0.41
1:C:51:ARG:HD2	4:C:1394:MTQ:S1'	2.61	0.41
1:A:201:ASP:HB3	1:A:202:HIS:HD2	1.86	0.41
1:D:291:VAL:HG13	1:D:336:TRP:HA	2.02	0.41
1:F:63:GLN:O	1:F:64:SER:HB3	2.20	0.41
1:C:63:GLN:O	1:C:64:SER:HB3	2.20	0.41
1:F:315:SER:O	1:F:339:PHE:HA	2.21	0.41
1:D:31:GLU:OE1	1:D:118:ASP:HB3	2.21	0.41
1:A:306:ASP:OD2	1:A:310:ASN:HB2	2.20	0.41
1:C:38:VAL:O	1:C:38:VAL:CG1	2.69	0.41
1:D:367:VAL:HG13	1:D:380:SER:OG	2.20	0.41
1:D:162:ARG:CD	5:D:2036:HOH:O	2.24	0.41
1:D:165:GLU:CA	5:D:2037:HOH:O	2.69	0.41
1:F:112:VAL:HG21	1:F:375:GLY:HA3	2.02	0.41
1:F:349:THR:HG23	5:F:2094:HOH:O	2.20	0.41
1:A:154:HIS:CE1	1:A:231:GLU:HB3	2.56	0.41
1:A:328:HIS:ND1	1:A:329:SER:N	2.68	0.41
1:B:182:ASN:C	1:B:182:ASN:OD1	2.59	0.41
1:B:199:ASN:HA	1:B:199:ASN:HD22	1.45	0.41
1:D:117:TRP:CE3	1:D:121:ALA:HB2	2.55	0.41
1:D:199:ASN:HB2	5:D:2050:HOH:O	2.20	0.41
1:B:38:VAL:HG22	1:B:338:LEU:HD22	2.03	0.41
1:E:289:TYR:CD1	1:E:289:TYR:C	2.94	0.41
1:B:264:PHE:HB2	1:B:265:PRO:HD2	2.04	0.40
1:C:325:ILE:O	1:C:331:SER:HB3	2.21	0.40
1:D:316:ARG:HB2	1:D:337:VAL:CG1	2.51	0.40
1:E:50:LYS:HE3	1:E:202:HIS:NE2	2.36	0.40
1:D:216:ALA:HB2	4:D:1394:MTQ:OM2	2.21	0.40
1:D:157:PHE:CD1	1:D:208:VAL:HG21	2.56	0.40
1:F:388:LEU:HA	1:F:388:LEU:HD23	1.91	0.40
1:F:57:PRO:HD2	1:F:221:TRP:CE2	2.56	0.40
1:D:219:VAL:HG11	5:D:2034:HOH:O	2.21	0.40
1:D:326:SER:CB	5:D:2068:HOH:O	2.69	0.40
5:D:2084:HOH:O	1:E:25:LYS:HE2	2.21	0.40
1:F:50:LYS:CE	1:F:202:HIS:CE1	2.90	0.40
1:B:245:PRO:HB2	5:B:2056:HOH:O	2.20	0.40
1:B:77:ARG:CG	1:B:77:ARG:HH11	2.30	0.40
1:C:374:ARG:HD2	1:C:374:ARG:HA	1.49	0.40
1:C:385:LEU:HA	1:C:385:LEU:HD12	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:ASN:HD22	1:D:255:TRP:N	2.17	0.40
1:E:164:LYS:HE2	5:E:2041:HOH:O	2.21	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	386/393 (98%)	369 (96%)	13 (3%)	4 (1%)	15	32
1	B	386/393 (98%)	371 (96%)	11 (3%)	4 (1%)	15	32
1	C	386/393 (98%)	369 (96%)	13 (3%)	4 (1%)	15	32
1	D	386/393 (98%)	370 (96%)	12 (3%)	4 (1%)	15	32
1	E	386/393 (98%)	370 (96%)	13 (3%)	3 (1%)	19	39
1	F	386/393 (98%)	368 (95%)	14 (4%)	4 (1%)	15	32
All	All	2316/2358 (98%)	2217 (96%)	76 (3%)	23 (1%)	15	32

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	380	SER
1	B	72	LEU
1	C	72	LEU
1	C	380	SER
1	D	72	LEU
1	E	72	LEU
1	F	72	LEU
1	B	380	SER
1	C	34	ARG

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Mol	Chain	Res	Type
1	D	380	SER
1	E	380	SER
1	F	380	SER
1	A	76	PRO
1	B	76	PRO
1	C	76	PRO
1	D	34	ARG
1	D	76	PRO
1	E	76	PRO
1	B	34	ARG
1	F	76	PRO
1	A	378	ASN
1	F	34	ARG

### 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	331/336 (98%)	294 (89%)	37 (11%)	6	10
1	B	331/336 (98%)	291 (88%)	40 (12%)	5	9
1	C	331/336 (98%)	286 (86%)	45 (14%)	3	6
1	D	331/336 (98%)	290 (88%)	41 (12%)	4	8
1	E	331/336 (98%)	287 (87%)	44 (13%)	4	7
1	F	331/336 (98%)	284 (86%)	47 (14%)	3	5
All	All	1986/2016 (98%)	1732 (87%)	254 (13%)	4	8

All (254) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	9	GLU
1	A	20	LEU
1	A	37	LEU
1	A	38	VAL

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Mol	Chain	Res	Type
1	A	51	ARG
1	A	58	ILE
1	A	63	GLN
1	A	64	SER
1	A	70	THR
1	A	72	LEU
1	A	77	ARG
1	A	81	ILE
1	A	87	LEU
1	A	110	ARG
1	A	119	VAL
1	A	132	LEU
1	A	177	LEU
1	A	178	SER
1	A	181	THR
1	A	184	GLU
1	A	199	ASN
1	A	208	VAL
1	A	222	LEU
1	A	254	ASN
1	A	258	ARG
1	A	265	PRO
1	A	278	MET
1	A	280	LYS
1	A	284	VAL
1	A	291	VAL
1	A	312	VAL
1	A	316	ARG
1	A	336	TRP
1	A	340	GLU
1	A	351	VAL
1	A	367	VAL
1	B	5	ARG
1	B	20	LEU
1	B	34	ARG
1	B	37	LEU
1	B	38	VAL
1	B	50	LYS
1	B	51	ARG
1	B	58	ILE
1	B	63	GLN
1	B	69	LEU

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Mol	Chain	Res	Type
1	B	70	THR
1	B	72	LEU
1	B	75	ASN
1	B	77	ARG
1	B	81	ILE
1	B	87	LEU
1	B	112	VAL
1	B	119	VAL
1	B	132	LEU
1	B	160	VAL
1	B	164	LYS
1	B	177	LEU
1	B	181	THR
1	B	199	ASN
1	B	208	VAL
1	B	222	LEU
1	B	254	ASN
1	B	258	ARG
1	B	278	MET
1	B	284	VAL
1	B	291	VAL
1	B	292	SER
1	B	316	ARG
1	B	319	GLU
1	B	336	TRP
1	B	340	GLU
1	B	351	VAL
1	B	367	VAL
1	B	369	SER
1	B	380	SER
1	C	5	ARG
1	C	9	GLU
1	C	17	HIS
1	C	20	LEU
1	C	37	LEU
1	C	38	VAL
1	C	51	ARG
1	C	53	HIS
1	C	58	ILE
1	C	61	HIS
1	C	63	GLN
1	C	64	SER

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Mol	Chain	Res	Type
1	C	69	LEU
1	C	70	THR
1	C	77	ARG
1	C	81	ILE
1	C	87	LEU
1	C	108	LYS
1	C	119	VAL
1	C	132	LEU
1	C	177	LEU
1	C	188	LEU
1	C	199	ASN
1	C	208	VAL
1	C	222	LEU
1	C	251	ASP
1	C	254	ASN
1	C	258	ARG
1	C	278	MET
1	C	280	LYS
1	C	284	VAL
1	C	291	VAL
1	C	309	LYS
1	C	313	GLU
1	C	316	ARG
1	C	319	GLU
1	C	327	GLU
1	C	336	TRP
1	C	340	GLU
1	C	344	ASP
1	C	351	VAL
1	C	367	VAL
1	C	374	ARG
1	C	380	SER
1	C	387	ARG
1	D	5	ARG
1	D	9	GLU
1	D	20	LEU
1	D	25	LYS
1	D	37	LEU
1	D	38	VAL
1	D	40	SER
1	D	51	ARG
1	D	60	ASP

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Mol	Chain	Res	Type
1	D	63	GLN
1	D	69	LEU
1	D	70	THR
1	D	72	LEU
1	D	77	ARG
1	D	81	ILE
1	D	86	SER
1	D	87	LEU
1	D	119	VAL
1	D	132	LEU
1	D	145	THR
1	D	177	LEU
1	D	178	SER
1	D	181	THR
1	D	196	GLU
1	D	199	ASN
1	D	222	LEU
1	D	224	SER
1	D	239	LYS
1	D	254	ASN
1	D	278	MET
1	D	280	LYS
1	D	284	VAL
1	D	291	VAL
1	D	302	ASP
1	D	316	ARG
1	D	319	GLU
1	D	336	TRP
1	D	340	GLU
1	D	344	ASP
1	D	351	VAL
1	D	367	VAL
1	E	9	GLU
1	E	16	ARG
1	E	17	HIS
1	E	20	LEU
1	E	37	LEU
1	E	38	VAL
1	E	39	SER
1	E	51	ARG
1	E	58	ILE
1	E	63	GLN

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Mol	Chain	Res	Type
1	E	64	SER
1	E	69	LEU
1	E	70	THR
1	E	72	LEU
1	E	77	ARG
1	E	81	ILE
1	E	87	LEU
1	E	119	VAL
1	E	132	LEU
1	E	160	VAL
1	E	177	LEU
1	E	178	SER
1	E	181	THR
1	E	188	LEU
1	E	196	GLU
1	E	199	ASN
1	E	208	VAL
1	E	222	LEU
1	E	224	SER
1	E	254	ASN
1	E	258	ARG
1	E	265	PRO
1	E	278	MET
1	E	280	LYS
1	E	284	VAL
1	E	287	LYS
1	E	291	VAL
1	E	319	GLU
1	E	336	TRP
1	E	340	GLU
1	E	344	ASP
1	E	351	VAL
1	E	367	VAL
1	E	387	ARG
1	F	5	ARG
1	F	9	GLU
1	F	20	LEU
1	F	21	LYS
1	F	35	SER
1	F	37	LEU
1	F	38	VAL
1	F	40	SER

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Mol	Chain	Res	Type
1	F	51	ARG
1	F	58	ILE
1	F	61	HIS
1	F	63	GLN
1	F	64	SER
1	F	69	LEU
1	F	70	THR
1	F	72	LEU
1	F	77	ARG
1	F	81	ILE
1	F	87	LEU
1	F	119	VAL
1	F	132	LEU
1	F	160	VAL
1	F	164	LYS
1	F	177	LEU
1	F	181	THR
1	F	188	LEU
1	F	196	GLU
1	F	199	ASN
1	F	205	PRO
1	F	208	VAL
1	F	222	LEU
1	F	226	ASN
1	F	254	ASN
1	F	258	ARG
1	F	265	PRO
1	F	278	MET
1	F	280	LYS
1	F	284	VAL
1	F	291	VAL
1	F	292	SER
1	F	309	LYS
1	F	336	TRP
1	F	340	GLU
1	F	344	ASP
1	F	351	VAL
1	F	367	VAL
1	F	387	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	17	HIS
1	A	63	GLN
1	A	74	GLN
1	A	91	ASN
1	A	254	ASN
1	A	323	GLN
1	A	382	HIS
1	B	91	ASN
1	B	199	ASN
1	B	254	ASN
1	B	323	GLN
1	B	328	HIS
1	C	53	HIS
1	C	91	ASN
1	C	149	ASN
1	C	154	HIS
1	C	202	HIS
1	C	254	ASN
1	C	323	GLN
1	C	328	HIS
1	D	17	HIS
1	D	154	HIS
1	D	167	ASN
1	D	199	ASN
1	D	202	HIS
1	D	254	ASN
1	D	382	HIS
1	E	53	HIS
1	E	199	ASN
1	E	254	ASN
1	E	323	GLN
1	F	17	HIS
1	F	53	HIS
1	F	199	ASN
1	F	202	HIS
1	F	254	ASN
1	F	323	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	MTQ	B	1394	1	20,30,30	4.46	10 (50%)	21,48,48	5.23	13 (61%)
3	GOL	D	1393	-	5,5,5	0.68	0	5,5,5	1.40	1 (20%)
4	MTQ	D	1394	1	20,30,30	3.71	14 (70%)	21,48,48	5.64	12 (57%)
3	GOL	F	1393	-	5,5,5	0.63	0	5,5,5	0.71	0
4	MTQ	F	1394	1	20,30,30	3.93	10 (50%)	21,48,48	4.92	9 (42%)
3	GOL	B	1393	-	5,5,5	0.97	0	5,5,5	0.91	0
4	MTQ	E	1394	1	20,30,30	4.26	10 (50%)	21,48,48	5.94	15 (71%)
3	GOL	E	1393	-	5,5,5	0.58	0	5,5,5	1.30	0
4	MTQ	C	1394	1	20,30,30	4.60	11 (55%)	21,48,48	5.41	13 (61%)
3	GOL	A	1393	-	5,5,5	0.78	0	5,5,5	1.67	1 (20%)
3	GOL	C	1393	-	5,5,5	0.56	0	5,5,5	1.30	1 (20%)
4	MTQ	A	1394	1	20,30,30	4.07	13 (65%)	21,48,48	6.52	14 (66%)

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
4	MTQ	B	1394	1	-	0/4/60/60	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	1393	-	-	0/4/4/4	-
4	MTQ	D	1394	1	-	1/4/60/60	0/4/4/4
3	GOL	F	1393	-	-	0/4/4/4	-
4	MTQ	F	1394	1	-	0/4/60/60	0/4/4/4
3	GOL	B	1393	-	-	2/4/4/4	-
4	MTQ	E	1394	1	-	1/4/60/60	0/4/4/4
3	GOL	E	1393	-	-	0/4/4/4	-
4	MTQ	C	1394	1	-	0/4/60/60	0/4/4/4
3	GOL	A	1393	-	-	2/4/4/4	-
3	GOL	C	1393	-	-	1/4/4/4	-
4	MTQ	A	1394	1	-	1/4/60/60	0/4/4/4

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1394	MTQ	O4'-C4'	11.23	1.50	1.43
4	E	1394	MTQ	O4'-C4'	10.95	1.50	1.43
4	C	1394	MTQ	O4'-C4'	8.87	1.49	1.43
4	F	1394	MTQ	O3'-C3'	8.36	1.51	1.36
4	F	1394	MTQ	C4'-C3'	-8.24	1.35	1.48
4	C	1394	MTQ	O3'-C3'	8.05	1.51	1.36
4	C	1394	MTQ	O4-C4	8.02	1.37	1.23
4	B	1394	MTQ	O3'-C3'	7.90	1.50	1.36
4	D	1394	MTQ	O3'-C3'	7.57	1.50	1.36
4	C	1394	MTQ	P-O4'	-7.42	1.36	1.60
4	E	1394	MTQ	C4'-C3'	-7.33	1.36	1.48
4	F	1394	MTQ	P-O4'	-6.94	1.37	1.60
4	C	1394	MTQ	C9-N5	6.80	1.50	1.32
4	E	1394	MTQ	P-O4'	-6.73	1.38	1.60
4	A	1394	MTQ	O3'-C3'	6.71	1.48	1.36
4	A	1394	MTQ	C4'-C3'	-6.58	1.38	1.48
4	A	1394	MTQ	O4'-C4'	6.51	1.47	1.43
4	B	1394	MTQ	O4-C4	6.29	1.34	1.23
4	B	1394	MTQ	P-O4'	-6.09	1.40	1.60
4	A	1394	MTQ	C6-N5	5.99	1.54	1.36
4	A	1394	MTQ	P-O4'	-5.96	1.41	1.60
4	D	1394	MTQ	P-O4'	-5.89	1.41	1.60
4	D	1394	MTQ	C4'-C3'	-5.86	1.39	1.48
4	A	1394	MTQ	C9-N5	5.71	1.47	1.32
4	E	1394	MTQ	C9-N5	5.69	1.47	1.32
4	E	1394	MTQ	C6-N5	5.66	1.53	1.36
4	F	1394	MTQ	C6-N5	5.54	1.52	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1394	MTQ	C6-N5	5.46	1.52	1.36
4	E	1394	MTQ	O3'-C3'	5.43	1.46	1.36
4	B	1394	MTQ	C4'-C3'	-5.39	1.39	1.48
4	C	1394	MTQ	C6-N5	4.95	1.51	1.36
4	B	1394	MTQ	C9-N5	4.82	1.45	1.32
4	C	1394	MTQ	C4'-C3'	-4.80	1.40	1.48
4	A	1394	MTQ	O4-C4	4.75	1.31	1.23
4	C	1394	MTQ	P-O1P	-4.67	1.35	1.50
4	D	1394	MTQ	O4'-C4'	4.61	1.46	1.43
4	B	1394	MTQ	C6-N5	4.56	1.50	1.36
4	D	1394	MTQ	C9-N5	4.54	1.44	1.32
4	F	1394	MTQ	C9-N5	4.52	1.44	1.32
4	D	1394	MTQ	O4-C4	4.42	1.31	1.23
4	F	1394	MTQ	P-O1P	-4.41	1.36	1.50
4	A	1394	MTQ	P-O1P	-4.30	1.36	1.50
4	A	1394	MTQ	C9-C10	4.14	1.55	1.43
4	B	1394	MTQ	P-O1P	-4.06	1.37	1.50
4	B	1394	MTQ	C9-C10	4.05	1.54	1.43
4	A	1394	MTQ	P-O2P	-3.77	1.40	1.54
4	E	1394	MTQ	P-O1P	-3.72	1.38	1.50
4	C	1394	MTQ	O3'-C7	3.71	1.51	1.45
4	F	1394	MTQ	O3'-C7	3.56	1.50	1.45
4	C	1394	MTQ	C10-N8	3.55	1.39	1.35
4	E	1394	MTQ	C9-C10	3.30	1.52	1.43
4	D	1394	MTQ	P-O1P	-3.22	1.40	1.50
4	D	1394	MTQ	C9-C10	3.19	1.52	1.43
4	C	1394	MTQ	C9-C10	3.17	1.52	1.43
4	E	1394	MTQ	C2-N3	-2.94	1.28	1.35
4	E	1394	MTQ	C1'-C6	2.94	1.43	1.36
4	D	1394	MTQ	C1'-C6	2.87	1.42	1.36
4	F	1394	MTQ	O4-C4	2.80	1.28	1.23
4	A	1394	MTQ	C1'-C6	2.79	1.42	1.36
4	F	1394	MTQ	C9-C10	2.77	1.51	1.43
4	D	1394	MTQ	C10-N1	2.77	1.38	1.32
4	B	1394	MTQ	P-O2P	-2.75	1.44	1.54
4	A	1394	MTQ	C2-N3	-2.67	1.29	1.35
4	D	1394	MTQ	O3'-C7	2.64	1.49	1.45
4	D	1394	MTQ	C4-N3	-2.53	1.33	1.38
4	A	1394	MTQ	C2-N2	-2.45	1.28	1.34
4	F	1394	MTQ	P-O2P	-2.32	1.45	1.54
4	D	1394	MTQ	P-O2P	-2.14	1.46	1.54

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1394	MTQ	C2'-C1'-C6	-25.18	98.04	123.96
4	E	1394	MTQ	C2'-C1'-C6	-22.23	101.08	123.96
4	D	1394	MTQ	C2'-C1'-C6	-20.79	102.56	123.96
4	B	1394	MTQ	C2'-C1'-C6	-19.57	103.82	123.96
4	F	1394	MTQ	C2'-C1'-C6	-17.80	105.64	123.96
4	C	1394	MTQ	C2'-C1'-C6	-14.44	109.09	123.96
4	E	1394	MTQ	C4-C9-N5	9.83	128.97	118.01
4	C	1394	MTQ	O3'-C7-N8	-8.35	99.69	108.43
4	C	1394	MTQ	N2-C2-N3	7.96	129.59	117.06
4	C	1394	MTQ	C4-C9-N5	7.08	125.91	118.01
4	A	1394	MTQ	O3'-C7-N8	-7.05	101.05	108.43
4	D	1394	MTQ	C4-C9-N5	7.03	125.85	118.01
4	F	1394	MTQ	O3'-C7-N8	6.89	115.64	108.43
4	B	1394	MTQ	C2'-C1'-S1'	6.47	129.57	115.81
4	A	1394	MTQ	C2'-C1'-S1'	6.24	129.09	115.81
4	A	1394	MTQ	O3'-C7-C6	-6.12	87.17	112.10
4	F	1394	MTQ	C4-C9-N5	6.10	124.81	118.01
4	D	1394	MTQ	O3'-C7-N8	-5.77	102.39	108.43
4	C	1394	MTQ	C1'-C2'-C3'	-5.61	117.23	123.82
4	C	1394	MTQ	C2'-C1'-S1'	5.51	127.53	115.81
4	C	1394	MTQ	O3'-C7-C6	-5.42	90.04	112.10
4	C	1394	MTQ	O3P-P-O1P	-5.36	89.70	110.68
4	C	1394	MTQ	O2P-P-O4'	5.31	120.87	106.73
4	A	1394	MTQ	O4'-P-O1P	5.29	121.31	106.47
4	F	1394	MTQ	C2'-C1'-S1'	5.22	126.91	115.81
4	C	1394	MTQ	N1-C2-N3	-5.05	118.23	126.43
4	A	1394	MTQ	C4-C9-N5	5.04	123.63	118.01
4	B	1394	MTQ	O3'-C7-C6	-5.04	91.57	112.10
4	E	1394	MTQ	O3'-C7-C6	-4.88	92.22	112.10
4	E	1394	MTQ	N1-C2-N3	-4.84	118.58	126.43
4	D	1394	MTQ	N2-C2-N3	4.82	124.64	117.06
4	D	1394	MTQ	C2'-C1'-S1'	4.52	125.42	115.81
4	B	1394	MTQ	O3'-C7-N8	-4.51	103.71	108.43
4	A	1394	MTQ	O4-C4-N3	4.46	127.83	120.23
4	B	1394	MTQ	N1-C2-N3	-4.21	119.59	126.43
4	D	1394	MTQ	O3'-C7-C6	-4.10	95.39	112.10
4	D	1394	MTQ	N1-C2-N3	-4.10	119.77	126.43
4	F	1394	MTQ	O3'-C7-C6	-4.09	95.46	112.10
4	B	1394	MTQ	O4-C4-N3	4.06	127.14	120.23
4	E	1394	MTQ	C2'-C1'-S1'	4.00	124.32	115.81
4	D	1394	MTQ	C1'-C2'-C3'	-3.98	119.14	123.82
4	D	1394	MTQ	O3P-P-O1P	3.90	125.94	110.68
4	C	1394	MTQ	C10-C9-N5	-3.78	115.75	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1394	MTQ	O2P-P-O4'	3.77	116.76	106.73
4	B	1394	MTQ	C4-C9-N5	3.69	122.12	118.01
4	E	1394	MTQ	C10-C9-N5	-3.68	115.97	124.48
4	F	1394	MTQ	C10-C9-N5	-3.60	116.16	124.48
4	D	1394	MTQ	O2P-P-O4'	-3.53	97.34	106.73
4	C	1394	MTQ	O4-C4-N3	3.52	126.23	120.23
4	E	1394	MTQ	O3P-P-O2P	3.45	120.81	107.64
4	A	1394	MTQ	C1'-C2'-C3'	-3.42	119.81	123.82
4	E	1394	MTQ	O4'-P-O1P	3.34	115.83	106.47
4	F	1394	MTQ	C1'-C2'-S2'	-3.27	108.85	115.81
4	F	1394	MTQ	O4'-C4'-C3'	-3.26	105.90	110.64
4	F	1394	MTQ	O4'-P-O1P	3.23	115.53	106.47
4	D	1394	MTQ	C10-C9-N5	-3.11	117.29	124.48
4	D	1394	MTQ	O2P-P-O1P	-3.10	98.53	110.68
4	E	1394	MTQ	C1'-C2'-S2'	-3.05	109.33	115.81
4	E	1394	MTQ	O2P-P-O1P	-2.93	99.21	110.68
3	A	1393	GOL	C3-C2-C1	-2.92	100.33	111.70
4	A	1394	MTQ	O2P-P-O1P	-2.87	99.43	110.68
4	E	1394	MTQ	N2-C2-N1	2.75	121.04	116.57
4	C	1394	MTQ	N2-C2-N1	-2.70	112.18	116.57
4	B	1394	MTQ	C10-C9-N5	-2.70	118.25	124.48
4	B	1394	MTQ	C1'-C2'-S2'	-2.62	110.24	115.81
4	A	1394	MTQ	N1-C2-N3	-2.60	122.21	126.43
4	A	1394	MTQ	O3P-P-O2P	2.55	117.37	107.64
4	A	1394	MTQ	N2-C2-N1	2.51	120.64	116.57
4	A	1394	MTQ	C1'-C2'-S2'	-2.49	110.51	115.81
4	A	1394	MTQ	C10-C9-N5	-2.45	118.82	124.48
4	B	1394	MTQ	N2-C2-N1	2.36	120.39	116.57
4	E	1394	MTQ	O3P-P-O4'	-2.35	100.48	106.73
4	E	1394	MTQ	O4-C4-N3	2.27	124.10	120.23
4	B	1394	MTQ	C1'-C2'-C3'	-2.19	121.25	123.82
4	E	1394	MTQ	N2-C2-N3	2.07	120.33	117.06
3	C	1393	GOL	O3-C3-C2	2.07	120.12	110.20
4	B	1394	MTQ	O3P-P-O2P	2.07	115.54	107.64
3	D	1393	GOL	C3-C2-C1	-2.04	103.77	111.70
4	E	1394	MTQ	C4-C9-C10	-2.04	115.06	117.40

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1393	GOL	O1-C1-C2-C3

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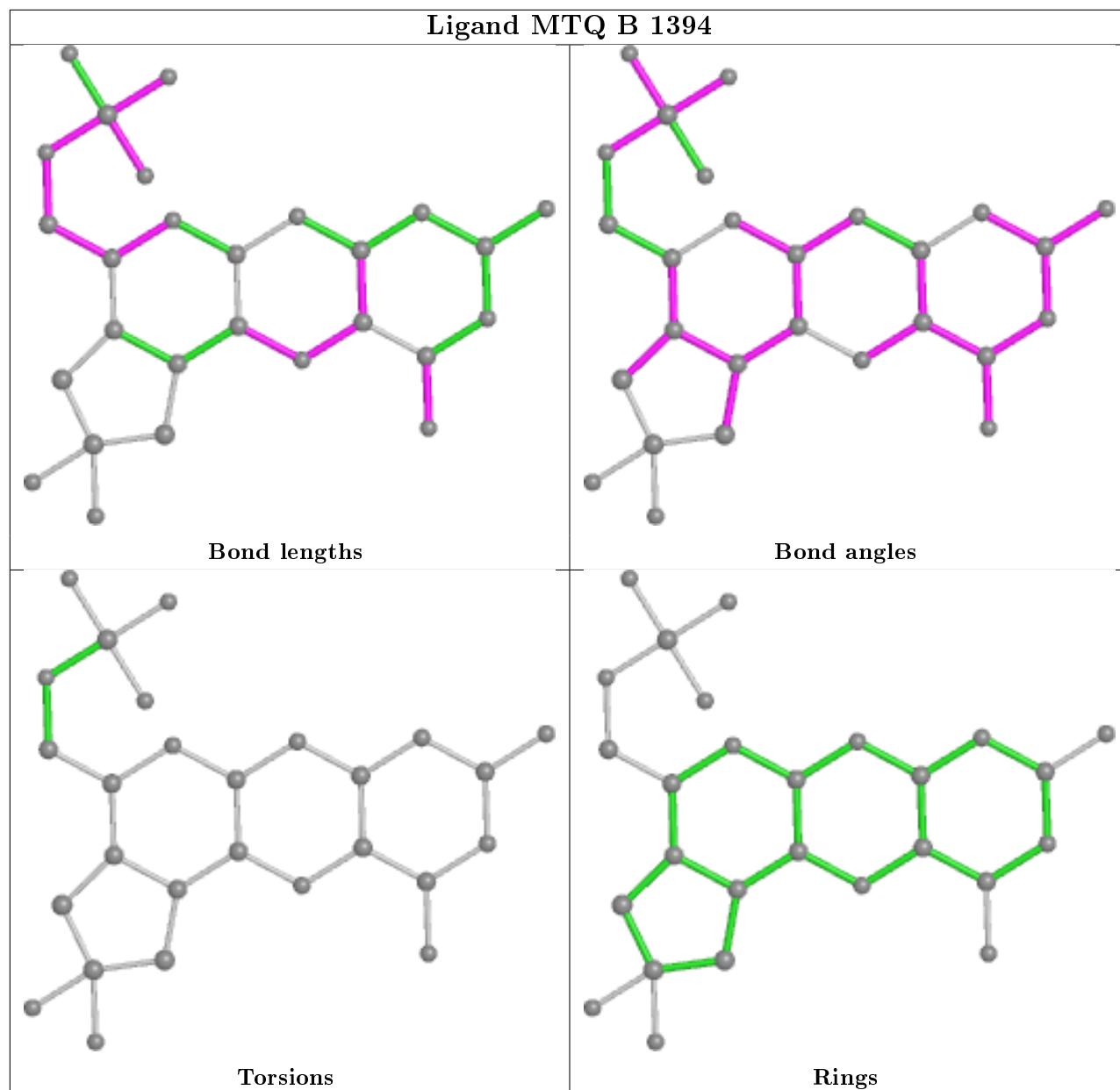
Mol	Chain	Res	Type	Atoms
3	B	1393	GOL	C1-C2-C3-O3
4	A	1394	MTQ	C4'-O4'-P-O2P
3	A	1393	GOL	O1-C1-C2-O2
3	B	1393	GOL	O2-C2-C3-O3
4	D	1394	MTQ	C4'-O4'-P-O3P
4	E	1394	MTQ	C4'-O4'-P-O2P
3	C	1393	GOL	O2-C2-C3-O3

There are no ring outliers.

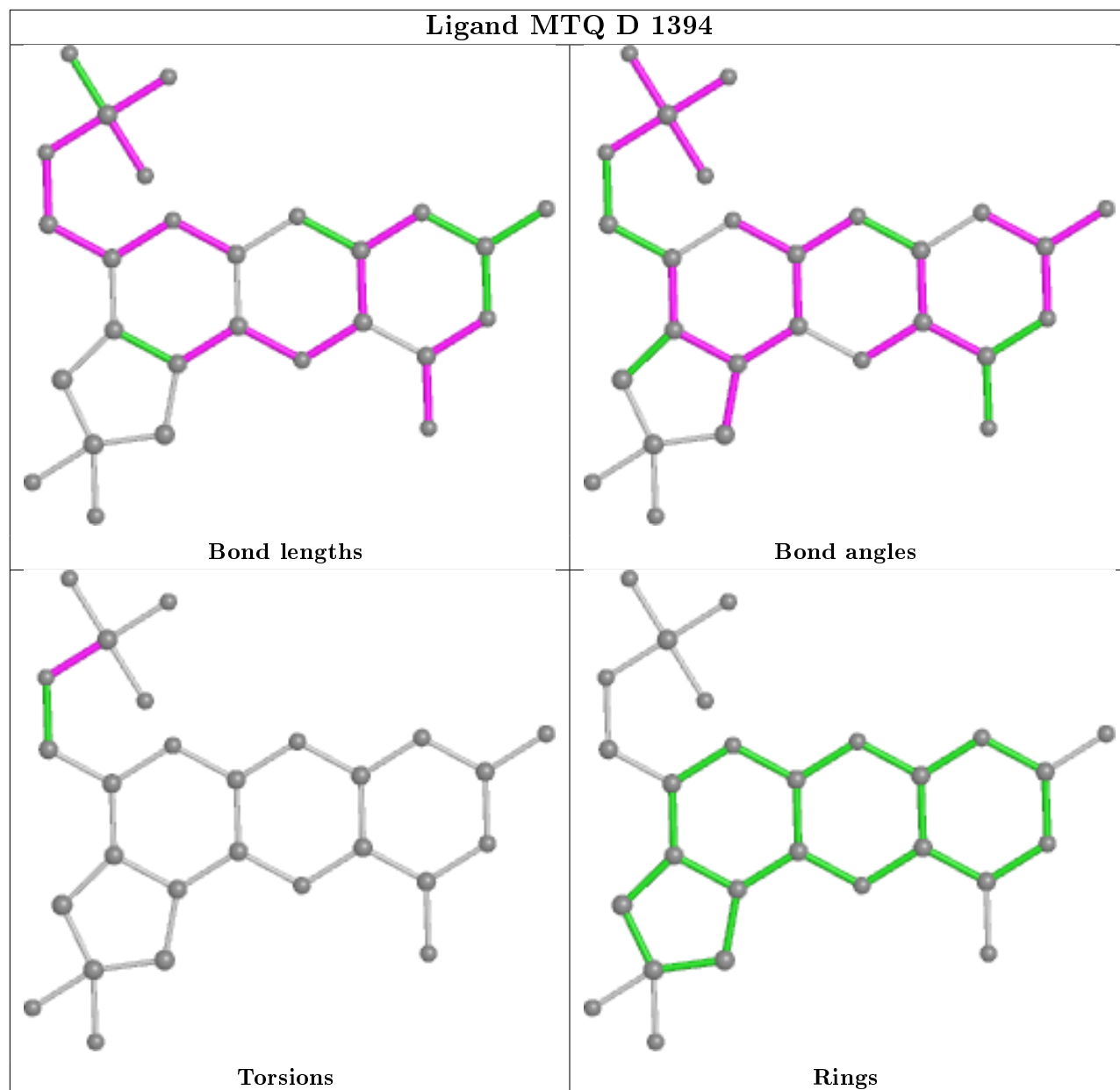
9 monomers are involved in 23 short contacts:

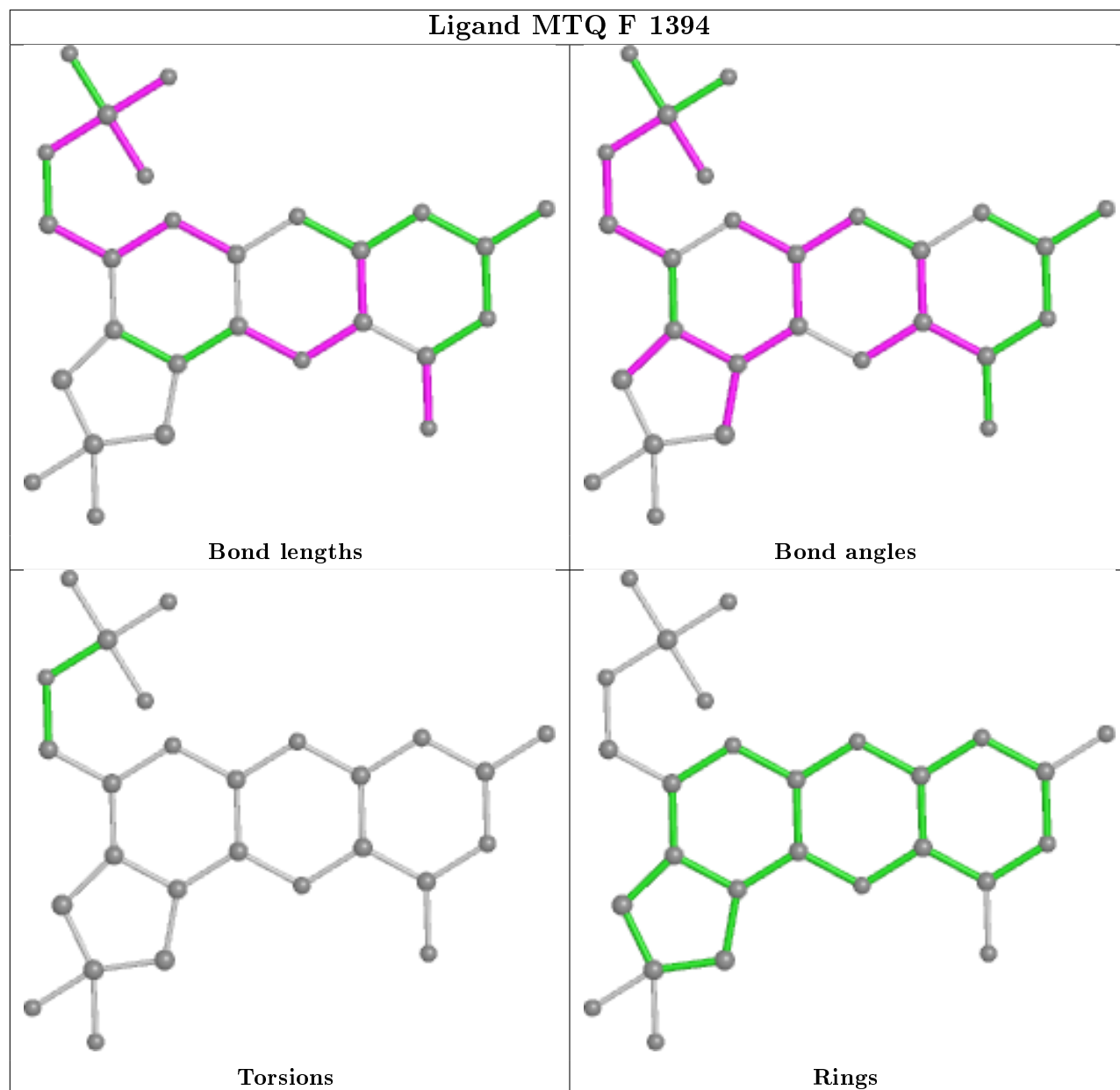
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1394	MTQ	2	0
3	D	1393	GOL	2	0
4	D	1394	MTQ	9	0
4	F	1394	MTQ	1	0
4	E	1394	MTQ	1	0
3	E	1393	GOL	1	0
4	C	1394	MTQ	3	0
3	C	1393	GOL	2	0
4	A	1394	MTQ	2	0

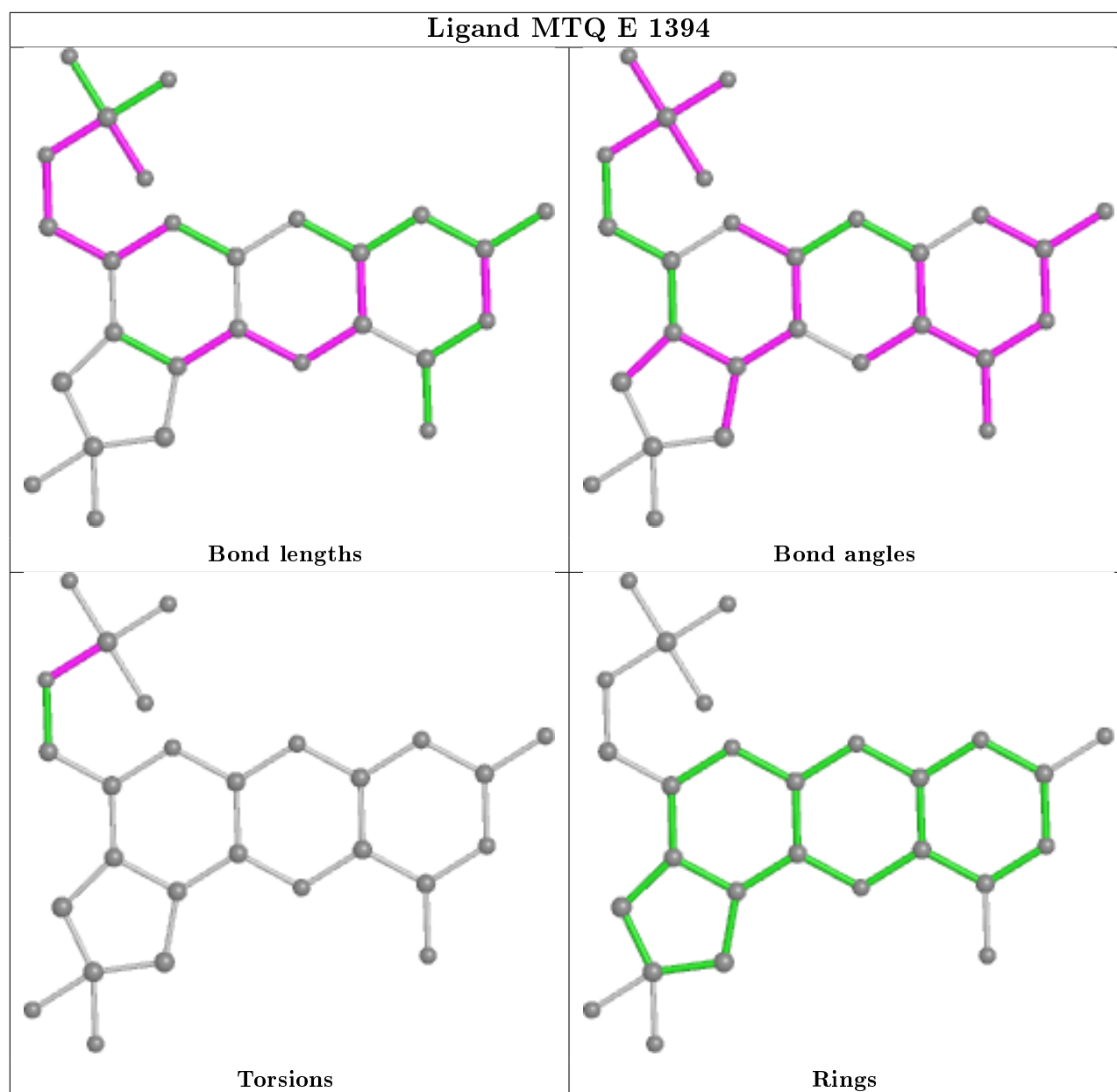
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



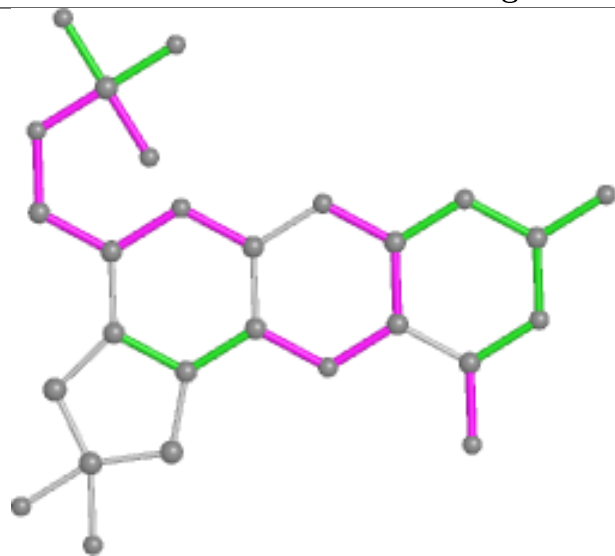




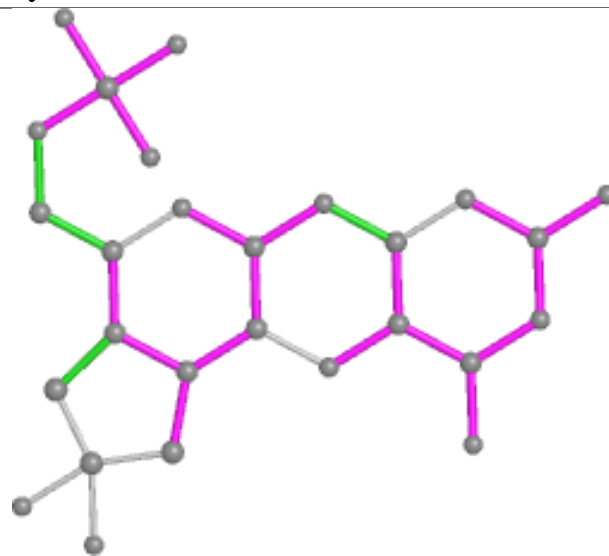




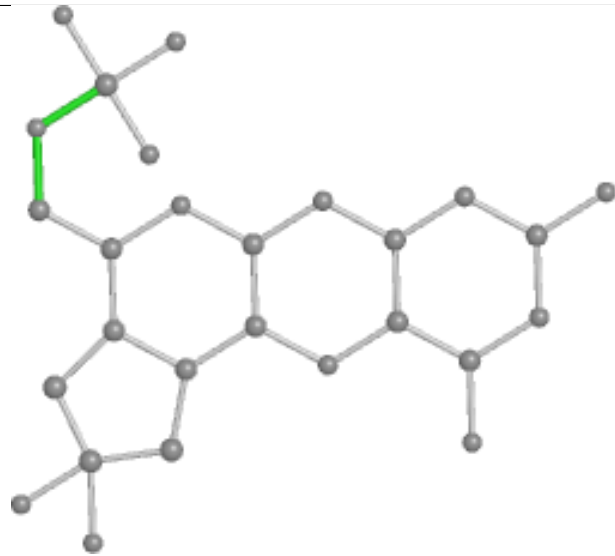
## Ligand MTQ C 1394



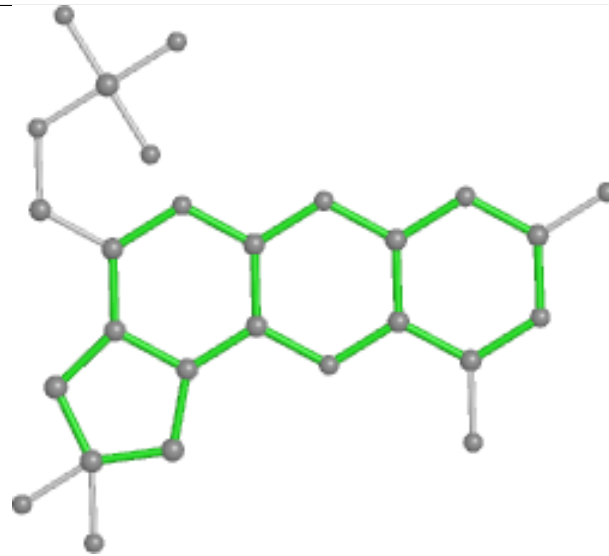
Bond lengths



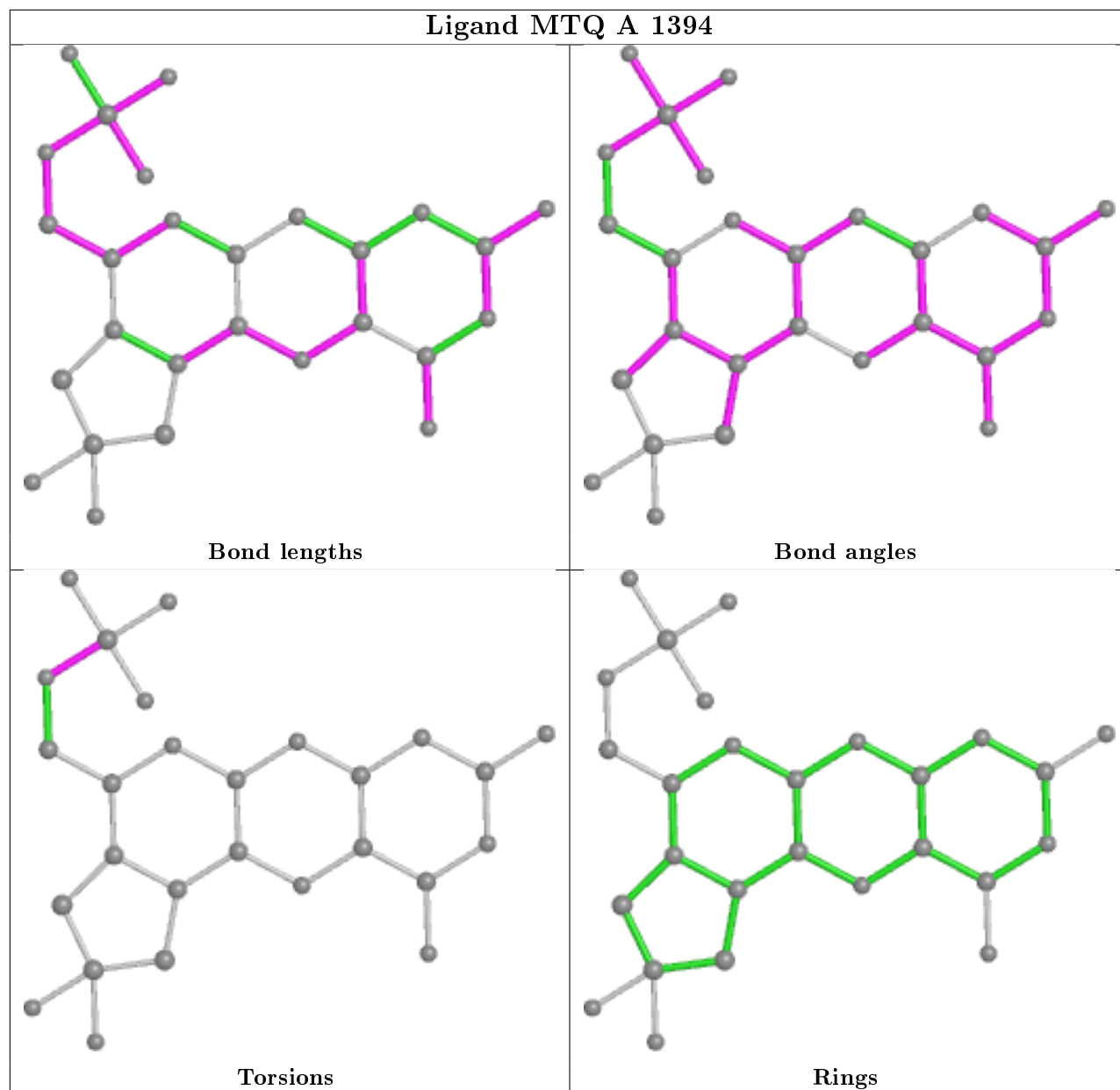
Bond angles



Torsions



Rings



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	388/393 (98%)	0.01	18 (4%)	32 26	39, 54, 78, 90	0
1	B	388/393 (98%)	-0.02	12 (3%)	49 42	39, 54, 78, 90	0
1	C	388/393 (98%)	0.09	20 (5%)	27 21	40, 55, 78, 90	0
1	D	388/393 (98%)	0.28	36 (9%)	8 6	39, 55, 78, 90	0
1	E	388/393 (98%)	0.08	17 (4%)	34 27	39, 54, 78, 90	0
1	F	388/393 (98%)	0.08	12 (3%)	49 42	39, 54, 78, 90	0
All	All	2328/2358 (98%)	0.09	115 (4%)	29 23	39, 54, 78, 90	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	389	GLY	8.7
1	B	389	GLY	7.7
1	F	2	PRO	6.7
1	D	2	PRO	6.5
1	F	389	GLY	6.2
1	B	2	PRO	5.8
1	D	389	GLY	5.8
1	C	2	PRO	5.8
1	A	2	PRO	4.7
1	A	389	GLY	4.5
1	D	388	LEU	4.4
1	D	3	GLY	4.4
1	E	2	PRO	4.3
1	D	344	ASP	4.0
1	D	63	GLN	3.9
1	D	321	GLY	3.7
1	D	280	LYS	3.7
1	A	280	LYS	3.6
1	D	82	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	346	SER	3.5
1	F	64	SER	3.5
1	C	61	HIS	3.5
1	D	64	SER	3.4
1	C	388	LEU	3.4
1	E	321	GLY	3.4
1	D	61	HIS	3.3
1	D	149	ASN	3.3
1	A	279	VAL	3.2
1	E	63	GLN	3.1
1	E	389	GLY	3.1
1	D	195	GLY	3.1
1	A	278	MET	3.0
1	C	278	MET	3.0
1	D	320	PRO	3.0
1	C	280	LYS	3.0
1	B	278	MET	3.0
1	D	278	MET	3.0
1	C	346	SER	2.9
1	F	321	GLY	2.9
1	E	349	THR	2.9
1	D	18	PRO	2.9
1	D	168	GLY	2.8
1	D	5	ARG	2.8
1	B	281	PRO	2.8
1	C	281	PRO	2.8
1	D	347	GLN	2.8
1	F	278	MET	2.7
1	A	321	GLY	2.7
1	D	39	SER	2.7
1	C	321	GLY	2.7
1	D	152	ALA	2.7
1	C	149	ASN	2.7
1	E	388	LEU	2.7
1	C	345	VAL	2.6
1	D	208	VAL	2.6
1	A	215	GLY	2.6
1	E	61	HIS	2.6
1	B	280	LYS	2.6
1	E	218	SER	2.6
1	D	279	VAL	2.6
1	C	64	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	60	ASP	2.5
1	E	208	VAL	2.5
1	D	72	LEU	2.5
1	B	64	SER	2.5
1	A	61	HIS	2.5
1	D	349	THR	2.5
1	A	219	VAL	2.4
1	D	11	SER	2.4
1	A	388	LEU	2.4
1	B	282	GLY	2.4
1	F	61	HIS	2.4
1	A	96	LEU	2.4
1	A	218	SER	2.4
1	C	75	ASN	2.4
1	E	219	VAL	2.4
1	F	96	LEU	2.3
1	B	321	GLY	2.3
1	E	281	PRO	2.3
1	B	344	ASP	2.3
1	E	278	MET	2.3
1	D	162	ARG	2.3
1	D	150	LEU	2.3
1	C	74	GLN	2.3
1	D	59	VAL	2.3
1	D	345	VAL	2.3
1	E	203	GLY	2.3
1	C	251	ASP	2.2
1	B	208	VAL	2.2
1	B	63	GLN	2.2
1	F	280	LYS	2.2
1	D	60	ASP	2.2
1	C	215	GLY	2.2
1	E	77	ARG	2.2
1	A	74	GLN	2.2
1	A	208	VAL	2.2
1	D	141	ILE	2.2
1	F	63	GLN	2.2
1	D	218	SER	2.1
1	C	112	VAL	2.1
1	C	322	LYS	2.1
1	F	207	ARG	2.1
1	A	207	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	61	HIS	2.1
1	D	138	LEU	2.1
1	D	58	ILE	2.1
1	F	202	HIS	2.1
1	E	74	GLN	2.0
1	A	209	VAL	2.0
1	F	216	ALA	2.0
1	C	63	GLN	2.0
1	A	346	SER	2.0
1	E	346	SER	2.0
1	A	222	LEU	2.0
1	E	280	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	GOL	A	1393	6/6	0.91	0.22	47,57,62,62	0
3	GOL	C	1393	6/6	0.92	0.18	52,57,60,64	0
3	GOL	D	1393	6/6	0.92	0.16	52,58,63,64	0
3	GOL	E	1393	6/6	0.94	0.19	47,56,62,63	0
3	GOL	B	1393	6/6	0.96	0.18	51,57,62,62	0
2	CS	D	1391	1/1	0.96	0.19	106,106,106,106	0
2	CS	C	1392	1/1	0.97	0.05	79,79,79,79	1
2	CS	E	1392	1/1	0.97	0.05	73,73,73,73	1
3	GOL	F	1393	6/6	0.97	0.17	45,57,61,63	0
2	CS	F	1392	1/1	0.97	0.04	70,70,70,70	1
2	CS	B	1392	1/1	0.98	0.03	67,67,67,67	1

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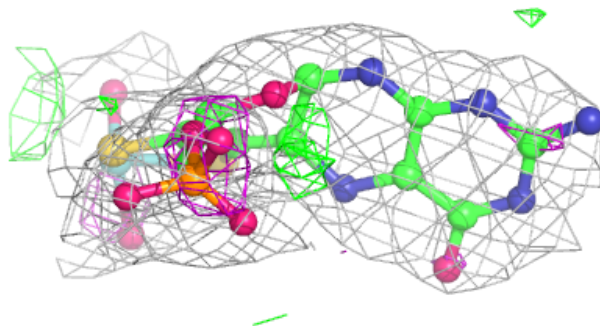
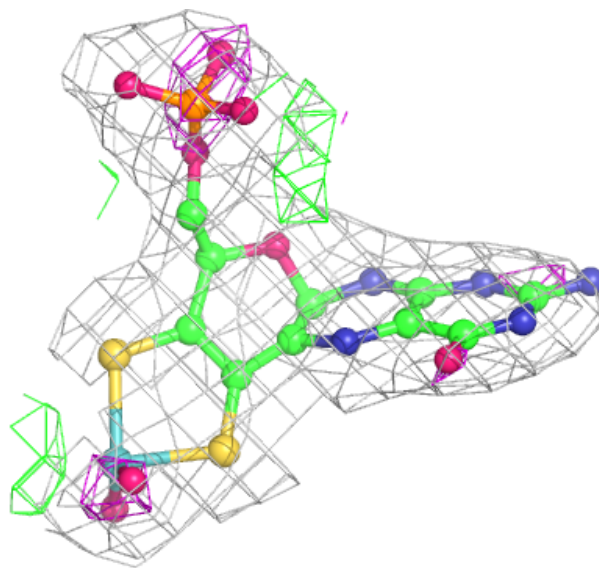
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CS	C	1391	1/1	0.98	0.04	80,80,80,80	0
4	MTQ	D	1394	27/27	0.98	0.15	35,42,51,56	0
2	CS	D	1392	1/1	0.98	0.11	81,81,81,81	1
4	MTQ	A	1394	27/27	0.99	0.19	33,40,44,49	0
2	CS	A	1392	1/1	0.99	0.04	69,69,69,69	1
2	CS	E	1391	1/1	0.99	0.06	68,68,68,68	0
4	MTQ	B	1394	27/27	0.99	0.18	33,40,46,51	0
2	CS	F	1391	1/1	0.99	0.05	73,73,73,73	0
4	MTQ	F	1394	27/27	0.99	0.20	32,39,44,49	0
2	CS	B	1391	1/1	0.99	0.04	73,73,73,73	0
4	MTQ	E	1394	27/27	0.99	0.19	29,39,44,47	0
4	MTQ	C	1394	27/27	0.99	0.15	34,42,50,51	0
2	CS	A	1391	1/1	0.99	0.07	67,67,67,67	0

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

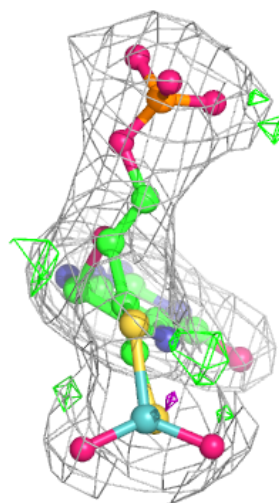
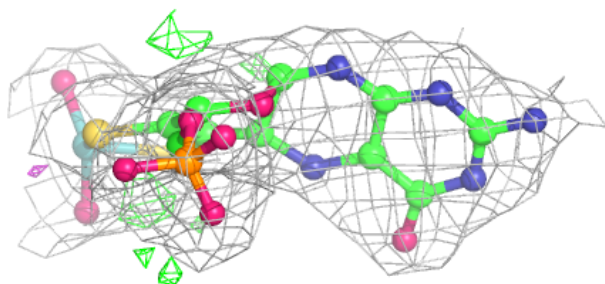
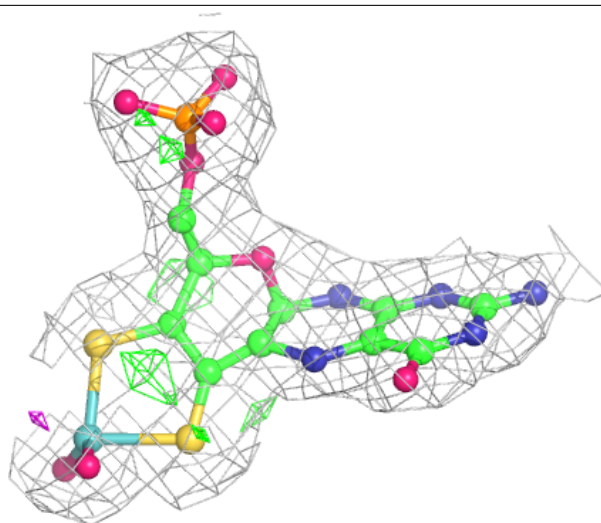
**Electron density around MTQ D 1394:**

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



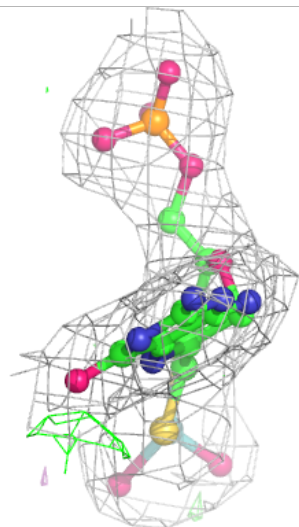
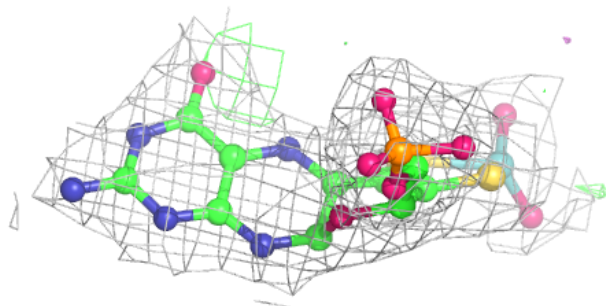
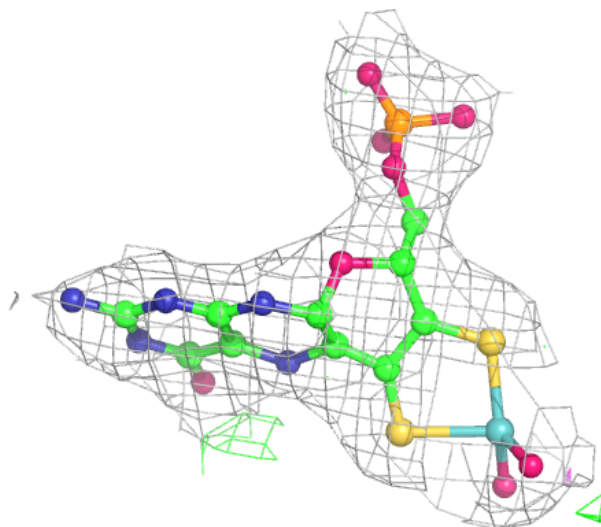
**Electron density around MTQ A 1394:**

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



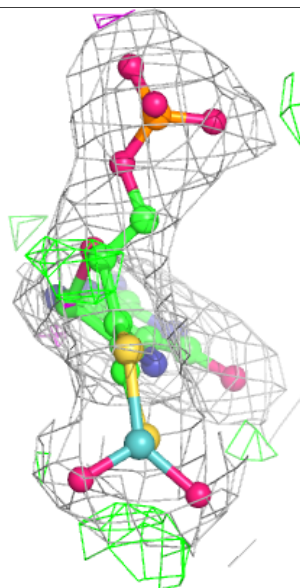
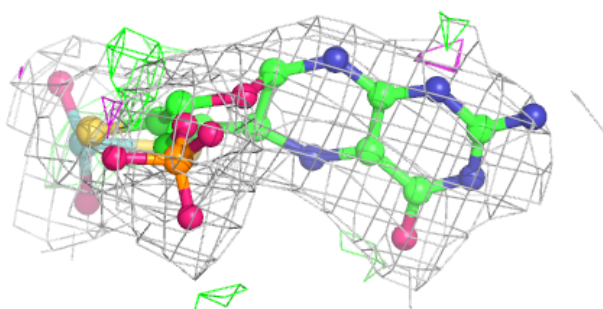
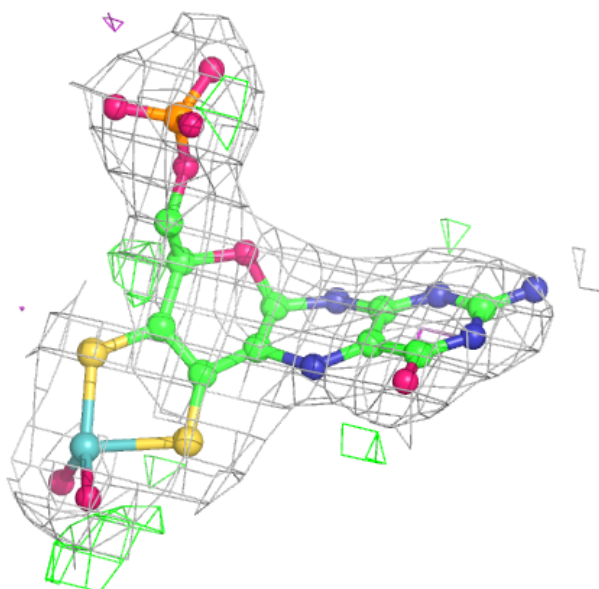
**Electron density around MTQ B 1394:**

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



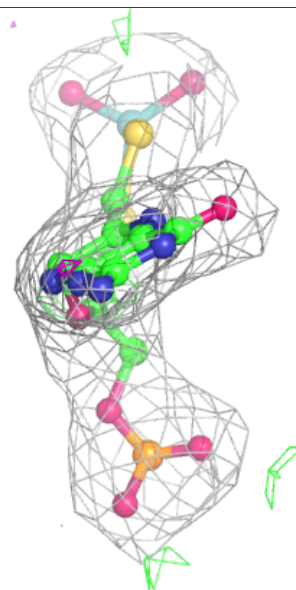
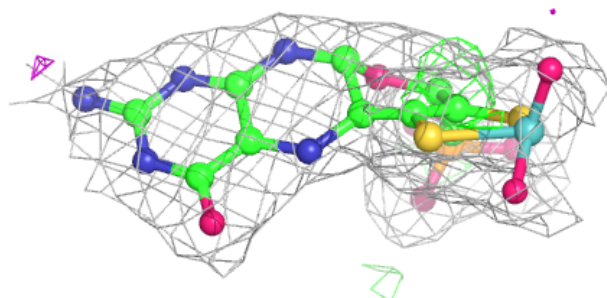
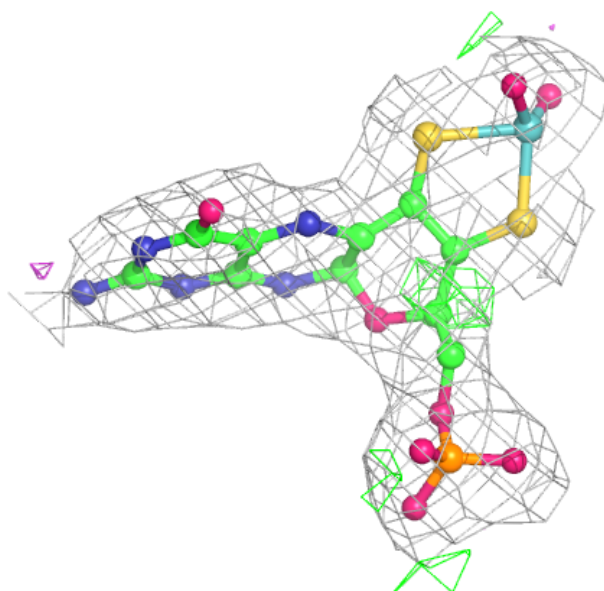
**Electron density around MTQ F 1394:**

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



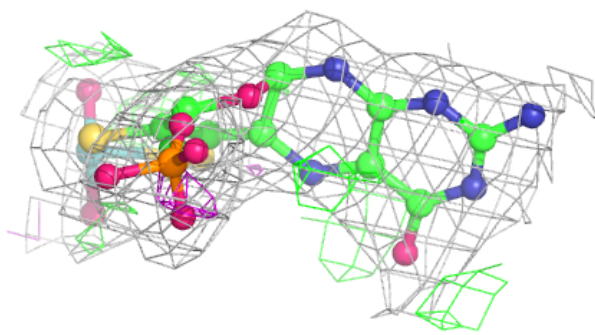
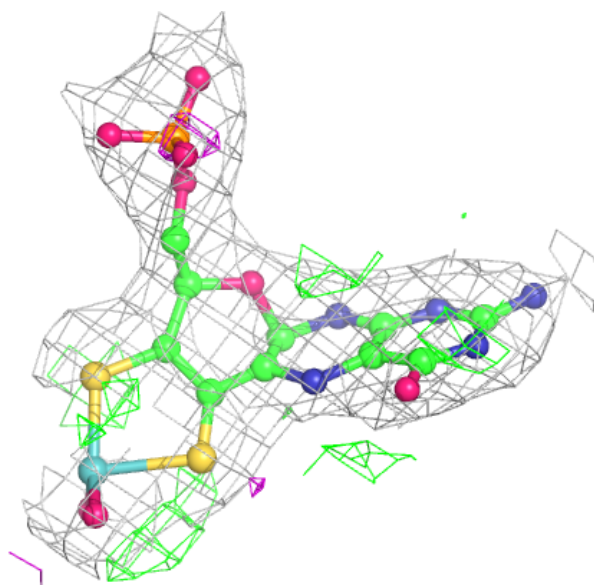
**Electron density around MTQ E 1394:**

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



**Electron density around MTQ C 1394:**

$2mF_o-DF_c$  (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.