



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:05 PM UTC

PDB ID : 1OGP / pdb_00001ogp
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

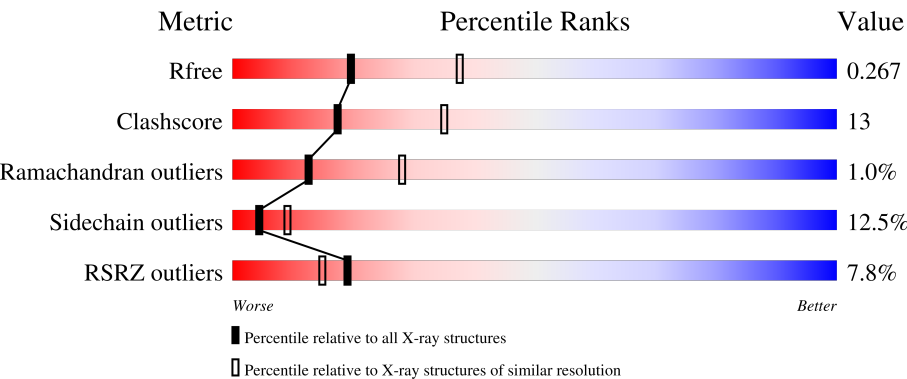
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	393	5% 69% 23% 6% ..
1	B	393	4% 69% 22% 6% ..
1	C	393	8% 61% 29% 7% ..
1	D	393	15% 55% 31% 9% ..
1	E	393	8% 63% 29% 6% ..

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Mol	Chain	Length	Quality of chain
1	F	393	

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 (CCD ID: CS) (formula: Cs).

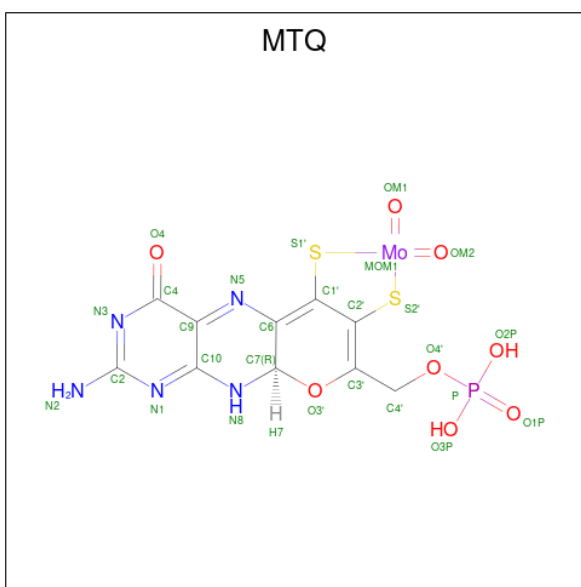
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cs	0	0
			2	2		
2	B	2	Total	Cs	0	0
			2	2		
2	C	2	Total	Cs	0	0
			2	2		
2	D	2	Total	Cs	0	0
			2	2		
2	E	2	Total	Cs	0	0
			2	2		
2	F	2	Total	Cs	0	0
			2	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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) (CCD ID: MTQ) (formula: $C_{10}H_8MoN_5O_8PS_2$).



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

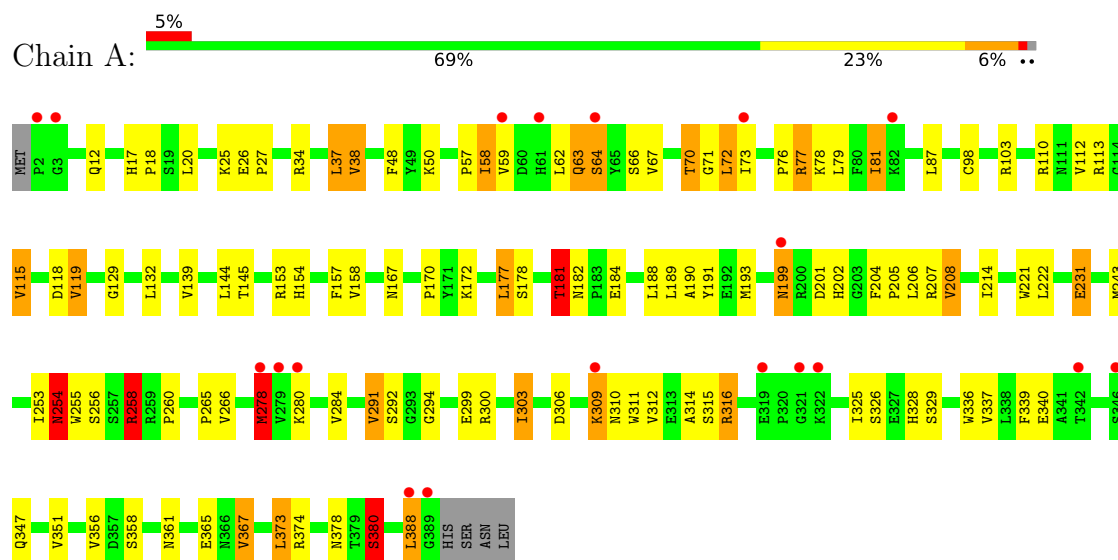
- Molecule 5 is water.

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

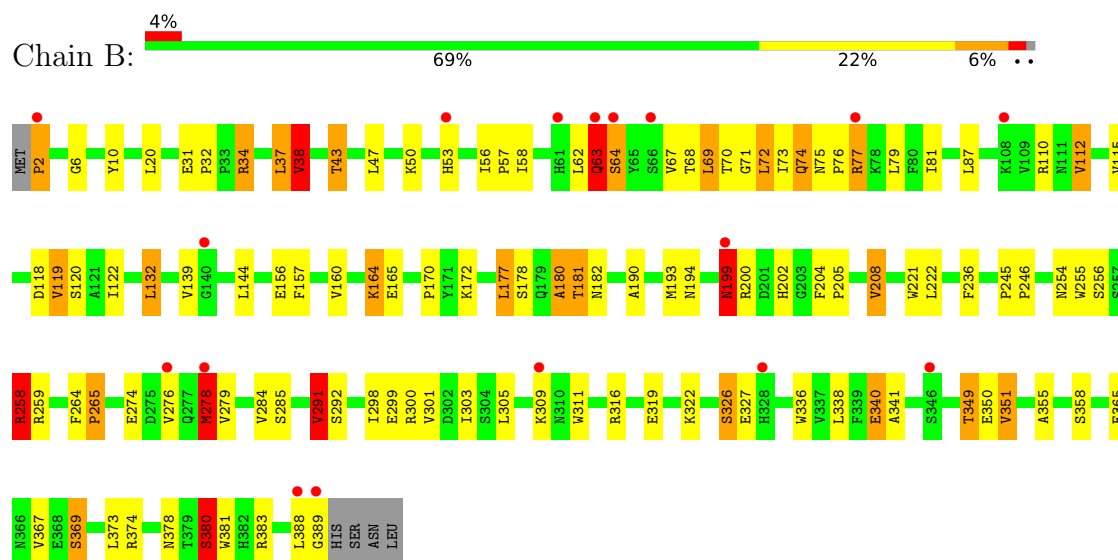
3 Residue-property plots [i](#)

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: SULFITE OXIDASE

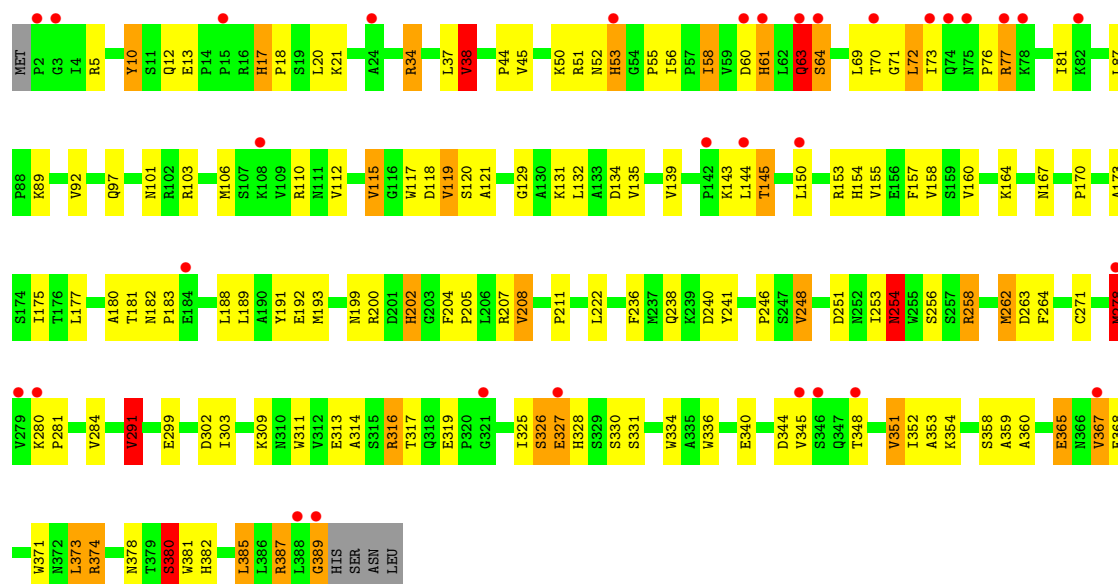


• Molecule 1: SULFITE OXIDASE

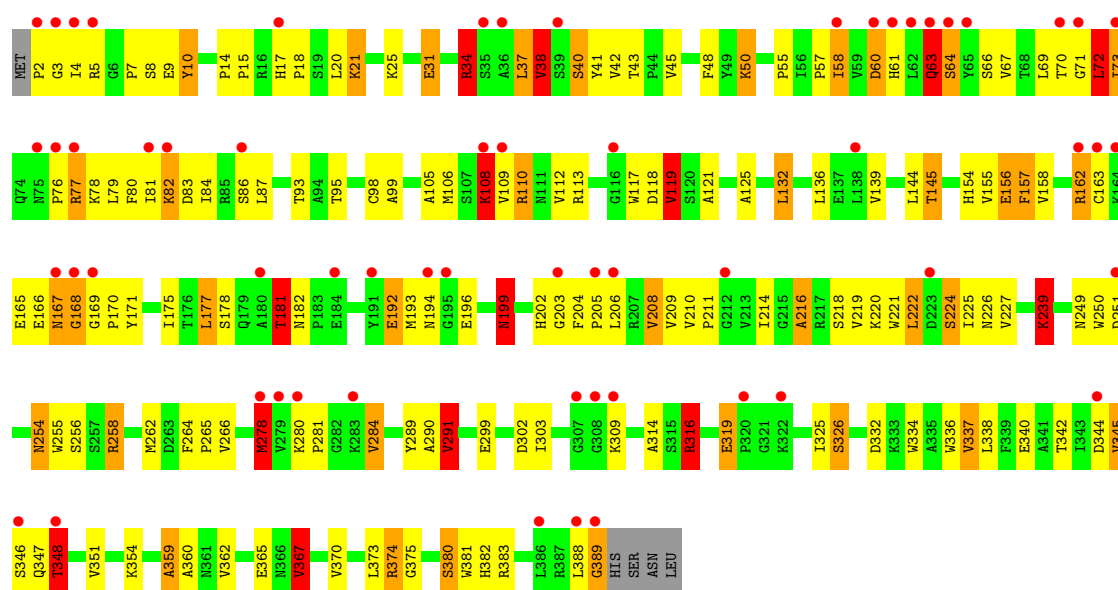


• Molecule 1: SULFITE OXIDASE

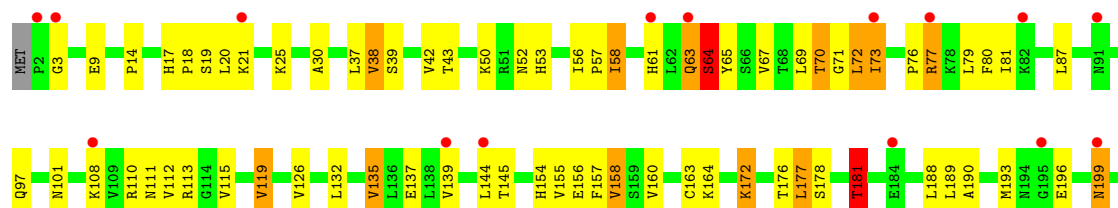


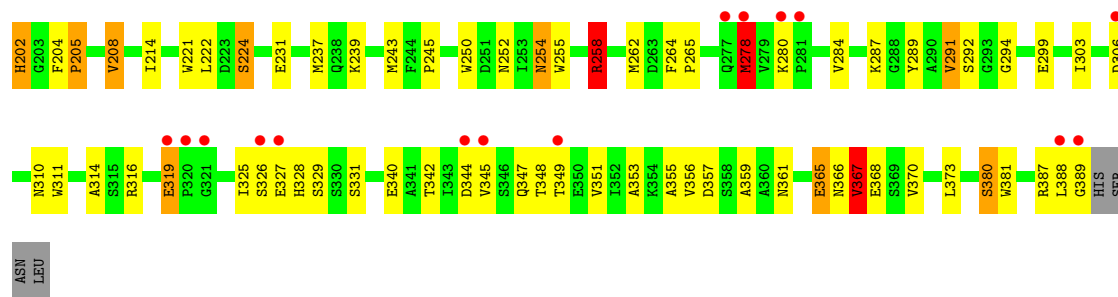


• Molecule 1: SULFITE OXIDASE

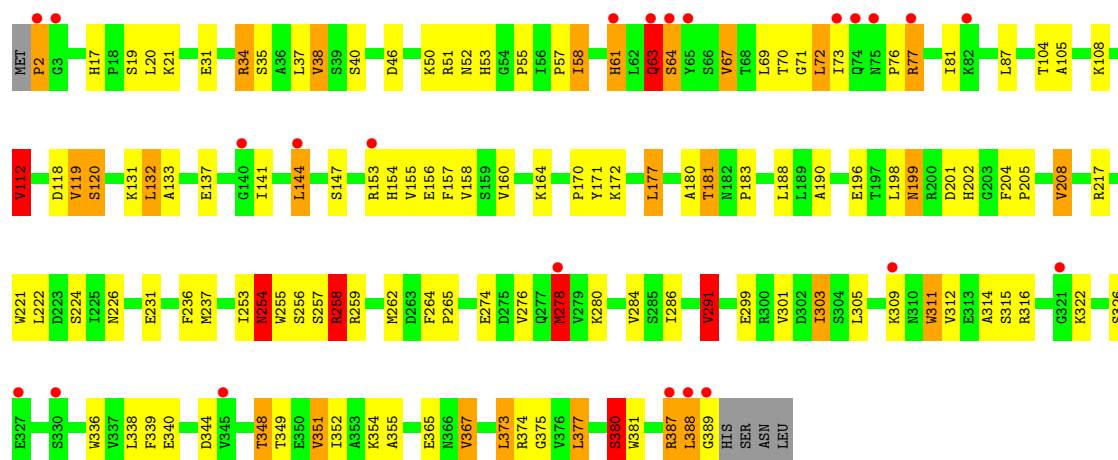


• Molecule 1: SULFITE OXIDASE





• Molecule 1: SULFITE OXIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	222.92Å 351.27Å 158.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	182.57 – 2.60 182.57 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (182.57-2.60) 99.0 (182.57-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	53.8	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CS, MTQ, GOL

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	1.83	34/3085 (1.1%)	1.49	23/4196 (0.5%)
1	B	1.81	47/3085 (1.5%)	1.52	30/4196 (0.7%)
1	C	1.89	47/3085 (1.5%)	1.50	21/4196 (0.5%)
1	D	2.04	62/3085 (2.0%)	1.62	39/4196 (0.9%)
1	E	1.94	54/3085 (1.8%)	1.54	30/4196 (0.7%)
1	F	1.88	48/3085 (1.6%)	1.53	27/4196 (0.6%)
All	All	1.90	292/18510 (1.6%)	1.53	170/25176 (0.7%)

All (292) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	278	MET	SD-CE	19.91	2.29	1.79
1	D	278	MET	SD-CE	15.71	2.18	1.79
1	B	115	VAL	CA-CB	-12.36	1.41	1.54
1	C	278	MET	SD-CE	12.04	2.09	1.79
1	D	359	ALA	CA-CB	-11.17	1.36	1.53
1	A	278	MET	SD-CE	11.04	2.07	1.79
1	F	355	ALA	CA-CB	-10.67	1.33	1.53
1	A	278	MET	CG-SD	10.58	2.07	1.80
1	D	214	ILE	CA-CB	10.37	1.64	1.54
1	B	278	MET	CG-SD	10.12	2.06	1.80
1	B	303	ILE	CA-CB	-10.09	1.41	1.54
1	F	237	MET	SD-CE	-9.91	1.54	1.79
1	F	253	ILE	C-O	-9.90	1.14	1.24
1	F	278	MET	SD-CE	9.53	2.03	1.79
1	B	112	VAL	CA-CB	9.47	1.67	1.54
1	C	262	MET	CG-SD	9.13	2.03	1.80
1	D	389	GLY	C-O	9.06	1.41	1.23
1	F	286	ILE	CA-CB	-8.98	1.43	1.53
1	B	358	SER	C-O	-8.83	1.12	1.24
1	D	266	VAL	CA-CB	-8.76	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	278	MET	CG-SD	8.46	2.01	1.80
1	D	93	THR	C-O	8.42	1.34	1.24
1	E	243	MET	SD-CE	-8.33	1.58	1.79
1	E	365	GLU	CA-C	8.27	1.63	1.52
1	E	245	PRO	C-O	-8.19	1.17	1.24
1	C	58	ILE	CA-CB	8.15	1.64	1.54
1	A	158	VAL	C-O	-8.13	1.15	1.24
1	E	52	ASN	C-O	-8.06	1.14	1.23
1	A	361	ASN	C-O	-8.04	1.14	1.23
1	D	337	VAL	CA-CB	-8.02	1.44	1.54
1	F	104	THR	CA-CB	-7.95	1.41	1.53
1	C	253	ILE	CA-CB	-7.82	1.45	1.54
1	A	214	ILE	CA-CB	7.82	1.61	1.54
1	D	290	ALA	CA-CB	-7.76	1.40	1.53
1	D	58	ILE	CA-CB	7.68	1.64	1.54
1	B	278	MET	CB-CG	7.66	1.75	1.52
1	C	92	VAL	CA-CB	-7.63	1.45	1.54
1	C	200	ARG	NE-CZ	7.57	1.41	1.33
1	F	365	GLU	CA-C	7.56	1.62	1.52
1	E	292	SER	C-O	-7.53	1.14	1.23
1	E	262	MET	SD-CE	-7.53	1.60	1.79
1	D	64	SER	CA-C	7.42	1.62	1.52
1	E	278	MET	CG-SD	7.42	1.99	1.80
1	F	311	TRP	C-O	-7.37	1.14	1.23
1	F	118	ASP	CA-C	7.35	1.62	1.52
1	F	274	GLU	C-O	-7.35	1.14	1.23
1	D	14	PRO	CA-C	-7.33	1.45	1.52
1	C	254	ASN	C-O	7.33	1.32	1.24
1	A	311	TRP	C-O	-7.32	1.14	1.23
1	D	258	ARG	CD-NE	-7.31	1.36	1.46
1	F	301	VAL	C-O	-7.30	1.16	1.24
1	C	291	VAL	CA-CB	7.20	1.66	1.55
1	D	227	VAL	CA-CB	-7.19	1.45	1.54
1	A	365	GLU	CA-C	7.17	1.61	1.52
1	E	112	VAL	CA-CB	7.16	1.63	1.54
1	D	125	ALA	C-O	7.11	1.32	1.23
1	B	349	THR	CA-CB	7.06	1.64	1.53
1	D	108	LYS	CG-CD	7.06	1.73	1.52
1	D	209	VAL	CA-CB	-7.05	1.45	1.54
1	D	382	HIS	CA-CB	-7.05	1.43	1.53
1	E	342	THR	CA-CB	-7.01	1.43	1.53
1	C	173	ALA	CA-CB	6.99	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	VAL	CA-CB	-6.99	1.47	1.54
1	A	253	ILE	C-O	-6.98	1.16	1.24
1	E	359	ALA	CA-CB	-6.98	1.43	1.53
1	B	276	VAL	C-O	-6.97	1.16	1.24
1	B	316	ARG	CB-CG	-6.96	1.31	1.52
1	C	311	TRP	C-O	-6.93	1.15	1.23
1	E	237	MET	SD-CE	-6.89	1.62	1.79
1	F	262	MET	SD-CE	-6.87	1.62	1.79
1	C	248	VAL	CA-CB	-6.86	1.45	1.54
1	B	6	GLY	C-O	-6.85	1.14	1.24
1	F	190	ALA	CA-CB	-6.85	1.43	1.53
1	C	353	ALA	CA-CB	-6.81	1.38	1.53
1	B	298	ILE	CA-CB	6.80	1.62	1.53
1	D	345	VAL	CA-CB	6.75	1.62	1.54
1	B	365	GLU	CA-C	6.74	1.61	1.52
1	E	214	ILE	CA-CB	6.68	1.60	1.54
1	D	264	PHE	N-CA	-6.68	1.39	1.45
1	E	101	ASN	C-O	-6.62	1.15	1.23
1	B	383	ARG	CD-NE	6.55	1.55	1.46
1	C	157	PHE	CA-C	-6.54	1.44	1.52
1	F	133	ALA	CA-CB	-6.53	1.43	1.53
1	F	64	SER	CA-C	6.46	1.61	1.52
1	D	258	ARG	NE-CZ	-6.44	1.25	1.33
1	F	224	SER	CA-C	-6.43	1.44	1.52
1	C	264	PHE	CA-CB	-6.42	1.46	1.53
1	A	278	MET	CB-CG	6.42	1.71	1.52
1	F	157	PHE	CA-C	-6.41	1.45	1.52
1	D	60	ASP	N-CA	6.41	1.54	1.46
1	F	155	VAL	C-O	-6.41	1.17	1.24
1	E	190	ALA	CA-CB	-6.41	1.44	1.53
1	D	156	GLU	CD-OE1	6.39	1.37	1.25
1	E	163	CYS	C-O	-6.32	1.16	1.24
1	A	189	LEU	C-O	-6.29	1.15	1.23
1	F	257	SER	C-O	-6.29	1.15	1.24
1	D	168	GLY	C-O	6.27	1.33	1.24
1	D	316	ARG	NE-CZ	6.24	1.40	1.33
1	B	199	ASN	CB-CG	-6.22	1.36	1.52
1	C	254	ASN	CA-CB	-6.21	1.43	1.53
1	A	358	SER	C-O	-6.19	1.16	1.24
1	D	181	THR	CA-CB	-6.18	1.44	1.53
1	F	316	ARG	CB-CG	-6.16	1.33	1.52
1	E	205	PRO	CG-CD	-6.15	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	240	ASP	CA-C	6.14	1.60	1.52
1	B	291	VAL	CA-C	-6.12	1.45	1.52
1	F	276	VAL	C-O	-6.09	1.17	1.24
1	F	157	PHE	C-O	-6.09	1.16	1.24
1	C	115	VAL	CA-CB	-6.06	1.48	1.54
1	C	389	GLY	C-O	6.05	1.35	1.23
1	D	43	THR	CA-CB	6.03	1.65	1.53
1	C	52	ASN	N-CA	6.00	1.53	1.46
1	A	316	ARG	CB-CG	-6.00	1.34	1.52
1	F	137	GLU	CA-C	5.98	1.60	1.52
1	F	305	LEU	C-O	-5.98	1.15	1.24
1	F	180	ALA	CA-CB	-5.97	1.43	1.53
1	A	167	ASN	CG-ND2	-5.97	1.20	1.33
1	B	180	ALA	CA-CB	-5.97	1.43	1.53
1	A	294	GLY	C-O	-5.96	1.15	1.23
1	B	258	ARG	NE-CZ	-5.95	1.26	1.33
1	F	217	ARG	C-O	-5.94	1.16	1.24
1	E	158	VAL	C-O	-5.92	1.17	1.24
1	A	356	VAL	CA-CB	5.91	1.61	1.54
1	F	55	PRO	CA-CB	5.91	1.61	1.53
1	B	193	MET	SD-CE	-5.91	1.64	1.79
1	E	250	TRP	C-O	-5.90	1.16	1.24
1	F	377	LEU	C-O	-5.90	1.16	1.23
1	E	111	ASN	CB-CG	-5.88	1.37	1.52
1	E	126	VAL	CA-CB	5.88	1.61	1.54
1	E	64	SER	CA-C	5.88	1.60	1.52
1	A	309	LYS	N-CA	5.87	1.53	1.46
1	A	172	LYS	C-O	-5.87	1.16	1.23
1	D	325	ILE	CA-CB	5.84	1.62	1.54
1	C	358	SER	C-O	-5.83	1.16	1.24
1	F	351	VAL	C-O	-5.83	1.17	1.24
1	D	319	GLU	N-CA	5.83	1.52	1.45
1	D	250	TRP	N-CA	5.81	1.54	1.46
1	F	105	ALA	CA-CB	-5.79	1.43	1.53
1	B	56	ILE	CA-C	-5.78	1.48	1.53
1	A	34	ARG	CB-CG	-5.76	1.35	1.52
1	F	198	LEU	C-O	-5.75	1.17	1.23
1	D	291	VAL	CA-CB	-5.75	1.46	1.55
1	A	243	MET	SD-CE	-5.73	1.65	1.79
1	A	182	ASN	C-O	-5.72	1.17	1.24
1	E	158	VAL	CA-CB	5.72	1.61	1.54
1	C	180	ALA	CA-CB	-5.72	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	68	THR	CA-CB	-5.71	1.45	1.53
1	E	155	VAL	CA-CB	-5.70	1.47	1.54
1	F	112	VAL	CA-CB	5.68	1.62	1.54
1	A	81	ILE	CA-CB	-5.68	1.46	1.54
1	C	10	TYR	CA-CB	5.65	1.60	1.53
1	E	327	GLU	N-CA	5.65	1.54	1.46
1	F	303	ILE	C-O	-5.64	1.18	1.24
1	E	56	ILE	CA-C	-5.64	1.47	1.52
1	D	262	MET	SD-CE	5.63	1.93	1.79
1	D	82	LYS	N-CA	5.62	1.53	1.46
1	F	387	ARG	NE-CZ	5.62	1.39	1.33
1	A	292	SER	C-O	-5.62	1.16	1.23
1	F	254	ASN	C-O	5.61	1.30	1.24
1	E	155	VAL	C-O	-5.61	1.18	1.24
1	B	316	ARG	C-O	-5.59	1.17	1.23
1	D	61	HIS	CA-CB	5.59	1.60	1.52
1	F	132	LEU	C-O	-5.59	1.17	1.24
1	C	302	ASP	CA-C	5.58	1.59	1.52
1	B	355	ALA	CA-CB	-5.57	1.43	1.53
1	E	345	VAL	CA-CB	5.57	1.61	1.54
1	B	122	ILE	CA-C	-5.57	1.45	1.52
1	F	264	PHE	C-O	-5.57	1.19	1.24
1	F	278	MET	CB-CG	5.56	1.69	1.52
1	C	352	ILE	CA-CB	-5.56	1.47	1.54
1	E	108	LYS	CD-CE	5.56	1.69	1.52
1	D	383	ARG	C-O	-5.55	1.17	1.24
1	D	63	GLN	N-CA	5.54	1.53	1.45
1	C	101	ASN	N-CA	5.53	1.53	1.46
1	D	192	GLU	CD-OE1	5.53	1.35	1.25
1	F	236	PHE	C-O	-5.53	1.16	1.24
1	D	374	ARG	CZ-NH1	5.52	1.40	1.32
1	E	42	VAL	CA-CB	-5.51	1.47	1.54
1	D	73	ILE	CA-C	5.50	1.59	1.52
1	E	258	ARG	CD-NE	-5.50	1.38	1.46
1	C	316	ARG	CB-CG	-5.49	1.35	1.52
1	E	380	SER	CB-OG	-5.49	1.31	1.42
1	B	305	LEU	C-O	-5.47	1.16	1.24
1	C	118	ASP	CA-C	5.46	1.60	1.52
1	C	345	VAL	CA-CB	5.46	1.61	1.54
1	F	141	ILE	CA-CB	-5.45	1.48	1.53
1	B	43	THR	CA-CB	-5.44	1.42	1.53
1	F	201	ASP	C-O	-5.44	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	14	PRO	C-O	-5.43	1.18	1.24
1	A	254	ASN	CA-CB	-5.42	1.45	1.53
1	B	157	PHE	C-O	-5.42	1.17	1.24
1	C	263	ASP	C-O	5.41	1.31	1.23
1	D	354	LYS	CB-CG	-5.41	1.36	1.52
1	E	252	ASN	N-CA	5.41	1.53	1.45
1	A	300	ARG	CB-CG	-5.40	1.36	1.52
1	B	300	ARG	NE-CZ	-5.40	1.27	1.33
1	E	58	ILE	C-O	-5.40	1.18	1.24
1	D	199	ASN	CB-CG	-5.39	1.38	1.52
1	A	207	ARG	C-O	-5.38	1.17	1.23
1	C	155	VAL	C-O	-5.38	1.18	1.24
1	B	265	PRO	CA-CB	-5.38	1.46	1.53
1	B	301	VAL	C-O	-5.38	1.18	1.24
1	E	79	LEU	C-O	-5.38	1.17	1.24
1	D	216	ALA	CA-CB	5.37	1.62	1.53
1	D	145	THR	CA-CB	5.37	1.61	1.53
1	A	190	ALA	CA-CB	-5.37	1.45	1.53
1	D	105	ALA	CA-CB	-5.36	1.44	1.53
1	C	60	ASP	N-CA	5.35	1.53	1.46
1	B	10	TYR	CA-C	5.35	1.59	1.53
1	A	157	PHE	C-O	-5.34	1.17	1.24
1	F	2	PRO	CB-CG	5.34	1.76	1.49
1	B	190	ALA	CA-CB	-5.33	1.45	1.53
1	B	350	GLU	CD-OE2	5.33	1.35	1.25
1	D	21	LYS	CD-CE	5.32	1.68	1.52
1	D	5	ARG	CZ-NH1	5.31	1.40	1.32
1	D	84	ILE	CA-CB	5.30	1.61	1.54
1	A	303	ILE	CA-CB	-5.30	1.47	1.54
1	F	316	ARG	C-O	-5.30	1.17	1.23
1	E	353	ALA	CA-CB	-5.29	1.44	1.53
1	E	349	THR	CA-CB	5.29	1.62	1.53
1	D	15	PRO	CG-CD	5.28	1.68	1.50
1	A	66	SER	CA-C	5.28	1.59	1.52
1	E	115	VAL	C-O	-5.28	1.18	1.24
1	A	266	VAL	CA-CB	5.28	1.60	1.54
1	A	79	LEU	CA-C	-5.27	1.46	1.52
1	D	4	ILE	CA-CB	5.27	1.62	1.54
1	B	74	GLN	N-CA	5.27	1.52	1.46
1	D	50	LYS	C-O	-5.27	1.18	1.24
1	A	311	TRP	CA-C	-5.26	1.46	1.52
1	A	118	ASP	CA-C	5.26	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	31	GLU	CA-C	5.25	1.58	1.52
1	E	264	PHE	C-O	-5.25	1.19	1.24
1	F	108	LYS	N-CA	5.24	1.52	1.46
1	E	258	ARG	NE-CZ	-5.24	1.27	1.33
1	E	355	ALA	CA-CB	-5.24	1.43	1.53
1	E	202	HIS	CA-CB	-5.23	1.45	1.53
1	D	162	ARG	CA-CB	5.23	1.61	1.53
1	E	73	ILE	CA-C	5.21	1.59	1.52
1	B	311	TRP	C-O	-5.21	1.17	1.23
1	C	240	ASP	CG-OD2	5.21	1.35	1.25
1	E	156	GLU	C-O	-5.20	1.17	1.24
1	C	160	VAL	CA-CB	-5.20	1.48	1.54
1	B	274	GLU	CA-C	-5.19	1.46	1.53
1	C	170	PRO	CA-CB	5.19	1.60	1.53
1	C	248	VAL	CB-CG2	5.18	1.69	1.52
1	C	44	PRO	C-O	5.18	1.29	1.23
1	C	12	GLN	CA-C	5.18	1.59	1.53
1	D	162	ARG	NE-CZ	5.17	1.38	1.33
1	D	167	ASN	CG-OD1	5.17	1.33	1.23
1	E	319	GLU	N-CA	5.17	1.51	1.45
1	E	135	VAL	C-O	-5.17	1.17	1.24
1	C	354	LYS	C-O	-5.17	1.17	1.23
1	D	218	SER	C-O	5.16	1.29	1.23
1	D	125	ALA	CA-CB	-5.16	1.44	1.53
1	C	238	GLN	CA-CB	-5.16	1.46	1.53
1	B	351	VAL	CA-CB	5.16	1.60	1.54
1	B	110	ARG	NE-CZ	5.15	1.38	1.33
1	D	99	ALA	C-O	-5.15	1.17	1.24
1	B	383	ARG	NE-CZ	5.15	1.38	1.33
1	E	380	SER	CA-C	-5.15	1.45	1.52
1	D	264	PHE	CA-C	-5.14	1.47	1.52
1	E	294	GLY	C-O	-5.13	1.16	1.23
1	B	200	ARG	CA-C	-5.13	1.46	1.52
1	D	119	VAL	CA-C	5.13	1.59	1.52
1	D	95	THR	C-O	5.13	1.30	1.24
1	F	52	ASN	C-O	-5.12	1.17	1.23
1	B	64	SER	CA-C	5.12	1.59	1.52
1	C	327	GLU	N-CA	5.11	1.54	1.46
1	D	175	ILE	CA-C	-5.11	1.46	1.52
1	E	224	SER	C-O	-5.10	1.17	1.23
1	B	156	GLU	C-O	-5.09	1.17	1.24
1	C	385	LEU	CA-C	-5.09	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	202	HIS	CA-CB	5.08	1.61	1.53
1	E	311	TRP	CA-C	-5.08	1.46	1.52
1	D	3	GLY	N-CA	5.07	1.51	1.45
1	C	97	GLN	N-CA	-5.07	1.40	1.46
1	B	178	SER	N-CA	5.06	1.52	1.46
1	E	157	PHE	C-O	-5.06	1.18	1.24
1	B	118	ASP	CA-C	5.06	1.59	1.52
1	B	327	GLU	N-CA	5.06	1.54	1.46
1	C	278	MET	CB-CG	5.06	1.67	1.52
1	D	348	THR	CA-CB	5.06	1.60	1.53
1	C	153	ARG	NE-CZ	5.05	1.38	1.33
1	E	80	PHE	C-O	-5.05	1.17	1.23
1	F	352	ILE	C-O	-5.05	1.19	1.24
1	E	356	VAL	C-O	-5.05	1.18	1.24
1	C	145	THR	CA-CB	5.04	1.60	1.53
1	F	326	SER	C-N	-5.03	1.27	1.33
1	B	285	SER	CA-C	5.02	1.59	1.52
1	B	278	MET	SD-CE	5.01	1.92	1.79
1	B	2	PRO	CB-CG	5.01	1.74	1.49
1	C	241	TYR	CD2-CE2	5.01	1.53	1.38

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	VAL	CB-CA-C	-12.41	93.71	111.34
1	B	208	VAL	CB-CA-C	-11.09	95.59	111.34
1	E	208	VAL	CB-CA-C	-10.50	96.83	111.21
1	C	326	SER	CA-C-N	-10.41	106.89	123.23
1	C	326	SER	C-N-CA	-10.41	106.89	123.23
1	F	326	SER	CA-C-N	-10.08	106.80	123.33
1	F	326	SER	C-N-CA	-10.08	106.80	123.33
1	A	326	SER	CA-C-N	-9.91	107.66	123.23
1	A	326	SER	C-N-CA	-9.91	107.66	123.23
1	B	326	SER	CA-C-N	-9.80	107.84	123.23
1	B	326	SER	C-N-CA	-9.80	107.84	123.23
1	D	326	SER	N-CA-C	9.80	121.91	111.03
1	E	326	SER	CA-C-N	-9.76	107.32	123.33
1	E	326	SER	C-N-CA	-9.76	107.32	123.33
1	D	326	SER	CA-C-N	-9.42	108.44	123.23
1	D	326	SER	C-N-CA	-9.42	108.44	123.23
1	B	119	VAL	N-CA-CB	-9.06	100.58	112.26
1	E	258	ARG	NE-CZ-NH2	-8.88	111.20	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	326	SER	N-CA-C	8.82	120.82	111.03
1	B	199	ASN	CB-CA-C	-8.80	91.01	110.19
1	F	258	ARG	NE-CZ-NH1	8.79	130.29	121.50
1	F	258	ARG	NE-CZ-NH2	-8.73	111.34	119.20
1	F	291	VAL	CB-CA-C	-8.51	95.16	110.48
1	B	389	GLY	CA-C-O	8.49	138.64	120.80
1	D	113	ARG	CB-CA-C	-8.33	96.56	109.89
1	E	291	VAL	CB-CA-C	-8.16	95.79	110.48
1	F	326	SER	N-CA-C	8.12	120.04	111.03
1	E	316	ARG	CG-CD-NE	-8.10	94.17	112.00
1	F	208	VAL	CB-CA-C	-8.01	99.96	111.34
1	E	326	SER	N-CA-C	8.00	119.91	111.03
1	B	67	VAL	CB-CA-C	-7.94	100.04	110.84
1	E	380	SER	CB-CA-C	-7.91	94.68	110.42
1	C	119	VAL	N-CA-CB	-7.90	102.07	112.26
1	C	326	SER	N-CA-C	7.84	119.73	111.03
1	A	380	SER	CB-CA-C	-7.80	94.90	110.42
1	B	291	VAL	CB-CA-C	-7.77	96.50	110.48
1	A	291	VAL	CB-CA-C	-7.75	96.53	110.48
1	C	208	VAL	CB-CA-C	-7.70	100.41	111.34
1	A	199	ASN	CB-CA-C	-7.68	93.44	110.19
1	D	291	VAL	CB-CA-C	-7.68	96.65	110.48
1	D	109	VAL	CB-CA-C	-7.65	102.02	112.04
1	F	326	SER	O-C-N	-7.46	113.97	122.03
1	A	119	VAL	N-CA-CB	-7.42	102.69	112.26
1	A	326	SER	N-CA-C	7.42	119.27	111.03
1	E	199	ASN	CB-CA-C	-7.39	94.08	110.19
1	C	158	VAL	CB-CA-C	-7.22	99.86	110.62
1	A	258	ARG	CG-CD-NE	-7.15	96.27	112.00
1	A	326	SER	O-C-N	-7.13	114.33	122.03
1	B	326	SER	O-C-N	-7.11	114.36	122.03
1	D	181	THR	N-CA-CB	-7.02	100.33	110.80
1	D	38	VAL	N-CA-CB	-7.02	102.94	112.28
1	C	326	SER	O-C-N	-6.99	114.48	122.03
1	A	38	VAL	CB-CA-C	6.97	120.16	111.65
1	F	259	ARG	NE-CZ-NH2	-6.96	112.93	119.20
1	F	119	VAL	N-CA-CB	-6.96	103.28	112.26
1	E	113	ARG	CB-CA-C	-6.95	98.76	109.89
1	D	326	SER	O-C-N	-6.90	114.57	122.03
1	C	327	GLU	N-CA-CB	6.88	123.35	110.56
1	A	316	ARG	CG-CD-NE	-6.86	96.91	112.00
1	D	199	ASN	CB-CA-C	-6.78	95.41	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	8	SER	CB-CA-C	-6.78	99.27	110.72
1	D	367	VAL	CB-CA-C	-6.73	103.23	112.04
1	C	291	VAL	CB-CA-C	-6.72	98.39	110.48
1	C	382	HIS	CB-CA-C	-6.68	100.23	110.26
1	D	63	GLN	N-CA-C	-6.64	100.66	110.48
1	E	208	VAL	N-CA-CB	6.59	119.66	110.56
1	E	258	ARG	NE-CZ-NH1	6.59	128.09	121.50
1	F	380	SER	CB-CA-C	-6.54	97.41	110.42
1	C	167	ASN	CB-CA-C	-6.52	102.47	111.73
1	B	278	MET	CG-SD-CE	6.51	115.22	100.90
1	E	389	GLY	CA-C-O	6.44	134.33	120.80
1	E	181	THR	N-CA-CB	-6.43	102.01	110.88
1	E	367	VAL	CB-CA-C	-6.42	103.67	111.88
1	D	258	ARG	CG-CD-NE	-6.33	98.06	112.00
1	F	258	ARG	CD-NE-CZ	6.33	133.26	124.40
1	D	302	ASP	CB-CA-C	-6.31	98.02	109.38
1	C	316	ARG	CB-CA-C	6.23	122.03	109.38
1	D	163	CYS	N-CA-C	6.20	119.01	108.90
1	E	119	VAL	N-CA-CB	-6.19	104.27	112.26
1	D	258	ARG	NE-CZ-NH2	-6.10	113.71	119.20
1	A	373	LEU	N-CA-C	6.09	118.42	111.11
1	F	46	ASP	CB-CA-C	-6.02	100.44	110.68
1	A	34	ARG	N-CA-CB	-6.02	100.31	110.49
1	E	70	THR	CB-CA-C	-6.02	99.99	112.44
1	F	388	LEU	N-CA-C	5.99	118.98	108.56
1	F	67	VAL	CB-CA-C	-5.99	102.69	110.84
1	E	43	THR	OG1-CB-CG2	-5.98	97.33	109.30
1	E	326	SER	O-C-N	-5.98	115.58	122.03
1	D	239	LYS	CA-CB-CG	5.97	126.04	114.10
1	D	370	VAL	N-CA-C	5.96	117.83	112.17
1	F	351	VAL	N-CA-C	5.96	116.88	108.36
1	C	351	VAL	N-CA-CB	5.96	118.14	110.99
1	C	61	HIS	CB-CA-C	-5.96	102.77	111.23
1	A	199	ASN	CA-CB-CG	5.95	118.55	112.60
1	A	258	ARG	NE-CZ-NH2	-5.95	113.84	119.20
1	D	166	GLU	CB-CA-C	5.89	120.51	111.02
1	C	365	GLU	CB-CG-CD	5.89	122.62	112.60
1	D	113	ARG	N-CA-CB	5.88	118.62	109.85
1	F	61	HIS	N-CA-C	5.87	117.01	107.32
1	B	63	GLN	N-CA-C	-5.85	100.95	110.20
1	B	258	ARG	NE-CZ-NH2	-5.84	113.94	119.20
1	E	63	GLN	N-CA-C	-5.82	101.66	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	10	TYR	CB-CA-C	-5.80	101.80	111.13
1	A	70	THR	CB-CA-C	-5.78	100.47	112.44
1	D	157	PHE	N-CA-C	-5.78	99.77	109.07
1	E	61	HIS	N-CA-C	5.77	116.84	107.32
1	D	170	PRO	CB-CA-C	-5.76	102.39	110.63
1	C	63	GLN	N-CA-C	-5.75	101.12	110.20
1	E	30	ALA	N-CA-C	5.68	117.47	108.79
1	B	38	VAL	N-CA-CB	-5.62	104.85	112.22
1	C	120	SER	N-CA-C	5.61	119.44	112.59
1	B	351	VAL	CB-CA-C	5.61	118.47	110.84
1	B	388	LEU	N-CA-C	5.61	118.52	107.98
1	B	119	VAL	N-CA-C	-5.61	107.52	112.90
1	F	63	GLN	N-CA-C	-5.60	101.35	110.20
1	D	362	VAL	CB-CA-C	-5.59	104.10	111.70
1	B	208	VAL	N-CA-CB	5.56	117.88	110.26
1	F	170	PRO	N-CA-C	5.56	120.96	111.68
1	A	63	GLN	N-CA-C	-5.56	101.42	110.20
1	F	34	ARG	N-CA-CB	-5.54	101.14	110.49
1	F	316	ARG	CB-CA-C	5.53	120.60	109.38
1	B	170	PRO	N-CA-C	5.52	120.89	111.68
1	D	373	LEU	CB-CA-C	-5.50	101.61	110.74
1	E	38	VAL	N-CA-CB	-5.50	105.01	112.16
1	D	34	ARG	N-CA-CB	-5.50	101.20	110.49
1	B	278	MET	CB-CG-SD	5.47	129.12	112.70
1	E	370	VAL	N-CA-C	5.46	117.46	112.43
1	A	181	THR	N-CA-CB	-5.44	103.37	110.88
1	F	373	LEU	N-CA-C	5.43	117.90	111.33
1	F	351	VAL	N-CA-CB	5.42	117.49	110.99
1	D	110	ARG	N-CA-CB	5.39	119.66	110.71
1	D	367	VAL	N-CA-CB	5.36	117.16	110.47
1	B	199	ASN	N-CA-C	5.33	116.97	110.41
1	E	316	ARG	CB-CA-C	5.30	120.15	109.38
1	C	380	SER	CB-CA-C	-5.30	99.88	110.42
1	D	389	GLY	CA-C-O	5.29	131.92	120.80
1	D	4	ILE	CB-CA-C	-5.29	101.51	111.30
1	F	316	ARG	CG-CD-NE	-5.29	100.37	112.00
1	E	115	VAL	CB-CA-C	-5.26	103.01	111.59
1	B	381	TRP	N-CA-CB	5.24	117.78	109.51
1	F	120	SER	N-CA-C	5.22	118.96	112.59
1	B	258	ARG	CG-CD-NE	-5.21	100.54	112.00
1	D	199	ASN	N-CA-CB	-5.20	103.26	110.38
1	D	316	ARG	CA-CB-CG	5.18	124.45	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	279	VAL	N-CA-C	5.17	117.18	108.81
1	D	38	VAL	CA-C-O	5.17	125.03	119.91
1	A	170	PRO	N-CA-C	5.16	120.30	111.68
1	F	348	THR	CB-CA-C	5.16	118.00	110.26
1	E	97	GLN	CB-CG-CD	5.13	121.32	112.60
1	B	119	VAL	CB-CA-C	5.13	117.56	111.20
1	F	144	LEU	N-CA-C	5.13	119.11	112.86
1	E	3	GLY	CA-C-O	5.12	125.55	119.10
1	B	34	ARG	N-CA-CB	-5.11	101.86	110.49
1	D	8	SER	CA-CB-OG	-5.11	100.88	111.10
1	D	345	VAL	N-CA-CB	5.10	117.89	111.46
1	A	388	LEU	N-CA-C	5.09	117.42	108.56
1	E	258	ARG	CG-CD-NE	-5.09	100.80	112.00
1	A	208	VAL	N-CA-CB	5.09	117.23	110.26
1	D	162	ARG	CG-CD-NE	-5.08	100.82	112.00
1	C	38	VAL	N-CA-CB	-5.08	105.56	112.16
1	B	63	GLN	N-CA-CB	5.06	117.70	110.06
1	D	250	TRP	N-CA-CB	5.06	119.25	110.39
1	B	259	ARG	NE-CZ-NH2	-5.06	114.65	119.20
1	D	342	THR	CB-CA-C	5.06	118.09	109.80
1	B	62	LEU	N-CA-C	5.05	116.47	111.07
1	B	369	SER	CA-CB-OG	-5.04	101.02	111.10
1	C	317	THR	OG1-CB-CG2	-5.04	99.22	109.30
1	A	278	MET	CB-CG-SD	5.04	127.80	112.70
1	E	67	VAL	CB-CA-C	-5.03	104.00	110.84
1	C	45	VAL	CB-CA-C	-5.02	105.47	112.04

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	64	0
1	B	3014	0	2998	59	0
1	C	3014	0	2998	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3014	0	2999	130	0
1	E	3014	0	2998	53	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	2	0
4	D	27	0	6	9	0
4	E	27	0	6	1	0
4	F	27	0	6	1	0
5	A	105	0	0	9	0
5	B	95	0	0	16	0
5	C	86	0	0	16	0
5	D	90	0	0	53	0
5	E	107	0	0	8	0
5	F	111	0	0	11	0
All	All	18888	0	18071	452	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 13.

All (452) 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:CG	1:B:278:MET:CB	1.75	1.59
1:B:2:PRO:CB	1:B:2:PRO:CG	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:CG	1:C:262:MET:SD	2.03	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:MET:CG	1:B:278:MET:SD	2.06	1.44
1:A:278:MET:SD	1:A:278:MET:CE	2.07	1.43
1:A:278:MET:SD	1:A:278:MET:CG	2.07	1.42
1:C:278:MET:SD	1:C:278:MET:CE	2.09	1.40
1:D:278:MET:SD	1:D:278:MET:CE	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
1:E:77:ARG:HG3	1:E:77:ARG:HH11	1.41	0.84
1:D:254:ASN:C	1:D:254:ASN:HD22	1.86	0.83
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:F:199:ASN:C	1:F:199:ASN:HD22	1.88	0.80
1:A:254:ASN:C	1:A:254:ASN:HD22	1.88	0.79
1:A:77:ARG:HG3	1:A:77:ARG:HH11	1.47	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:HG3	1:C:77:ARG:NH1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:50:LYS:HE3	1:F:202:HIS:CE1	2.21	0.76
1:D:72:LEU:HD13	5:D:2056:HOH:O	1.86	0.75
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:C:193:MET:HE1	1:C:202:HIS:CD2	2.23	0.73
1:D:192:GLU:HB3	5:D:2048:HOH:O	1.89	0.73
1:C:254:ASN:HD22	1:C:254:ASN:C	1.96	0.72
1:D:157:PHE:C	5:D:2034:HOH:O	2.33	0.71
1:D:78:LYS:HG2	5:D:2011:HOH:O	1.90	0.71
1:D:98:CYS:SG	4:D:1394:MTQ:S2'	2.89	0.70
1:D:108:LYS:HD2	5:E:2005:HOH:O	1.91	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:E:254:ASN:C	1:E:254:ASN:HD22	1.99	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
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:225:ILE:C	5:D:2055:HOH:O	2.36	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:A:202:HIS:CG	5:A:2061:HOH:O	2.47	0.67
1:F:254:ASN:C	1:F:254:ASN:HD22	2.02	0.67
1:F:50:LYS:CE	1:F:202:HIS:HE1	2.08	0.66
4:E:1394:MTQ:MOM1	4:E:1394:MTQ:OM2	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:A:254:ASN:C	1:A:254:ASN:ND2	2.51	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:OM1	4:A:1394:MTQ:MOM1	1.69	0.64
1:A:177:LEU:O	1:A:181:THR:HB	1.98	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
1:B:73:ILE:HG12	1:B:139:VAL:CG1	2.29	0.63
4:B:1394:MTQ:OM2	4:B:1394:MTQ:MOM1	1.70	0.63
1:C:254:ASN:C	1:C:254:ASN:ND2	2.56	0.62
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:OM1	4:D:1394:MTQ:MOM1	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
1:F:53:HIS:HD2	1:F:171:TYR:CD1	2.18	0.62
1:F:303:ILE:HD12	1:F:314:ALA:HB2	1.81	0.62
1:A:144:LEU:HD11	1:B:144:LEU:HD11	1.82	0.62
1:C:387:ARG:CG	1:C:387:ARG:HH11	2.12	0.62
1:C:13:GLU:OE1	1:C:56:ILE:HG12	2.00	0.62
1:D:389:GLY:C	5:D:2088:HOH:O	2.43	0.62
1:C:246:PRO:HD2	5:D:2069:HOH:O	2.00	0.61
1:D:156:GLU:C	5:D:2033:HOH:O	2.44	0.61
1:C:299:GLU:OE2	1:D:258:ARG:HD3	2.01	0.61
1:D:254:ASN:C	1:D:254:ASN:ND2	2.55	0.61
1:B:77:ARG:HH11	1:B:77:ARG:HG3	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:D:79:LEU:C	5:D:2013:HOH:O	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:25:LYS:HE2	1:D:239:LYS:NZ	2.17	0.59
1:D:21:LYS:CE	5:E:2028:HOH:O	2.42	0.59
1:E:77:ARG:HH11	1:E:77:ARG:CG	2.13	0.59
1:E:154:HIS:CD2	1:E:176:THR:HA	2.32	0.59
1:F:53:HIS:CD2	1:F:171:TYR:CE1	2.90	0.59
1:B:254:ASN:C	1:B:254:ASN:HD22	2.09	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:78:LYS:C	5:D:2013:HOH:O	2.43	0.59
1:D:66:SER:HB2	5:D:2013:HOH:O	2.01	0.59
1:D:203:GLY:HA2	1:D:221:TRP:CD1	2.38	0.59
1:E:193:MET:HE1	1:E:202:HIS:CE1	2.38	0.59
1:F:153:ARG:C	1:F:154:HIS:ND1	2.60	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:F:388:LEU:C	5:F:2109:HOH:O	2.46	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
1:D:332:ASP:C	5:D:2077:HOH:O	2.46	0.58
4:D:1394:MTQ:OM1	4:D:1394:MTQ:S1'	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:C:106:MET:HE3	1:C:378:ASN:HB2	1.87	0.57
1:E:328:HIS:HD2	1:E:329:SER:N	2.02	0.57
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:E:254:ASN:C	1:E:254:ASN:ND2	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:77:ARG:HH11	1:F:77:ARG:CG	2.10	0.55
1:F:199:ASN:C	1:F:199:ASN:ND2	2.57	0.55
1:D:63:GLN:O	1:D:64:SER:OG	2.17	0.55
1:B:278:MET:CA	5:B:2062:HOH:O	2.54	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:E:366:ASN:HB2	5:E:2100:HOH:O	2.06	0.54
1:B:254:ASN:C	1:B:254:ASN:ND2	2.64	0.54
1:F:254:ASN:C	1:F:254:ASN:ND2	2.64	0.54
1:C:145:THR:O	1:C:181:THR:HG21	2.08	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: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:34:ARG:HB2	5:C:2024:HOH:O	2.07	0.53
1:C:326:SER:HB3	5:C:2067:HOH:O	2.08	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:34:ARG:HB2	5:D:2027:HOH:O	2.07	0.52
1:D:203:GLY:HA2	1:D:221:TRP:NE1	2.24	0.52
1:D:289:TYR:CD1	1:D:289:TYR:C	2.86	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:17:HIS:HD2	1:D:18:PRO:HD2	1.69	0.52
1:D:117:TRP:N	5:D:2019:HOH:O	2.43	0.52
1:A:113:ARG:NH1	5:A:2039:HOH:O	2.21	0.52
1:A:77:ARG:HG3	1:A:77:ARG:NH1	2.14	0.52
1:C:328:HIS:HD2	1:C:330:SER:H	1.58	0.52
1:D:136:LEU:C	5:D:2029:HOH:O	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:69:LEU:CD1	1:B:79:LEU:HD12	2.42	0.50
1:B:278:MET:CG	1:B:278:MET:CA	2.83	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:D:169:GLY:C	5:D:2040:HOH:O	2.52	0.50
1:A:202:HIS:ND1	5:A:2061:HOH:O	2.40	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:37:LEU:HD22	1:A:336:TRP:HH2	1.77	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:B:165:GLU:O	5:B:2033[A]:HOH:O	2.20	0.49
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:B:278:MET:H	1:B:278:MET:HG3	1.77	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:C:38:VAL:HG13	1:C:38:VAL:O	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:21:LYS:HE2	5:E:2005:HOH:O	2.13	0.48
1:E:139:VAL:HG12	1:E:139:VAL:O	2.14	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: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
5:A:2012:HOH:O	1:D:239:LYS:HG2	2.13	0.47
1:C:150:LEU:HD12	5:C:2014:HOH:O	2.13	0.47
1:D:106:MET:SD	1:D:375:GLY:HA2	2.54	0.47
1:A:193:MET:HE1	1:A:202:HIS:HD1	1.78	0.47
1:C:202:HIS:O	1:C:207:ARG:HD2	2.15	0.47
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: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:51:ARG:CZ	1:C:53:HIS:CE1	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:O	1:F:38:VAL:HG13	2.14	0.46
1:A:367:VAL:HG13	1:A:380:SER:OG	2.14	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:347:GLN:HG2	1:D:348:THR:N	2.29	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:O	1:D:119:VAL:HG13	2.16	0.46
1:A:193:MET:HE1	1:A:202:HIS:ND1	2.31	0.46
1:B:291:VAL:HG13	1:B:336:TRP:HA	1.97	0.46
1:F:51:ARG:NH2	1:F:53:HIS:HE1	2.14	0.45
1:F:154:HIS:CD2	1:F:231:GLU:HA	2.51	0.45
1:B:182:ASN:OD1	1:B:182:ASN:C	2.59	0.45
1:E:289:TYR:CD1	1:E:289:TYR:C	2.94	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:A:193:MET:HE1	1:A:202:HIS:CE1	2.52	0.45
1:B:254:ASN:ND2	1:B:256:SER:H	2.14	0.45
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:50:LYS:HE3	1:C:202:HIS:CE1	2.51	0.45
1:C:117:TRP:CE3	1:C:121:ALA:HB2	2.52	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:63:GLN:O	1:A:64:SER:HB3	2.15	0.45
1:A:374:ARG:HD2	1:A:374:ARG:HA	1.75	0.45
1:D:139:VAL:HG12	1:D:139:VAL:O	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:7:PRO:HD3	1:D:57:PRO:HA	1.98	0.44
1:D:45:VAL:HG23	1:D:194:ASN:HD22	1.81	0.44
1:D:157:PHE:CB	5:D:2034:HOH:O	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:ALA:HA	4:D:1394:MTQ:S1'	2.58	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:E:357:ASP:CG	1:E:361:ASN:HB2	2.43	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:HD12	1:B:373:LEU:HA	1.64	0.44
1:C:204:PHE:CD1	1:C:205:PRO:HA	2.53	0.44
1:A:373:LEU:HA	1:A:373:LEU:HD12	1.70	0.44
1:D:18:PRO:HG2	5:D:2006:HOH:O	2.18	0.44
1:B:340:GLU:OE2	1:B:341:ALA:C	2.61	0.43
1:D:37:LEU:HD22	1:D:336:TRP:HH2	1.83	0.43
1:D:41:TYR:HA	1:D:338:LEU:HD11	1.99	0.43
1:D:281:PRO:CB	5:D:2078:HOH:O	2.65	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: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:40:SER:OG	1:D:42:VAL:O	2.36	0.43
1:D:220:LYS:NZ	4:D:1394:MTQ:O1P	2.49	0.43
1:B:374:ARG:HD2	1:B:374:ARG:HA	1.66	0.43
1:F:53:HIS:CD2	1:F:171:TYR:HE1	2.34	0.43
1:D:57:PRO:HD2	1:D:221:TRP:CD2	2.54	0.43
1:E:193:MET:HE1	1:E:202:HIS:ND1	2.34	0.43
1:E:347:GLN:HG2	1:E:348:THR:N	2.34	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: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:HD12	1:A:62:LEU:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD22	1:B:132:LEU:O	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:HA	1:E:373:LEU:HD12	1.71	0.42
1:E:306:ASP:OD2	1:E:310:ASN:HB2	2.18	0.42
1:D:45:VAL:HG22	1:D:193:MET:HE2	2.01	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:F:153:ARG:O	1:F:154:HIS:ND1	2.51	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:C:367:VAL:O	1:C:368:GLU:C	2.63	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:A:58:ILE:HG13	1:A:59:VAL:N	2.32	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:C:134:ASP:OD1	1:C:143:LYS:NZ	2.48	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
1:F:367:VAL:HG22	5:F:2101:HOH:O	2.20	0.41
1:D:77:ARG:HH11	1:D:77:ARG:CG	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:D:182:ASN:OD1	1:D:182:ASN:C	2.63	0.41
1:A:201:ASP:HB3	1:A:202:HIS:HD2	1.86	0.41
1:D:249:ASN:OD1	1:D:249:ASN:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:199:ASN:HD22	1:B:199:ASN:HA	1.45	0.41
1:C:175:ILE:HG22	1:C:262:MET:HE1	2.03	0.41
1:D:117:TRP:CE3	1:D:121:ALA:HB2	2.55	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:D:199:ASN:HB2	5:D:2050:HOH:O	2.20	0.41
1:E:65:TYR:CD2	1:E:65:TYR:C	2.99	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:B:38:VAL:HG22	1:B:338:LEU:HD22	2.03	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:157:PHE:CD1	1:D:208:VAL:HG21	2.56	0.40
1:D:216:ALA:HB2	4:D:1394:MTQ:OM2	2.21	0.40
1:F:57:PRO:HD2	1:F:221:TRP:CE2	2.56	0.40
1:F:388:LEU:HD23	1:F:388:LEU:HA	1.91	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:E:367:VAL:O	1:E:368:GLU:C	2.64	0.40
1:F:50:LYS:CE	1:F:202:HIS:CE1	2.90	0.40
1:B:77:ARG:HH11	1:B:77:ARG:CG	2.30	0.40
1:B:245:PRO:HB2	5:B:2056:HOH:O	2.20	0.40
1:C:374:ARG:HA	1:C:374:ARG:HD2	1.49	0.40
1:C:385:LEU:HD12	1:C:385:LEU:HA	1.95	0.40
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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	386/393 (98%)	369 (96%)	13 (3%)	4 (1%)	12	28
1	B	386/393 (98%)	371 (96%)	11 (3%)	4 (1%)	12	28
1	C	386/393 (98%)	369 (96%)	13 (3%)	4 (1%)	12	28
1	D	386/393 (98%)	370 (96%)	12 (3%)	4 (1%)	12	28
1	E	386/393 (98%)	370 (96%)	13 (3%)	3 (1%)	16	34
1	F	386/393 (98%)	368 (95%)	14 (4%)	4 (1%)	12	28
All	All	2316/2358 (98%)	2217 (96%)	76 (3%)	23 (1%)	12	28

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
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

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Mol	Chain	Res	Type
1	F	76	PRO
1	A	378	ASN
1	F	34	ARG

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	331/336 (98%)	295 (89%)	36 (11%)	6	13
1	B	331/336 (98%)	295 (89%)	36 (11%)	6	13
1	C	331/336 (98%)	286 (86%)	45 (14%)	3	7
1	D	331/336 (98%)	287 (87%)	44 (13%)	4	8
1	E	331/336 (98%)	288 (87%)	43 (13%)	4	8
1	F	331/336 (98%)	287 (87%)	44 (13%)	4	8
All	All	1986/2016 (98%)	1738 (88%)	248 (12%)	4	9

All (248) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	37	LEU
1	A	38	VAL
1	A	58	ILE
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	112	VAL
1	A	119	VAL
1	A	132	LEU
1	A	139	VAL

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Mol	Chain	Res	Type
1	A	177	LEU
1	A	178	SER
1	A	181	THR
1	A	184	GLU
1	A	188	LEU
1	A	199	ASN
1	A	208	VAL
1	A	222	LEU
1	A	231	GLU
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	309	LYS
1	A	312	VAL
1	A	340	GLU
1	A	351	VAL
1	A	367	VAL
1	B	20	LEU
1	B	37	LEU
1	B	38	VAL
1	B	50	LYS
1	B	58	ILE
1	B	63	GLN
1	B	69	LEU
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

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Mol	Chain	Res	Type
1	B	208	VAL
1	B	222	LEU
1	B	258	ARG
1	B	278	MET
1	B	284	VAL
1	B	291	VAL
1	B	292	SER
1	B	309	LYS
1	B	319	GLU
1	B	340	GLU
1	B	349	THR
1	B	351	VAL
1	B	367	VAL
1	B	369	SER
1	B	380	SER
1	C	17	HIS
1	C	20	LEU
1	C	37	LEU
1	C	38	VAL
1	C	53	HIS
1	C	58	ILE
1	C	61	HIS
1	C	63	GLN
1	C	64	SER
1	C	69	LEU
1	C	70	THR
1	C	72	LEU
1	C	77	ARG
1	C	81	ILE
1	C	87	LEU
1	C	112	VAL
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

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Mol	Chain	Res	Type
1	C	280	LYS
1	C	281	PRO
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	340	GLU
1	C	344	ASP
1	C	348	THR
1	C	351	VAL
1	C	367	VAL
1	C	373	LEU
1	C	374	ARG
1	C	380	SER
1	C	387	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	58	ILE
1	D	60	ASP
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	108	LYS
1	D	110	ARG
1	D	112	VAL
1	D	119	VAL
1	D	132	LEU
1	D	145	THR
1	D	177	LEU
1	D	178	SER

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Mol	Chain	Res	Type
1	D	181	THR
1	D	196	GLU
1	D	199	ASN
1	D	208	VAL
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	309	LYS
1	D	316	ARG
1	D	319	GLU
1	D	340	GLU
1	D	344	ASP
1	D	348	THR
1	D	351	VAL
1	D	367	VAL
1	E	9	GLU
1	E	19	SER
1	E	20	LEU
1	E	37	LEU
1	E	38	VAL
1	E	39	SER
1	E	58	ILE
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	110	ARG
1	E	119	VAL
1	E	132	LEU
1	E	137	GLU
1	E	160	VAL
1	E	172	LYS
1	E	177	LEU
1	E	178	SER

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Mol	Chain	Res	Type
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	340	GLU
1	E	344	ASP
1	E	351	VAL
1	E	367	VAL
1	E	387	ARG
1	F	20	LEU
1	F	21	LYS
1	F	35	SER
1	F	37	LEU
1	F	38	VAL
1	F	40	SER
1	F	58	ILE
1	F	61	HIS
1	F	63	GLN
1	F	67	VAL
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	112	VAL
1	F	119	VAL
1	F	132	LEU
1	F	147	SER
1	F	160	VAL

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Mol	Chain	Res	Type
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	208	VAL
1	F	222	LEU
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	309	LYS
1	F	312	VAL
1	F	340	GLU
1	F	344	ASP
1	F	348	THR
1	F	351	VAL
1	F	367	VAL
1	F	387	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	17	HIS
1	A	63	GLN
1	A	74	GLN
1	A	111	ASN
1	A	199	ASN
1	A	254	ASN
1	A	323	GLN
1	A	382	HIS
1	B	63	GLN
1	B	91	ASN
1	B	199	ASN
1	B	254	ASN
1	B	323	GLN
1	B	328	HIS

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Mol	Chain	Res	Type
1	B	366	ASN
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	C	361	ASN
1	D	17	HIS
1	D	63	GLN
1	D	91	ASN
1	D	111	ASN
1	D	124	ASN
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	124	ASN
1	F	199	ASN
1	F	202	HIS
1	F	226	ASN
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 ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	1394	1	22,30,30	4.24	14 (63%)	19,48,48	6.59	14 (73%)
4	MTQ	F	1394	1	22,30,30	4.17	12 (54%)	19,48,48	4.90	8 (42%)
4	MTQ	E	1394	1	22,30,30	4.02	11 (50%)	19,48,48	5.99	15 (78%)
3	GOL	D	1393	-	5,5,5	0.72	0	5,5,5	1.48	1 (20%)
3	GOL	B	1393	-	5,5,5	0.99	0	5,5,5	0.98	0
4	MTQ	C	1394	1	22,30,30	4.52	12 (54%)	19,48,48	5.65	13 (68%)
4	MTQ	D	1394	1	22,30,30	4.00	15 (68%)	19,48,48	5.73	12 (63%)
3	GOL	A	1393	-	5,5,5	0.79	0	5,5,5	1.78	1 (20%)
3	GOL	C	1393	-	5,5,5	0.58	0	5,5,5	1.37	1 (20%)
3	GOL	F	1393	-	5,5,5	0.64	0	5,5,5	0.76	0
3	GOL	E	1393	-	5,5,5	0.59	0	5,5,5	1.38	0
4	MTQ	B	1394	1	22,30,30	4.18	11 (50%)	19,48,48	5.24	13 (68%)

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	A	1394	1	-	1/4/60/60	0/4/4/4
4	MTQ	F	1394	1	-	0/4/60/60	0/4/4/4
4	MTQ	E	1394	1	-	1/4/60/60	0/4/4/4
3	GOL	D	1393	-	-	0/4/4/4	-
3	GOL	B	1393	-	-	2/4/4/4	-

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

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1394	MTQ	O3'-C3'	8.85	1.51	1.36
4	D	1394	MTQ	C2'-C3'	8.68	1.64	1.38
4	A	1394	MTQ	C2'-C3'	8.64	1.64	1.38
4	F	1394	MTQ	C4'-C3'	-8.54	1.35	1.48
4	C	1394	MTQ	O3'-C3'	8.53	1.51	1.36
4	B	1394	MTQ	O3'-C3'	8.37	1.50	1.36
4	D	1394	MTQ	O3'-C3'	8.02	1.50	1.36
4	C	1394	MTQ	C2'-C3'	7.93	1.62	1.38
4	C	1394	MTQ	P-O4'	-7.59	1.36	1.60
4	E	1394	MTQ	C4'-C3'	-7.59	1.36	1.48
4	B	1394	MTQ	O4'-C4'	7.55	1.50	1.43
4	F	1394	MTQ	C2'-C3'	7.38	1.60	1.38
4	E	1394	MTQ	O4'-C4'	7.35	1.50	1.43
4	C	1394	MTQ	O4-C4	7.28	1.37	1.23
4	A	1394	MTQ	O3'-C3'	7.12	1.48	1.36
4	F	1394	MTQ	P-O4'	-7.11	1.37	1.60
4	C	1394	MTQ	C9-N5	6.92	1.50	1.33
4	E	1394	MTQ	P-O4'	-6.89	1.38	1.60
4	A	1394	MTQ	C4'-C3'	-6.82	1.38	1.48
4	B	1394	MTQ	C2'-C3'	6.69	1.58	1.38
4	E	1394	MTQ	C2'-C3'	6.38	1.57	1.38
4	B	1394	MTQ	P-O4'	-6.23	1.40	1.60
4	A	1394	MTQ	P-O4'	-6.11	1.41	1.60
4	A	1394	MTQ	C6-N5	6.10	1.54	1.36
4	D	1394	MTQ	C4'-C3'	-6.07	1.39	1.48
4	D	1394	MTQ	P-O4'	-6.04	1.41	1.60
4	C	1394	MTQ	O4'-C4'	5.91	1.49	1.43
4	A	1394	MTQ	C9-N5	5.81	1.47	1.33
4	E	1394	MTQ	C9-N5	5.78	1.47	1.33
4	E	1394	MTQ	O3'-C3'	5.77	1.46	1.36
4	E	1394	MTQ	C6-N5	5.77	1.53	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1394	MTQ	O4-C4	5.73	1.34	1.23
4	F	1394	MTQ	C6-N5	5.64	1.52	1.36
4	B	1394	MTQ	C4'-C3'	-5.58	1.39	1.48
4	D	1394	MTQ	C6-N5	5.57	1.52	1.36
4	C	1394	MTQ	C6-N5	5.04	1.51	1.36
4	C	1394	MTQ	C4'-C3'	-4.96	1.40	1.48
4	B	1394	MTQ	C9-N5	4.89	1.45	1.33
4	C	1394	MTQ	P-O1P	-4.82	1.35	1.50
4	B	1394	MTQ	C6-N5	4.65	1.50	1.36
4	D	1394	MTQ	C9-N5	4.60	1.44	1.33
4	F	1394	MTQ	C9-N5	4.59	1.44	1.33
4	F	1394	MTQ	P-O1P	-4.55	1.36	1.50
4	A	1394	MTQ	P-O1P	-4.44	1.36	1.50
4	A	1394	MTQ	O4-C4	4.35	1.31	1.23
4	A	1394	MTQ	O4'-C4'	4.27	1.47	1.43
4	B	1394	MTQ	P-O1P	-4.19	1.37	1.50
4	A	1394	MTQ	C9-C10	4.18	1.55	1.43
4	B	1394	MTQ	C9-C10	4.09	1.54	1.43
4	D	1394	MTQ	O4-C4	4.05	1.31	1.23
4	A	1394	MTQ	P-O2P	-3.90	1.40	1.54
4	E	1394	MTQ	P-O1P	-3.84	1.38	1.50
4	C	1394	MTQ	O3'-C7	3.71	1.51	1.45
4	C	1394	MTQ	C10-N8	3.67	1.39	1.35
4	F	1394	MTQ	O3'-C7	3.56	1.50	1.45
4	E	1394	MTQ	C9-C10	3.33	1.52	1.43
4	D	1394	MTQ	P-O1P	-3.32	1.40	1.50
4	D	1394	MTQ	C9-C10	3.22	1.52	1.43
4	C	1394	MTQ	C9-C10	3.19	1.52	1.43
4	E	1394	MTQ	C2-N3	-3.06	1.28	1.35
4	E	1394	MTQ	C1'-C6	3.04	1.43	1.36
4	D	1394	MTQ	C1'-C6	2.97	1.42	1.36
4	D	1394	MTQ	O4'-C4'	2.95	1.46	1.43
4	D	1394	MTQ	C10-N1	2.95	1.38	1.32
4	A	1394	MTQ	C1'-C6	2.89	1.42	1.36
4	B	1394	MTQ	P-O2P	-2.84	1.44	1.54
4	F	1394	MTQ	C9-C10	2.78	1.51	1.43
4	A	1394	MTQ	C2-N3	-2.78	1.29	1.35
4	D	1394	MTQ	O3'-C7	2.64	1.49	1.45
4	D	1394	MTQ	C4-N3	-2.63	1.33	1.38
4	F	1394	MTQ	O4-C4	2.59	1.28	1.23
4	A	1394	MTQ	C2-N2	-2.49	1.28	1.34
4	F	1394	MTQ	P-O2P	-2.40	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1394	MTQ	P-O2P	-2.20	1.46	1.54
4	F	1394	MTQ	C2-N3	-2.02	1.30	1.35

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1394	MTQ	C2'-C1'-C6	-23.36	98.04	123.78
4	E	1394	MTQ	C2'-C1'-C6	-20.61	101.08	123.78
4	D	1394	MTQ	C2'-C1'-C6	-19.26	102.56	123.78
4	B	1394	MTQ	C2'-C1'-C6	-18.12	103.82	123.78
4	F	1394	MTQ	C2'-C1'-C6	-16.47	105.64	123.78
4	C	1394	MTQ	C2'-C1'-C6	-13.33	109.09	123.78
4	E	1394	MTQ	C4-C9-N5	9.99	128.97	118.00
4	C	1394	MTQ	O3'-C7-N8	-9.61	99.69	108.56
4	A	1394	MTQ	O3'-C7-N8	-8.14	101.05	108.56
4	C	1394	MTQ	N2-C2-N3	8.09	129.59	117.09
4	F	1394	MTQ	O3'-C7-N8	7.68	115.64	108.56
4	C	1394	MTQ	C4-C9-N5	7.20	125.91	118.00
4	D	1394	MTQ	C4-C9-N5	7.15	125.85	118.00
4	D	1394	MTQ	O3'-C7-N8	-6.69	102.39	108.56
4	A	1394	MTQ	O3'-C7-C6	-6.27	87.17	112.09
4	F	1394	MTQ	C4-C9-N5	6.20	124.81	118.00
4	B	1394	MTQ	C2'-C1'-S1'	6.10	129.57	115.59
4	A	1394	MTQ	C2'-C1'-S1'	5.89	129.09	115.59
4	C	1394	MTQ	O3'-C7-C6	-5.55	90.04	112.09
4	A	1394	MTQ	O4'-P-O1P	5.50	121.31	106.44
4	C	1394	MTQ	C1'-C2'-C3'	-5.47	117.23	123.70
4	C	1394	MTQ	O2P-P-O4'	5.45	120.87	106.67
4	C	1394	MTQ	O3P-P-O1P	-5.42	89.70	110.83
4	B	1394	MTQ	O3'-C7-N8	-5.25	103.71	108.56
4	C	1394	MTQ	C2'-C1'-S1'	5.21	127.53	115.59
4	C	1394	MTQ	N1-C2-N3	-5.18	118.23	126.44
4	B	1394	MTQ	O3'-C7-C6	-5.16	91.57	112.09
4	A	1394	MTQ	C4-C9-N5	5.13	123.63	118.00
4	E	1394	MTQ	O3'-C7-C6	-5.00	92.22	112.09
4	E	1394	MTQ	N1-C2-N3	-4.96	118.58	126.44
4	F	1394	MTQ	C2'-C1'-S1'	4.94	126.91	115.59
4	D	1394	MTQ	N2-C2-N3	4.89	124.64	117.09
4	A	1394	MTQ	O4-C4-N3	4.48	127.83	120.27
4	E	1394	MTQ	O4-C4-C9	-4.38	111.70	122.35
4	B	1394	MTQ	N1-C2-N3	-4.32	119.59	126.44
4	D	1394	MTQ	C2'-C1'-S1'	4.29	125.42	115.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1394	MTQ	O4-C4-C9	-4.26	111.99	122.35
4	C	1394	MTQ	O4-C4-C9	-4.25	112.01	122.35
4	D	1394	MTQ	N1-C2-N3	-4.21	119.77	126.44
4	D	1394	MTQ	O3'-C7-C6	-4.20	95.39	112.09
4	F	1394	MTQ	O3'-C7-C6	-4.19	95.46	112.09
4	B	1394	MTQ	O4-C4-N3	4.08	127.14	120.27
4	D	1394	MTQ	O3P-P-O1P	3.88	125.94	110.83
4	B	1394	MTQ	O2P-P-O4'	3.87	116.76	106.67
4	A	1394	MTQ	O4-C4-C9	-3.85	112.97	122.35
4	D	1394	MTQ	C1'-C2'-C3'	-3.85	119.14	123.70
4	E	1394	MTQ	C2'-C1'-S1'	3.81	124.32	115.59
4	B	1394	MTQ	C4-C9-N5	3.75	122.12	118.00
4	D	1394	MTQ	O2P-P-O4'	-3.58	97.34	106.67
4	C	1394	MTQ	O4-C4-N3	3.53	126.23	120.27
4	E	1394	MTQ	O4'-P-O1P	3.47	115.83	106.44
4	E	1394	MTQ	O3P-P-O2P	3.47	120.81	107.80
4	F	1394	MTQ	O4'-P-O1P	3.36	115.53	106.44
4	A	1394	MTQ	C1'-C2'-C3'	-3.29	119.81	123.70
4	D	1394	MTQ	O2P-P-O1P	-3.16	98.53	110.83
3	A	1393	GOL	C3-C2-C1	-3.13	100.33	111.80
4	E	1394	MTQ	O2P-P-O1P	-2.98	99.21	110.83
4	F	1394	MTQ	C1'-C2'-S2'	-2.94	108.85	115.59
4	A	1394	MTQ	O2P-P-O1P	-2.93	99.43	110.83
4	E	1394	MTQ	N2-C2-N1	2.81	121.04	116.57
4	C	1394	MTQ	N2-C2-N1	-2.75	112.18	116.57
4	F	1394	MTQ	O4-C4-C9	-2.75	115.66	122.35
4	E	1394	MTQ	C1'-C2'-S2'	-2.73	109.33	115.59
4	A	1394	MTQ	N1-C2-N3	-2.67	122.21	126.44
4	A	1394	MTQ	N2-C2-N1	2.56	120.64	116.57
4	A	1394	MTQ	O3P-P-O2P	2.55	117.37	107.80
4	B	1394	MTQ	N2-C2-N1	2.40	120.39	116.57
4	E	1394	MTQ	O3P-P-O4'	-2.37	100.48	106.67
4	B	1394	MTQ	C1'-C2'-S2'	-2.34	110.24	115.59
4	E	1394	MTQ	O4-C4-N3	2.27	124.10	120.27
4	A	1394	MTQ	C1'-C2'-S2'	-2.22	110.51	115.59
3	D	1393	GOL	C3-C2-C1	-2.19	103.77	111.80
3	C	1393	GOL	O3-C3-C2	2.17	120.12	110.38
4	E	1394	MTQ	N2-C2-N3	2.09	120.33	117.09
4	B	1394	MTQ	O4-C4-C9	-2.08	117.29	122.35
4	B	1394	MTQ	C1'-C2'-C3'	-2.07	121.25	123.70
4	B	1394	MTQ	O3P-P-O2P	2.06	115.54	107.80
4	E	1394	MTQ	C4-C9-C10	-2.06	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
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

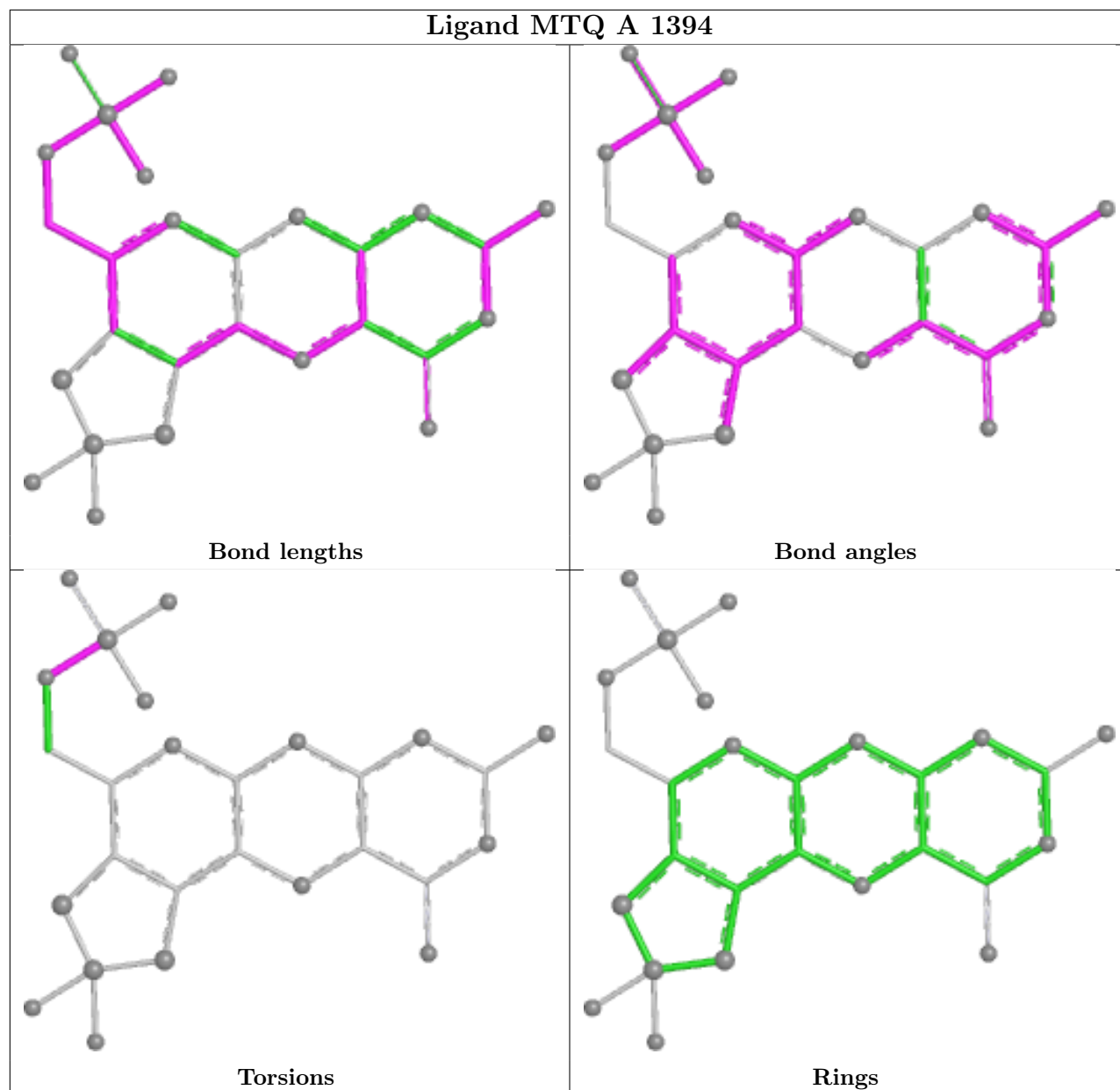
There are no ring outliers.

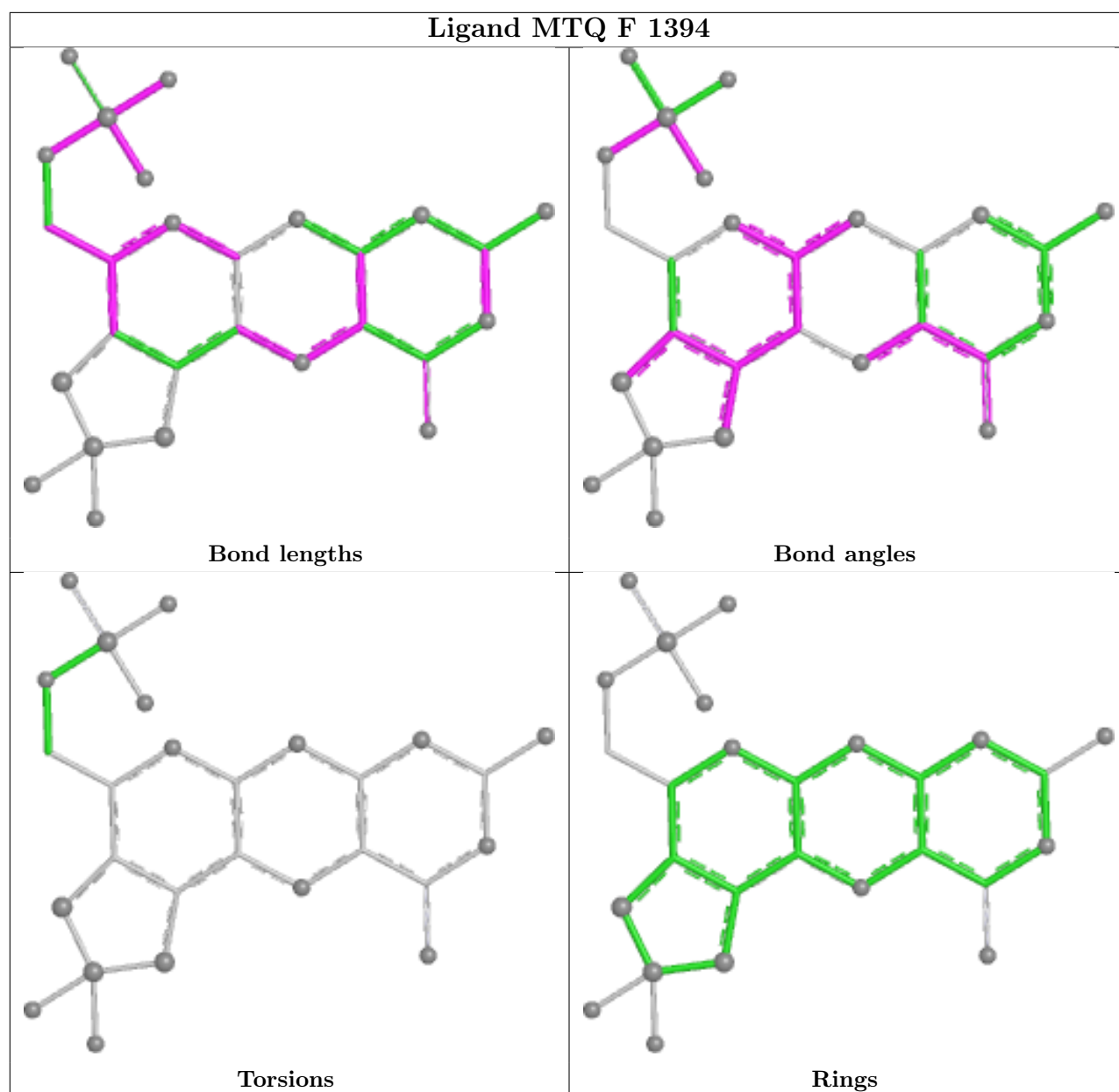
9 monomers are involved in 22 short contacts:

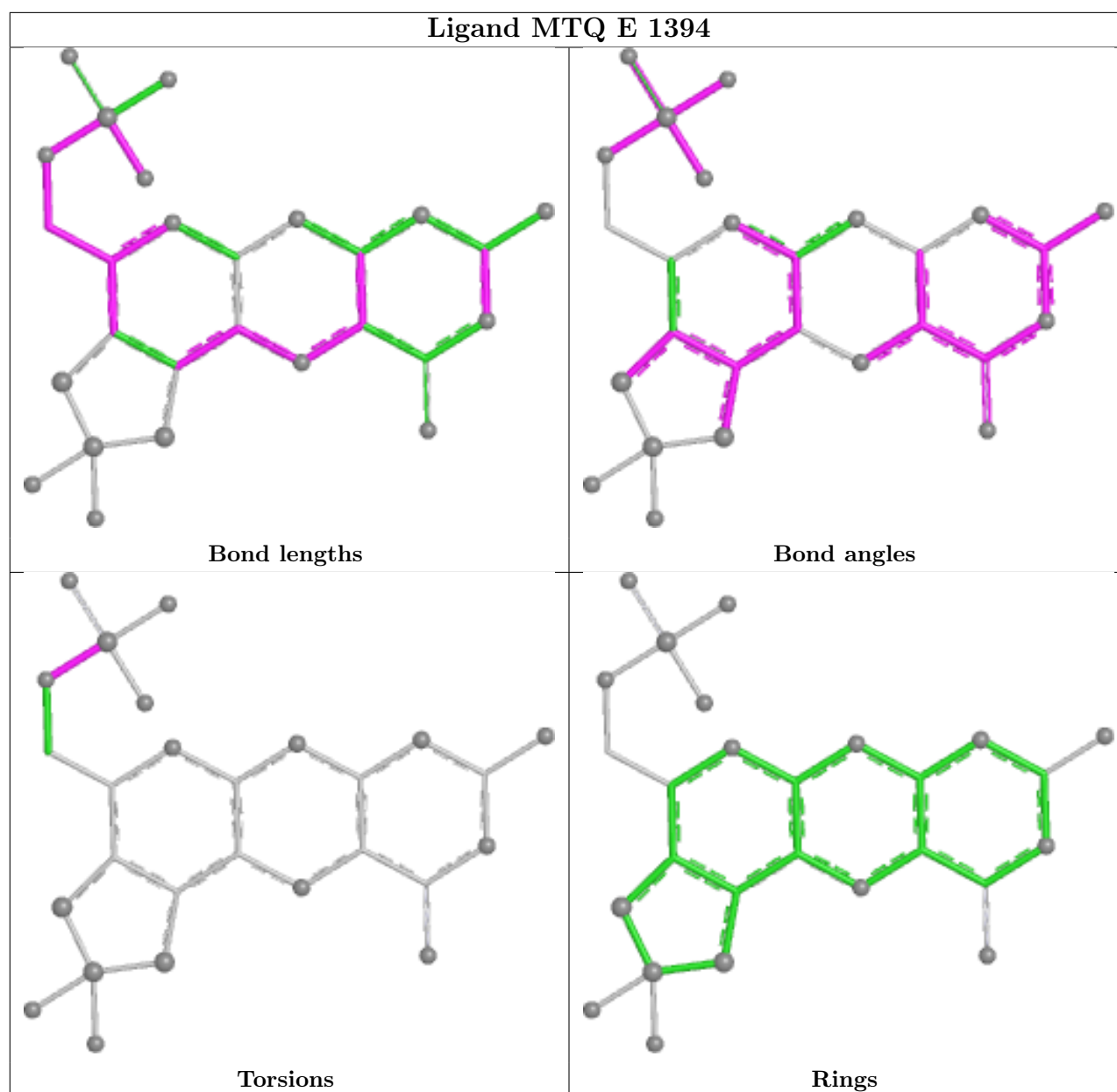
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1394	MTQ	2	0
4	F	1394	MTQ	1	0
4	E	1394	MTQ	1	0
3	D	1393	GOL	2	0
4	C	1394	MTQ	2	0
4	D	1394	MTQ	9	0
3	C	1393	GOL	2	0
3	E	1393	GOL	1	0
4	B	1394	MTQ	2	0

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.

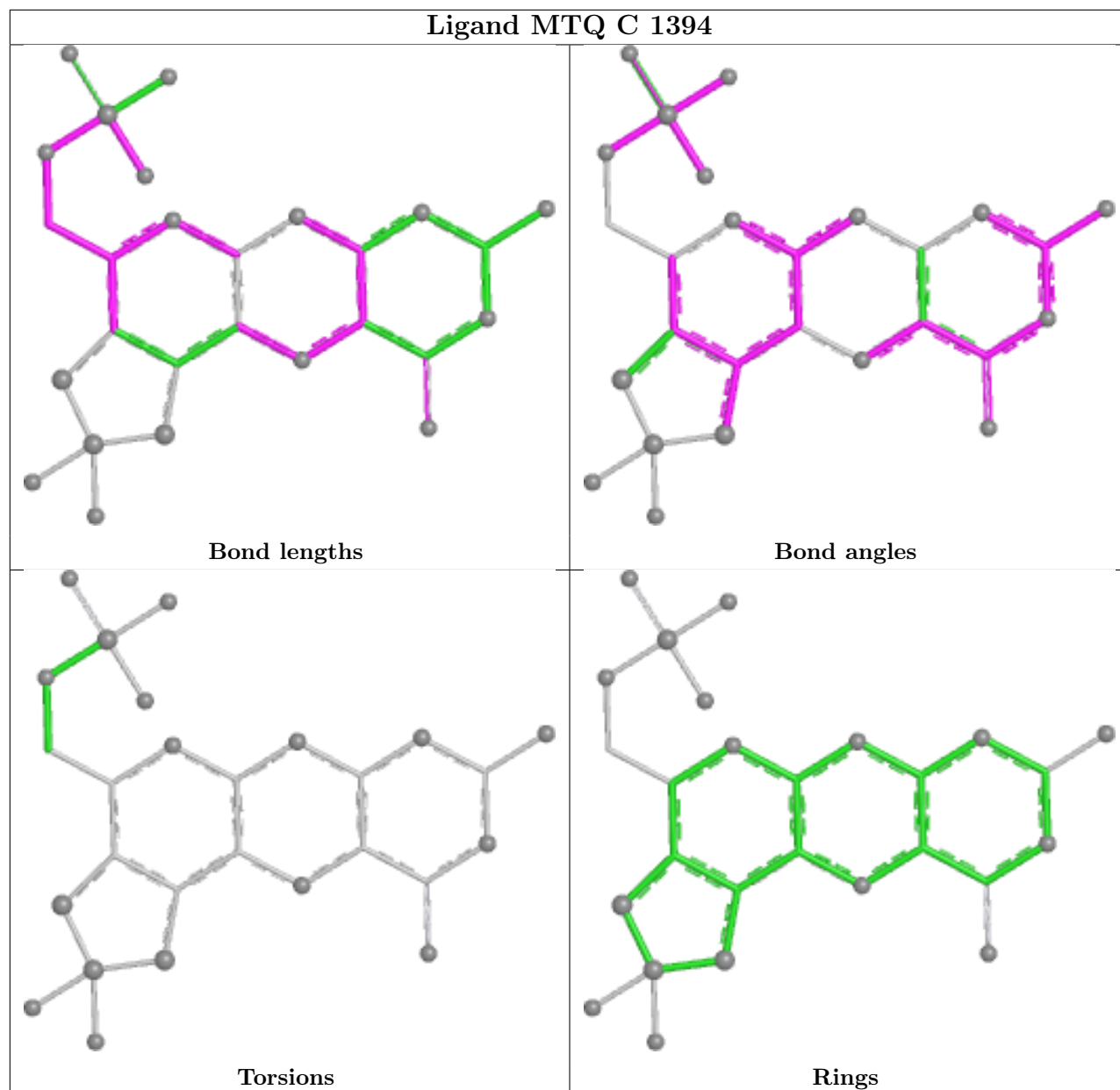
Ligand MTQ A 1394



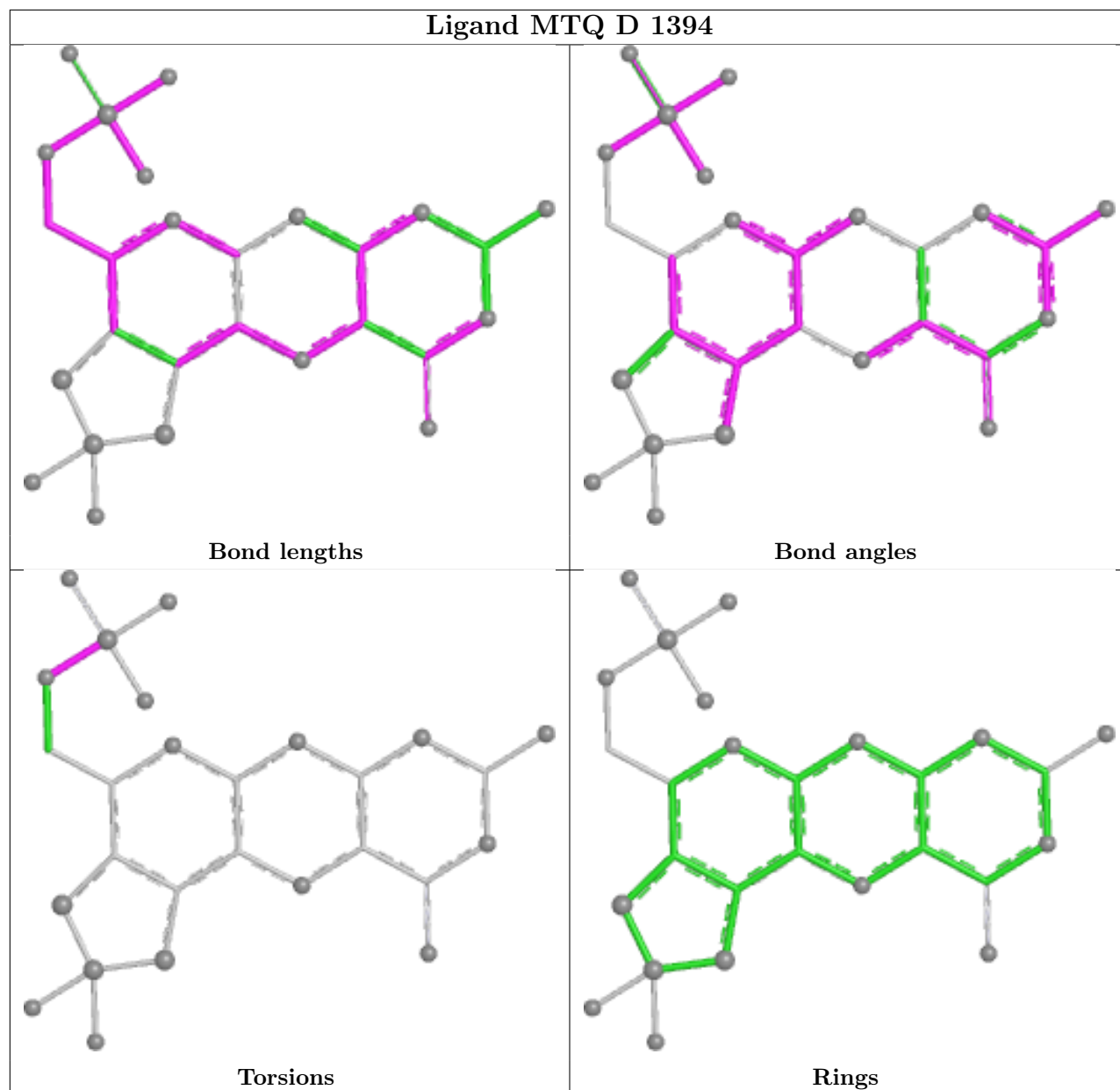


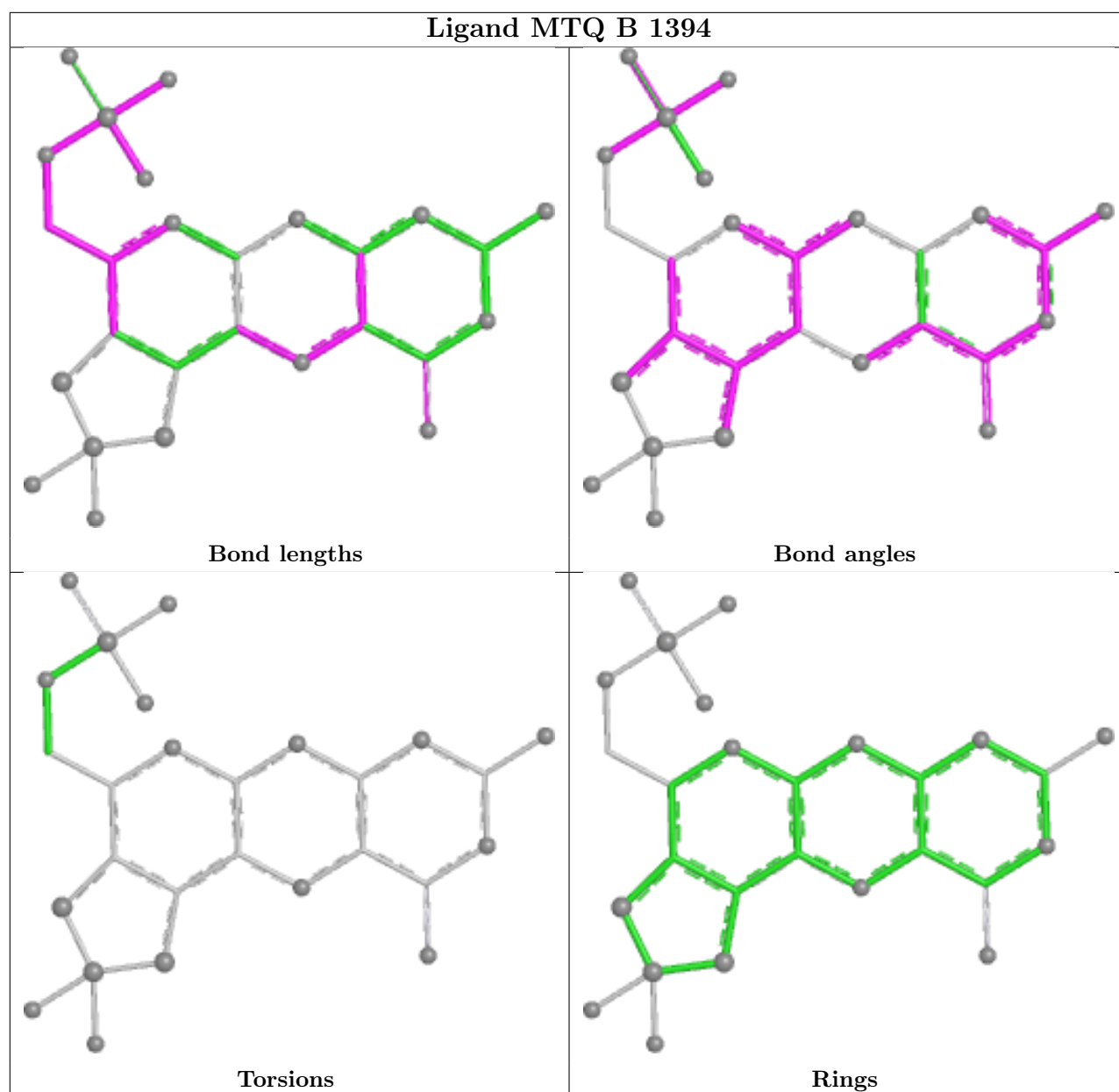


Ligand MTQ C 1394



Ligand MTQ D 1394





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	388/393 (98%)	0.41	19 (4%)	35 29	39, 54, 78, 90	0
1	B	388/393 (98%)	0.41	17 (4%)	39 33	39, 54, 78, 90	0
1	C	388/393 (98%)	0.73	32 (8%)	17 14	40, 55, 78, 90	0
1	D	388/393 (98%)	1.16	60 (15%)	5 4	39, 55, 78, 90	0
1	E	388/393 (98%)	0.51	30 (7%)	19 15	39, 54, 78, 90	0
1	F	388/393 (98%)	0.50	23 (5%)	28 23	39, 54, 78, 90	0
All	All	2328/2358 (98%)	0.62	181 (7%)	19 15	39, 54, 78, 90	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	389	GLY	14.3
1	F	2	PRO	12.2
1	F	389	GLY	11.2
1	B	2	PRO	10.0
1	D	389	GLY	9.1
1	A	2	PRO	8.8
1	B	389	GLY	8.7
1	D	2	PRO	8.2
1	E	2	PRO	7.5
1	C	2	PRO	6.9
1	A	389	GLY	5.7
1	E	278	MET	5.7
1	D	168	GLY	5.2
1	D	3	GLY	5.1
1	E	389	GLY	4.9
1	F	278	MET	4.6
1	D	4	ILE	4.6
1	D	82	LYS	4.5
1	D	388	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	64	SER	4.5
1	A	280	LYS	4.3
1	F	64	SER	4.3
1	D	278	MET	4.2
1	E	388	LEU	4.1
1	C	278	MET	4.0
1	D	63	GLN	4.0
1	C	70	THR	4.0
1	C	75	ASN	3.9
1	D	108	LYS	3.9
1	E	77	ARG	3.8
1	A	278	MET	3.8
1	B	278	MET	3.8
1	E	61	HIS	3.7
1	E	63	GLN	3.7
1	D	280	LYS	3.6
1	C	280	LYS	3.6
1	B	388	LEU	3.4
1	A	3	GLY	3.4
1	F	61	HIS	3.3
1	D	58	ILE	3.3
1	D	169	GLY	3.3
1	B	64	SER	3.2
1	E	3	GLY	3.2
1	C	388	LEU	3.2
1	A	321	GLY	3.2
1	D	61	HIS	3.2
1	D	70	THR	3.1
1	D	76	PRO	3.1
1	F	144	LEU	3.1
1	D	322	LYS	3.0
1	C	327	GLU	3.0
1	B	63	GLN	3.0
1	F	309	LYS	3.0
1	C	82	LYS	3.0
1	D	283	LYS	3.0
1	B	328	HIS	2.9
1	E	326	SER	2.9
1	B	77	ARG	2.9
1	D	344	ASP	2.9
1	F	388	LEU	2.9
1	F	73	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	116	GLY	2.8
1	D	307	GLY	2.8
1	A	73	ILE	2.8
1	A	82	LYS	2.8
1	F	63	GLN	2.7
1	D	35	SER	2.7
1	B	199	ASN	2.7
1	C	367	VAL	2.7
1	D	279	VAL	2.7
1	B	108	LYS	2.7
1	C	61	HIS	2.7
1	C	345	VAL	2.7
1	E	108	LYS	2.7
1	D	65	TYR	2.7
1	F	387	ARG	2.7
1	A	309	LYS	2.7
1	A	388	LEU	2.6
1	D	203	GLY	2.6
1	B	346	SER	2.6
1	D	138	LEU	2.6
1	A	279	VAL	2.6
1	D	109	VAL	2.6
1	E	199	ASN	2.6
1	E	73	ILE	2.6
1	D	162	ARG	2.6
1	F	77	ARG	2.6
1	B	309	LYS	2.6
1	C	74	GLN	2.6
1	E	349	THR	2.5
1	D	5	ARG	2.5
1	B	61	HIS	2.5
1	E	184	GLU	2.5
1	D	195	GLY	2.5
1	D	39	SER	2.5
1	D	81	ILE	2.5
1	E	319	GLU	2.5
1	E	281	PRO	2.5
1	A	346	SER	2.5
1	F	153	ARG	2.5
1	C	3	GLY	2.5
1	D	309	LYS	2.5
1	E	91	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	60	ASP	2.5
1	B	276	VAL	2.5
1	C	73	ILE	2.4
1	D	386	LEU	2.4
1	F	330	SER	2.4
1	E	321	GLY	2.4
1	F	321	GLY	2.4
1	C	77	ARG	2.4
1	C	150	LEU	2.4
1	D	62	LEU	2.4
1	C	64	SER	2.4
1	D	223	ASP	2.4
1	D	75	ASN	2.4
1	B	53	HIS	2.4
1	D	164	LYS	2.4
1	D	36	ALA	2.4
1	D	73	ILE	2.4
1	E	82	LYS	2.4
1	F	3	GLY	2.4
1	E	345	VAL	2.4
1	E	327	GLU	2.3
1	F	327	GLU	2.3
1	F	140	GLY	2.3
1	D	191	TYR	2.3
1	F	65	TYR	2.3
1	C	348	THR	2.3
1	D	184	GLU	2.3
1	D	320	PRO	2.3
1	D	180	ALA	2.3
1	C	53	HIS	2.3
1	C	78	LYS	2.3
1	A	199	ASN	2.3
1	E	306	ASP	2.3
1	B	140	GLY	2.3
1	C	142	PRO	2.2
1	E	320	PRO	2.2
1	E	344	ASP	2.2
1	D	212	GLY	2.2
1	C	108	LYS	2.2
1	D	205	PRO	2.2
1	C	144	LEU	2.2
1	D	71	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	61	HIS	2.2
1	A	319	GLU	2.1
1	D	77	ARG	2.1
1	D	348	THR	2.1
1	F	74	GLN	2.1
1	F	75	ASN	2.1
1	C	321	GLY	2.1
1	D	86	SER	2.1
1	F	345	VAL	2.1
1	C	24	ALA	2.1
1	C	63	GLN	2.1
1	C	279	VAL	2.1
1	E	139	VAL	2.1
1	C	346	SER	2.1
1	A	322	LYS	2.1
1	E	277	GLN	2.1
1	D	206	LEU	2.1
1	E	21	LYS	2.1
1	D	167	ASN	2.1
1	C	184	GLU	2.0
1	D	346	SER	2.0
1	A	342	THR	2.0
1	D	17	HIS	2.0
1	D	308	GLY	2.0
1	A	59	VAL	2.0
1	D	163	CYS	2.0
1	C	60	ASP	2.0
1	D	251	ASP	2.0
1	E	280	LYS	2.0
1	F	82	LYS	2.0
1	A	64	SER	2.0
1	B	66	SER	2.0
1	C	15	PRO	2.0
1	E	144	LEU	2.0
1	D	194	ASN	2.0
1	E	195	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

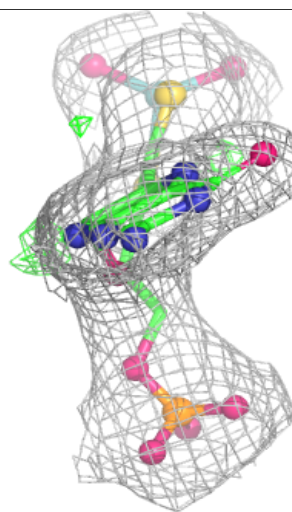
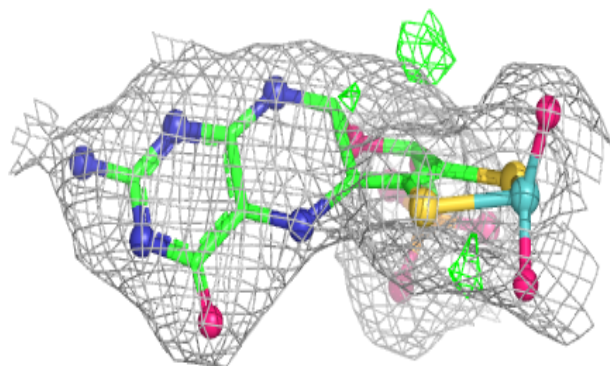
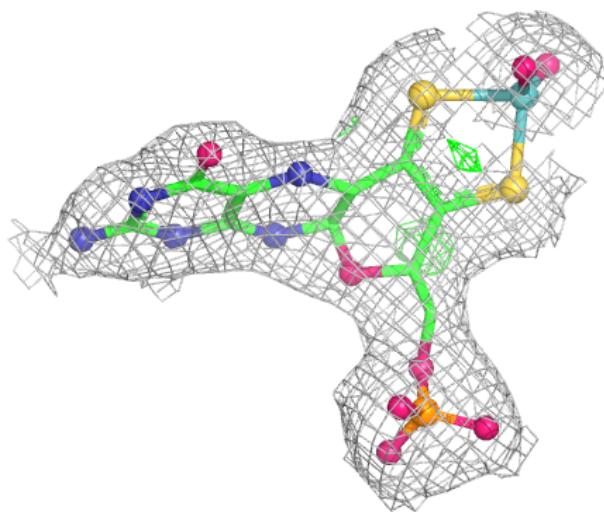
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	1393	6/6	0.92	0.15	47,57,62,62	0
3	GOL	C	1393	6/6	0.92	0.12	52,57,60,64	0
3	GOL	D	1393	6/6	0.93	0.14	52,58,63,64	0
2	CS	D	1391	1/1	0.95	0.23	106,106,106,106	0
3	GOL	E	1393	6/6	0.95	0.10	47,56,62,63	0
2	CS	D	1392	1/1	0.96	0.08	81,81,81,81	1
2	CS	E	1392	1/1	0.97	0.05	73,73,73,73	1
2	CS	C	1391	1/1	0.97	0.07	80,80,80,80	0
3	GOL	B	1393	6/6	0.97	0.09	51,57,62,62	0
3	GOL	F	1393	6/6	0.97	0.08	45,57,61,63	0
2	CS	C	1392	1/1	0.98	0.04	79,79,79,79	1
2	CS	F	1392	1/1	0.98	0.04	70,70,70,70	1
2	CS	B	1391	1/1	0.99	0.05	73,73,73,73	0
2	CS	B	1392	1/1	0.99	0.04	67,67,67,67	1
2	CS	E	1391	1/1	0.99	0.04	68,68,68,68	0
2	CS	A	1391	1/1	0.99	0.03	67,67,67,67	0
2	CS	F	1391	1/1	0.99	0.05	73,73,73,73	0
2	CS	A	1392	1/1	0.99	0.03	69,69,69,69	1
4	MTQ	A	1394	27/27	0.99	0.05	33,40,44,49	0
4	MTQ	B	1394	27/27	0.99	0.05	33,40,46,51	0
4	MTQ	C	1394	27/27	0.99	0.06	34,42,50,51	0
4	MTQ	D	1394	27/27	0.99	0.07	35,42,51,56	0
4	MTQ	E	1394	27/27	0.99	0.05	29,39,44,47	0
4	MTQ	F	1394	27/27	0.99	0.06	32,39,44,49	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.

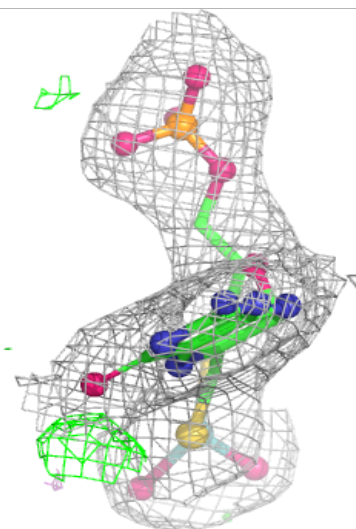
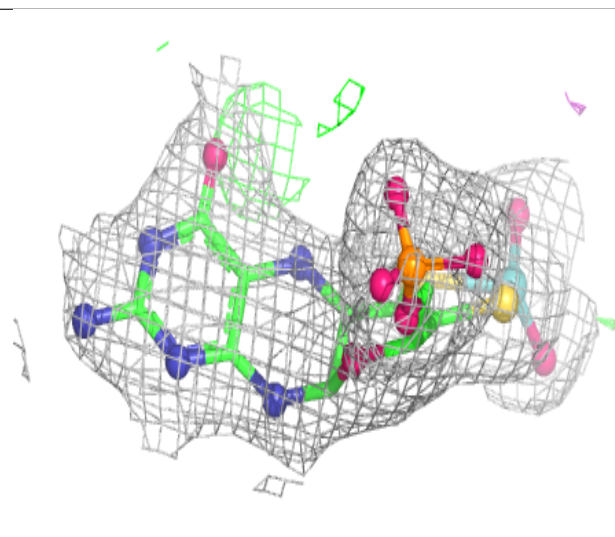
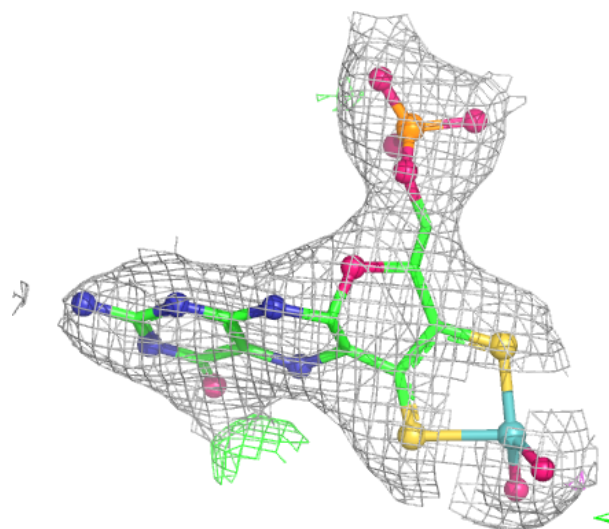
Electron density around MTQ A 1394:

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



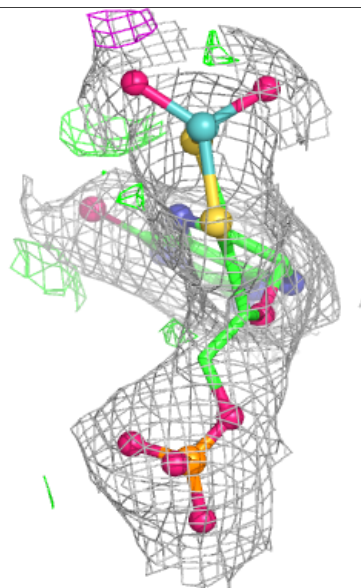
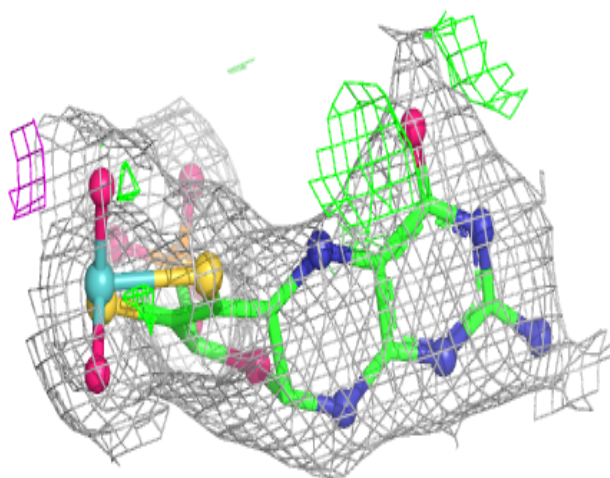
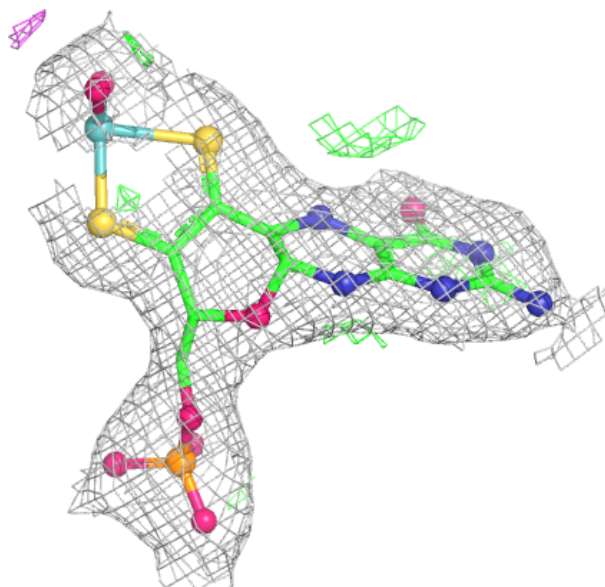
Electron density around MTQ B 1394:

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



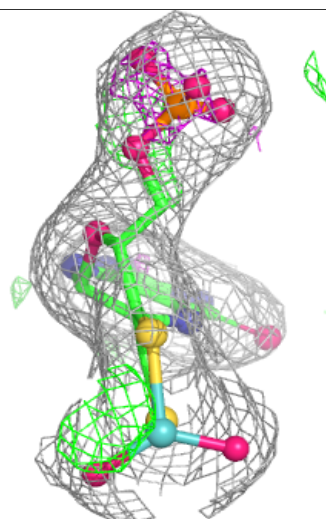
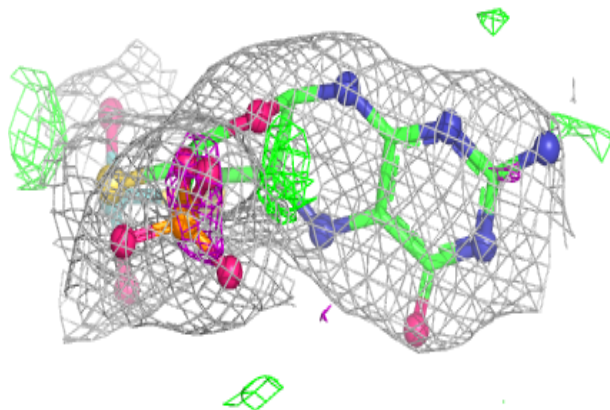
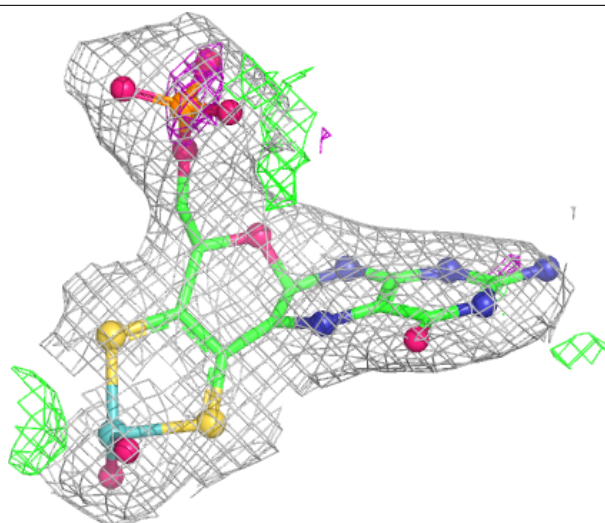
Electron density around MTQ C 1394:

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



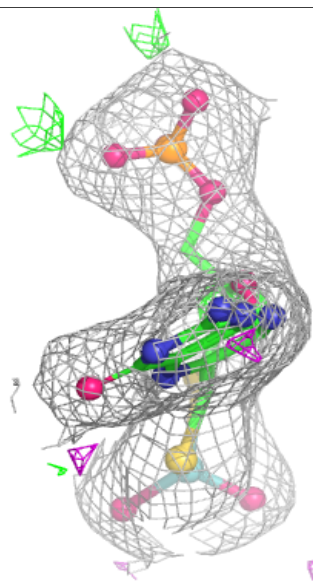
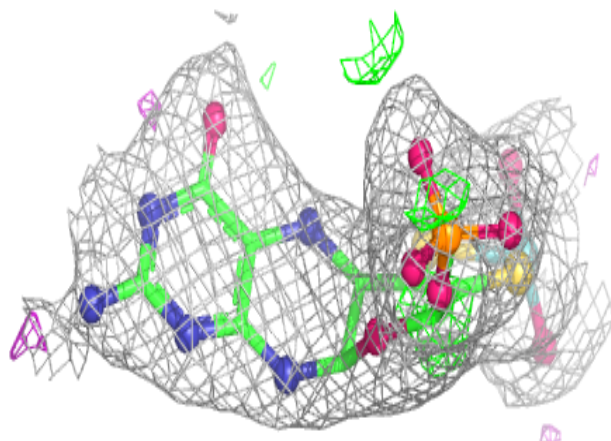
Electron density around MTQ D 1394:

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



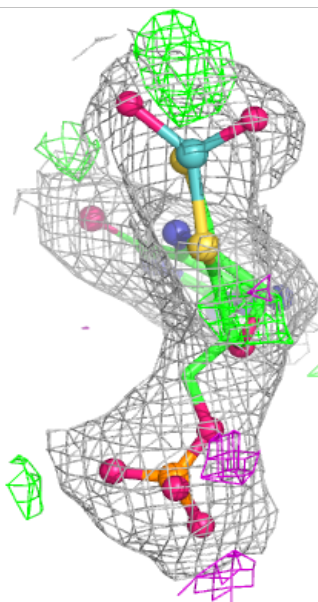
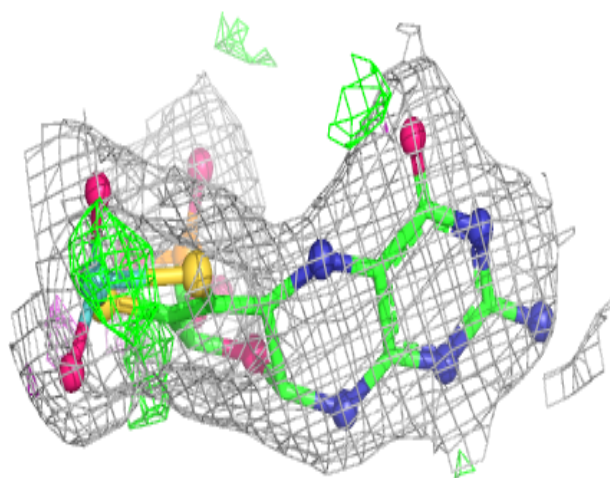
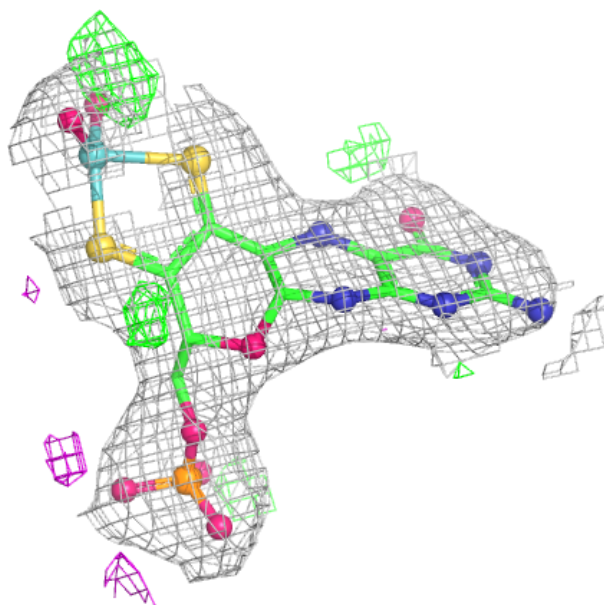
Electron density around MTQ E 1394:

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



Electron density around MTQ 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.