



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 03:33 AM EDT

PDB ID : 1G8K / pdb_00001g8k
Title : CRYSTAL STRUCTURE ANALYSIS OF ARSENITE OXIDASE FROM AL-CALIGENES FAECALIS
Authors : Ellis, P.J.; Conrads, T.; Hille, R.; Kuhn, P.
Deposited on : 2000-11-17
Resolution : 1.64 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

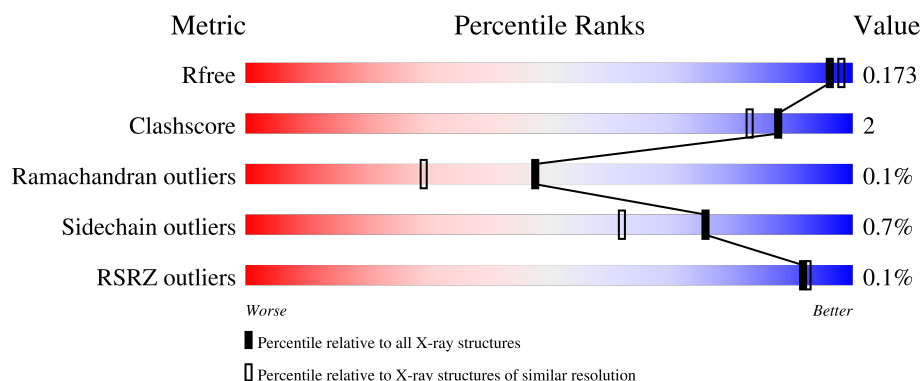
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	825	 91% 8%
1	C	825	 90% 8% .
1	E	825	 89% 10%
1	G	825	 90% 9% .
2	B	133	 94% 6%

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Mol	Chain	Length	Quality of chain
2	D	133	95% 5%
2	F	133	95% 5%
2	H	133	% 93% 7%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 34251 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 ARSENITE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	822	Total 6455	C 4060	N 1136	O 1219	S 40	67	0	0
1	C	822	Total 6455	C 4060	N 1136	O 1219	S 40	44	0	0
1	E	822	Total 6455	C 4060	N 1136	O 1219	S 40	37	0	0
1	G	822	Total 6455	C 4060	N 1136	O 1219	S 40	61	0	0

- Molecule 2 is a protein called ARSENITE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total 965	C 604	N 158	O 195	S 8	0	0	0
2	D	133	Total 965	C 604	N 158	O 195	S 8	0	0	0
2	F	133	Total 965	C 604	N 158	O 195	S 8	0	0	0
2	H	133	Total 965	C 604	N 158	O 195	S 8	0	0	0

- Molecule 3 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Hg 2	0	0
3	B	1	Total 1	Hg 1	0	0
3	C	2	Total 2	Hg 2	0	0
3	D	1	Total 1	Hg 1	0	0

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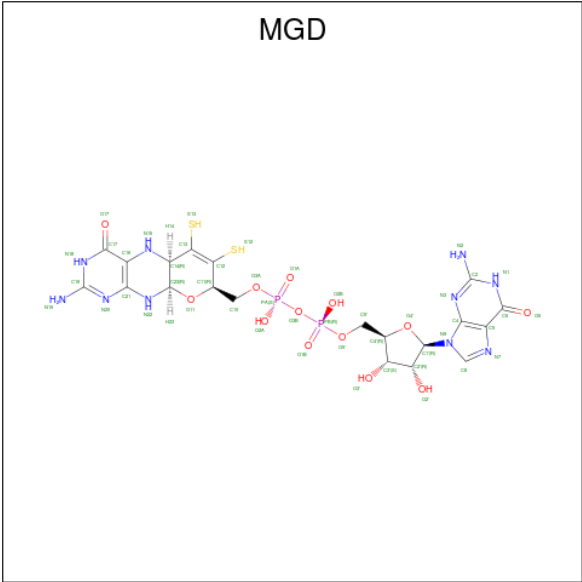
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	2	Total	Hg	0	0
			2	2		
3	F	1	Total	Hg	0	0
			1	1		
3	G	2	Total	Hg	0	0
			2	2		
3	H	1	Total	Hg	0	0
			1	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		
4	C	2	Total	Ca	0	0
			2	2		
4	E	2	Total	Ca	0	0
			2	2		
4	G	2	Total	Ca	0	0
			2	2		

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	
			47	20	10	13	2	2	
5	A	1	Total	C	N	O	P	S	
			47	20	10	13	2	2	
5	C	1	Total	C	N	O	P	S	
			47	20	10	13	2	2	
5	C	1	Total	C	N	O	P	S	
			47	20	10	13	2	2	
5	E	1	Total	C	N	O	P	S	
			47	20	10	13	2	2	
5	E	1	Total	C	N	O	P	S	
			47	20	10	13	2	2	
5	G	1	Total	C	N	O	P	S	
			47	20	10	13	2	2	
5	G	1	Total	C	N	O	P	S	
			47	20	10	13	2	2	

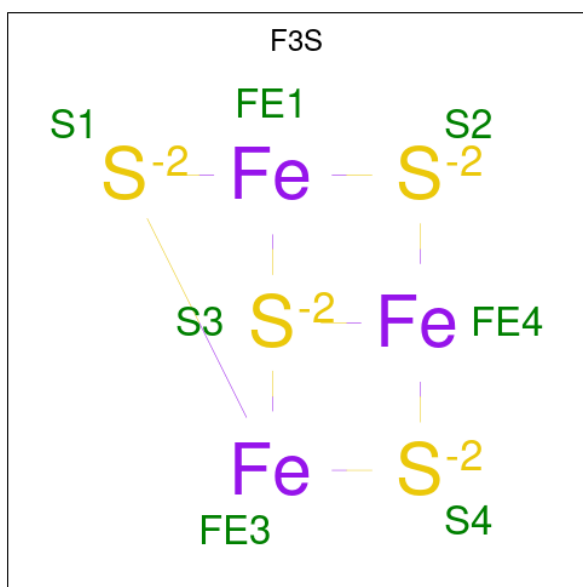
- Molecule 6 is OXYGEN ATOM (CCD ID: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O		
			1	1	0	0
6	C	1	Total	O		
			1	1	0	0
6	E	1	Total	O		
			1	1	0	0
6	G	1	Total	O		
			1	1	0	0

- Molecule 7 is MOLYBDENUM(IV) ION (CCD ID: 4MO) (formula: Mo).

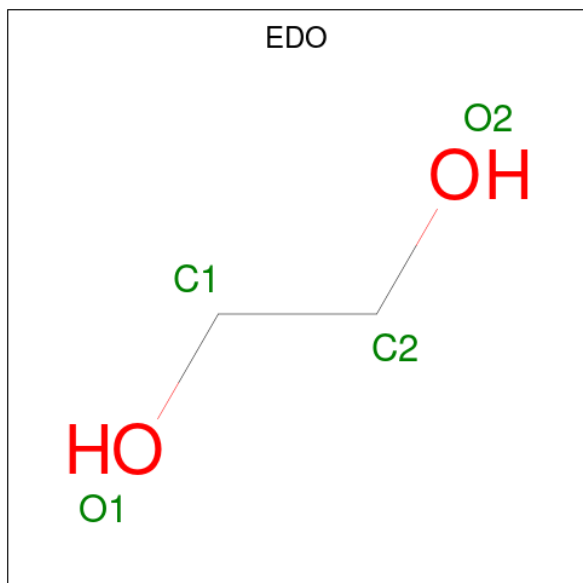
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mo		
			1	1	0	0
7	C	1	Total	Mo		
			1	1	0	0
7	E	1	Total	Mo		
			1	1	0	0
7	G	1	Total	Mo		
			1	1	0	0

- Molecule 8 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe₃S₄).



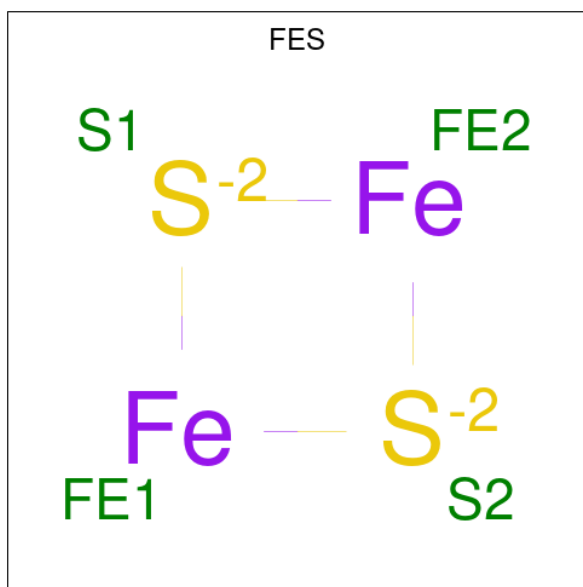
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	Fe	S	0	0
			7	3	4		
8	C	1	Total	Fe	S	0	0
			7	3	4		
8	E	1	Total	Fe	S	0	0
			7	3	4		
8	G	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	C	1	Total C O 4 2 2	0	0
9	C	1	Total C O 4 2 2	0	0
9	E	1	Total C O 4 2 2	0	0
9	E	1	Total C O 4 2 2	0	0
9	E	1	Total C O 4 2 2	0	0
9	G	1	Total C O 4 2 2	0	0
9	G	1	Total C O 4 2 2	0	0

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Fe S 4 2 2	0	0
10	D	1	Total Fe S 4 2 2	0	0
10	F	1	Total Fe S 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	H	1	Total 4	Fe 2	S 2	0	0

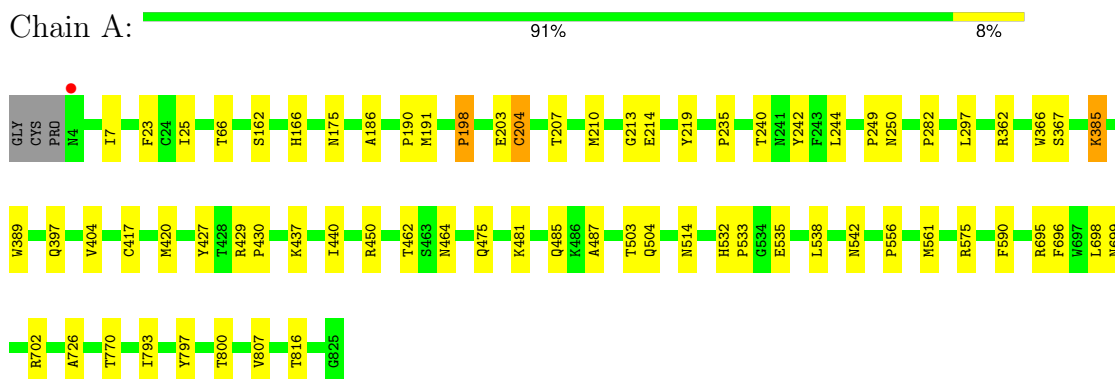
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	804	Total 804	O 804	0	0
11	B	165	Total 165	O 165	0	0
11	C	908	Total 908	O 908	0	0
11	D	157	Total 157	O 157	0	0
11	E	878	Total 878	O 878	0	0
11	F	162	Total 162	O 162	0	0
11	G	849	Total 849	O 849	0	0
11	H	164	Total 164	O 164	0	0

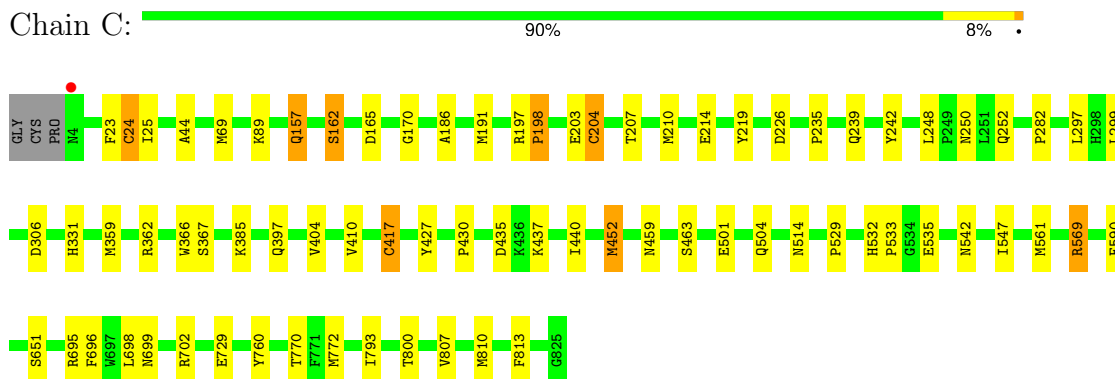
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

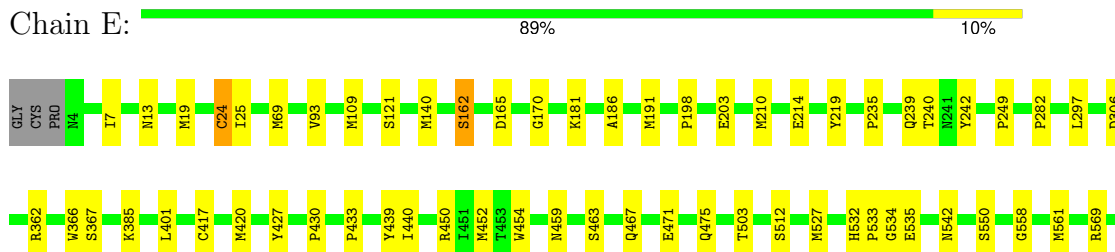
• Molecule 1: ARSENITE OXIDASE



• Molecule 1: ARSENITE OXIDASE



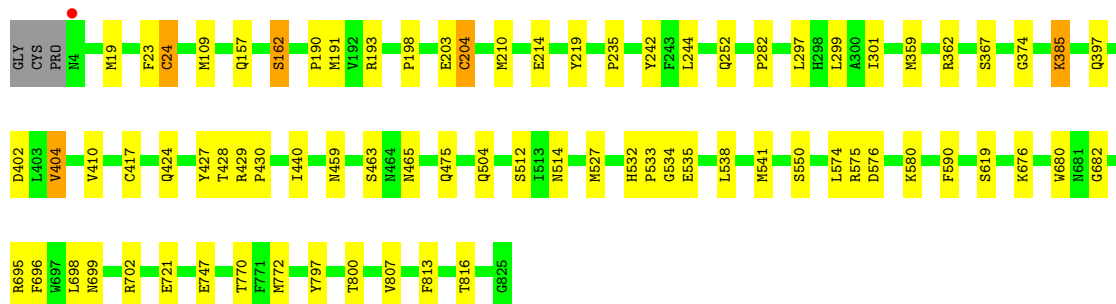
• Molecule 1: ARSENITE OXIDASE





• Molecule 1: ARSENITE OXIDASE

Chain G: 90% 9%



• Molecule 2: ARSENITE OXIDASE

Chain B: 94% 6%



• Molecule 2: ARSENITE OXIDASE

Chain D: 95% 5%



• Molecule 2: ARSENITE OXIDASE

Chain F: 95% 5%



• Molecule 2: ARSENITE OXIDASE

Chain H: 93% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.74Å 109.52Å 117.64Å 97.71° 90.00° 96.43°	Depositor
Resolution (Å)	17.80 – 1.64 17.80 – 1.64	Depositor EDS
% Data completeness (in resolution range)	(Not available) (17.80-1.64) 93.5 (17.80-1.64)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.65Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.154 , 0.179 0.149 , 0.173	Depositor DCC
R_{free} test set	25621 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	13.2	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	34251	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: HG, 4MO, CA, EDO, MGD, FES, F3S, O

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	1.05	3/6616 (0.0%)	1.14	36/8969 (0.4%)
1	C	1.12	10/6616 (0.2%)	1.16	31/8969 (0.3%)
1	E	1.18	10/6616 (0.2%)	1.22	32/8969 (0.4%)
1	G	1.14	7/6616 (0.1%)	1.20	34/8969 (0.4%)
2	B	1.15	1/986 (0.1%)	1.21	4/1349 (0.3%)
2	D	1.07	0/986	1.19	2/1349 (0.1%)
2	F	1.07	0/986	1.17	3/1349 (0.2%)
2	H	1.08	0/986	1.16	5/1349 (0.4%)
All	All	1.12	31/30408 (0.1%)	1.18	147/41272 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
1	E	0	2
1	G	0	2
All	All	0	7

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	191	MET	SD-CE	-12.96	1.47	1.79
1	G	191	MET	SD-CE	-9.95	1.54	1.79
1	C	191	MET	SD-CE	-9.34	1.56	1.79
1	G	210	MET	SD-CE	8.27	2.00	1.79
1	A	191	MET	SD-CE	-7.67	1.60	1.79
1	C	452	MET	SD-CE	6.99	1.97	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	109	MET	SD-CE	6.88	1.96	1.79
1	C	561	MET	SD-CE	-6.55	1.63	1.79
1	A	210	MET	SD-CE	6.47	1.95	1.79
1	G	772	MET	SD-CE	6.43	1.95	1.79
1	E	140	MET	CG-SD	6.36	1.96	1.80
1	E	772	MET	SD-CE	6.34	1.95	1.79
1	C	69	MET	SD-CE	-6.26	1.63	1.79
1	A	561	MET	SD-CE	-6.13	1.64	1.79
1	E	93	VAL	CA-CB	6.01	1.61	1.54
1	E	730	MET	SD-CE	6.00	1.94	1.79
1	C	772	MET	SD-CE	5.89	1.94	1.79
1	E	210	MET	SD-CE	5.89	1.94	1.79
1	E	19	MET	SD-CE	5.87	1.94	1.79
1	E	750	ASN	C-O	5.85	1.28	1.24
1	C	529	PRO	C-O	5.83	1.29	1.23
1	G	541	MET	SD-CE	-5.78	1.65	1.79
1	C	547	ILE	CA-CB	5.76	1.61	1.54
1	C	210	MET	SD-CE	5.74	1.94	1.79
1	E	240	THR	CA-CB	5.64	1.62	1.53
2	B	90	ALA	CA-CB	5.62	1.61	1.53
1	C	44	ALA	CA-CB	5.49	1.61	1.53
1	C	810	MET	SD-CE	5.31	1.92	1.79
1	G	404	VAL	CA-CB	5.21	1.60	1.54
1	E	69	MET	SD-CE	-5.02	1.67	1.79
1	G	19	MET	SD-CE	5.00	1.92	1.79

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	242	TYR	N-CA-C	-9.17	101.23	111.14
1	C	242	TYR	N-CA-C	-8.99	101.43	111.14
1	C	695	ARG	N-CA-C	8.75	122.07	111.40
1	E	242	TYR	N-CA-C	-8.63	101.82	111.14
1	E	695	ARG	N-CA-C	8.53	121.81	111.40
1	G	695	ARG	N-CA-C	8.35	121.59	111.40
1	A	695	ARG	N-CA-C	8.09	121.64	111.69
1	C	702	ARG	N-CA-C	7.68	121.85	110.48
2	B	82	PHE	N-CA-C	7.53	122.42	113.23
1	C	535	GLU	N-CA-C	-7.41	104.23	113.28
1	A	242	TYR	N-CA-C	-7.30	102.50	111.40
1	G	385	LYS	N-CA-C	7.25	121.39	112.54
1	E	430	PRO	N-CA-C	-7.17	101.96	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	162	SER	N-CA-C	-6.95	96.94	108.34
1	G	367	SER	N-CA-C	6.91	121.95	112.90
1	G	204	CYS	N-CA-C	6.88	119.68	110.88
1	G	702	ARG	N-CA-C	6.85	120.62	110.48
1	G	535	GLU	N-CA-C	-6.85	104.93	113.28
1	E	702	ARG	N-CA-C	6.83	121.17	110.32
1	E	535	GLU	N-CA-C	-6.81	104.97	113.28
1	E	214	GLU	N-CA-C	6.80	121.17	113.01
1	E	440	ILE	N-CA-C	6.79	116.93	110.42
1	E	235	PRO	N-CA-C	6.76	122.78	113.65
1	C	430	PRO	N-CA-C	-6.61	102.64	110.70
1	A	367	SER	N-CA-C	6.60	121.55	112.90
1	G	696	PHE	N-CA-C	6.57	120.54	109.76
1	C	437	LYS	N-CA-C	-6.53	98.57	108.96
1	C	440	ILE	N-CA-C	6.53	117.22	110.36
1	E	24	CYS	N-CA-C	6.53	118.44	110.41
1	A	535	GLU	N-CA-C	-6.51	105.34	113.28
2	H	57	SER	N-CA-C	-6.47	100.70	110.28
1	E	807	VAL	N-CA-C	-6.46	105.44	111.45
1	E	367	SER	N-CA-C	6.40	121.29	112.90
1	E	816	THR	N-CA-C	6.38	122.54	114.31
1	G	807	VAL	N-CA-C	-6.38	105.52	111.45
1	C	214	GLU	N-CA-C	6.35	120.28	112.54
1	A	385	LYS	N-CA-C	6.35	120.28	112.54
1	G	430	PRO	N-CA-C	-6.34	102.97	110.70
1	E	198	PRO	N-CA-C	6.33	125.50	112.47
1	E	696	PHE	N-CA-C	6.32	120.13	109.76
1	G	427	TYR	N-CA-C	6.30	119.00	108.73
1	G	235	PRO	N-CA-C	6.29	122.14	113.65
1	A	389	TRP	N-CA-C	-6.25	105.50	112.57
1	G	214	GLU	N-CA-C	6.22	120.13	112.54
1	A	430	PRO	N-CA-C	-6.19	103.15	110.70
1	A	203	GLU	N-CA-C	-6.16	105.72	113.18
1	G	429	ARG	N-CA-C	6.13	115.36	108.25
2	D	57	SER	N-CA-C	-6.12	101.22	110.28
1	C	427	TYR	N-CA-C	6.11	118.69	108.73
1	E	417	CYS	N-CA-C	-6.11	97.14	108.02
1	A	696	PHE	N-CA-C	6.11	119.43	109.59
1	G	504	GLN	N-CA-C	-6.09	105.85	113.28
1	A	204	CYS	N-CA-C	6.06	118.64	110.88
1	A	487	ALA	N-CA-C	6.01	118.67	110.55
1	C	24	CYS	N-CA-C	6.01	117.80	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	696	PHE	N-CA-C	5.98	119.57	109.76
2	F	57	SER	N-CA-C	-5.97	100.77	110.20
1	A	702	ARG	N-CA-C	5.95	119.78	110.32
1	E	427	TYR	N-CA-C	5.95	118.43	108.73
1	C	250	ASN	N-CA-C	-5.89	104.78	111.14
1	G	244	LEU	N-CA-C	5.87	117.75	111.36
2	D	82	PHE	N-CA-C	5.86	120.38	113.23
1	A	816	THR	N-CA-C	5.85	122.25	114.12
1	C	514	ASN	N-CA-CB	-5.85	102.00	111.24
2	B	123	GLY	N-CA-C	-5.84	106.40	111.95
2	H	82	PHE	N-CA-C	5.78	119.63	112.58
1	A	23	PHE	N-CA-C	5.78	123.11	110.80
1	E	203	GLU	N-CA-C	-5.78	106.19	113.18
1	G	374	GLY	N-CA-C	5.75	119.74	113.58
1	C	204	CYS	N-CA-C	5.75	118.24	110.88
1	A	198	PRO	N-CA-C	5.73	124.27	112.47
1	G	203	GLU	N-CA-C	-5.72	106.25	113.18
1	G	24	CYS	N-CA-C	5.70	117.42	110.41
1	A	462	THR	N-CA-C	5.70	122.04	114.12
1	C	165	ASP	N-CA-C	-5.68	104.55	113.02
1	C	417	CYS	N-CA-C	-5.67	95.85	107.70
1	G	534	GLY	N-CA-C	-5.65	107.17	113.79
1	G	190	PRO	N-CA-C	-5.65	106.78	114.80
1	A	213	GLY	N-CA-C	-5.64	104.76	111.36
1	G	198	PRO	N-CA-C	5.63	124.07	112.47
1	G	550	SER	N-CA-C	-5.62	100.08	109.24
1	A	514	ASN	N-CA-CB	-5.62	102.36	111.24
2	F	8	ALA	N-CA-C	-5.59	98.09	107.99
1	G	813	PHE	N-CA-C	-5.59	105.26	111.36
1	A	235	PRO	N-CA-C	5.58	121.90	113.81
1	C	203	GLU	N-CA-C	-5.58	106.43	113.18
1	G	109	MET	N-CA-C	-5.58	102.64	110.50
1	E	165	ASP	N-CA-C	-5.57	104.72	113.02
1	C	807	VAL	N-CA-C	-5.55	106.40	111.67
1	C	813	PHE	N-CA-C	-5.55	105.31	111.36
1	C	331	HIS	N-CA-C	5.54	120.75	112.94
1	A	214	GLU	N-CA-C	5.52	119.27	112.54
1	C	306	ASP	N-CA-C	5.52	118.01	111.33
2	F	82	PHE	N-CA-C	5.51	119.95	113.23
1	A	166	HIS	N-CA-C	5.49	118.56	109.94
1	E	420	MET	N-CA-C	-5.49	106.09	112.89
2	H	64	GLY	N-CA-C	5.48	122.88	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	424	GLN	N-CA-C	-5.45	103.71	110.41
1	C	198	PRO	N-CA-C	5.45	123.69	112.47
1	E	534	GLY	N-CA-C	-5.45	107.42	113.79
1	A	726	ALA	N-CA-C	-5.44	102.34	110.23
1	G	514	ASN	N-CA-CB	-5.44	102.65	111.24
1	A	429	ARG	N-CA-C	5.44	114.56	108.25
1	E	162	SER	N-CA-C	-5.42	99.58	108.41
1	C	367	SER	N-CA-C	5.41	119.99	112.90
1	A	250	ASN	N-CA-C	-5.38	105.33	111.14
1	A	240	THR	N-CA-C	5.38	120.19	111.37
1	C	23	PHE	N-CA-C	5.36	122.21	110.80
1	E	181	LYS	N-CA-C	-5.34	105.45	111.28
1	C	239	GLN	N-CA-C	-5.32	102.46	110.06
1	A	427	TYR	N-CA-C	5.31	117.39	108.73
1	A	420	MET	N-CA-C	-5.31	106.31	112.89
1	E	584	ALA	N-CA-C	5.31	117.07	111.28
1	C	226	ASP	N-CA-C	-5.30	105.17	111.69
1	E	699	ASN	N-CA-C	-5.30	103.49	110.43
1	E	109	MET	N-CA-C	-5.29	103.54	110.53
1	G	816	THR	N-CA-C	5.29	121.13	114.31
1	G	440	ILE	N-CA-C	5.28	115.49	110.42
1	A	244	LEU	N-CA-C	5.28	117.12	111.36
1	E	813	PHE	N-CA-C	-5.27	105.62	111.36
1	E	454	TRP	N-CA-C	-5.25	100.75	109.46
2	H	8	ALA	N-CA-C	-5.25	98.84	108.02
1	A	464	ASN	N-CA-C	-5.24	103.48	110.55
1	A	175	ASN	N-CA-C	5.22	117.05	111.36
2	B	57	SER	N-CA-C	-5.22	102.56	110.28
1	A	504	GLN	N-CA-C	-5.21	106.88	113.18
1	E	550	SER	N-CA-C	-5.20	100.25	108.73
1	A	162	SER	N-CA-C	-5.20	98.77	108.02
1	A	440	ILE	N-CA-C	5.19	115.81	110.36
1	G	465	ASN	N-CA-C	-5.19	104.22	111.39
1	C	197	ARG	CB-CA-C	5.17	116.94	109.45
1	C	162	SER	N-CA-C	-5.14	99.90	108.34
2	B	22	PRO	N-CA-C	5.13	119.15	111.14
1	C	504	GLN	N-CA-C	-5.12	106.54	112.89
1	G	747	GLU	N-CA-C	-5.11	101.38	109.96
1	G	23	PHE	N-CA-C	5.10	121.65	110.80
1	C	235	PRO	CA-C-N	-5.08	113.47	120.28
1	C	235	PRO	C-N-CA	-5.08	113.47	120.28
2	H	39	LEU	N-CA-C	5.08	117.72	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	726	ALA	N-CA-C	-5.08	102.87	110.23
1	A	807	VAL	N-CA-C	-5.07	106.74	111.45
1	E	13	ASN	N-CA-C	5.05	118.48	112.72
1	A	190	PRO	N-CA-C	-5.04	107.62	114.98
1	E	239	GLN	N-CA-C	-5.04	102.86	110.06
1	G	301	ILE	N-CA-C	5.03	117.63	110.09
1	E	306	ASP	N-CA-C	5.01	117.40	111.33
1	A	556	PRO	N-CA-C	-5.01	104.59	110.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	219	TYR	Sidechain
1	A	797	TYR	Sidechain
1	C	219	TYR	Sidechain
1	E	219	TYR	Sidechain
1	E	439	TYR	Sidechain
1	G	219	TYR	Sidechain
1	G	797	TYR	Sidechain

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	6455	0	6220	20	0
1	C	6455	0	6221	25	0
1	E	6455	0	6220	28	0
1	G	6455	0	6221	23	0
2	B	965	0	934	3	0
2	D	965	0	933	3	0
2	F	965	0	933	2	0
2	H	965	0	933	6	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	2	0	0	0	0
3	F	1	0	0	0	0
3	G	2	0	0	1	0
3	H	1	0	0	0	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
4	E	2	0	0	0	0
4	G	2	0	0	0	0
5	A	94	0	44	2	0
5	C	94	0	44	2	0
5	E	94	0	44	2	0
5	G	94	0	44	1	0
6	A	1	0	0	0	0
6	C	1	0	0	1	0
6	E	1	0	0	1	0
6	G	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	1	0
7	E	1	0	0	1	0
7	G	1	0	0	0	0
8	A	7	0	0	0	0
8	C	7	0	0	0	0
8	E	7	0	0	0	0
8	G	7	0	0	0	0
9	A	8	0	12	0	0
9	C	8	0	12	0	0
9	E	12	0	18	0	0
9	G	8	0	12	0	0
10	B	4	0	0	0	0
10	D	4	0	0	0	0
10	F	4	0	0	0	0
10	H	4	0	0	0	0
11	A	804	0	0	3	0
11	B	165	0	0	3	0
11	C	908	0	0	5	0
11	D	157	0	0	1	0
11	E	878	0	0	3	0
11	F	162	0	0	0	0
11	G	849	0	0	7	0
11	H	164	0	0	4	0
All	All	34251	0	28845	112	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 2.

All (112) 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:E:561:MET:HE1	1:E:569:ARG:HH11	1.19	0.99
1:C:157:GLN:HG2	11:C:7662:HOH:O	1.72	0.89
1:E:561:MET:HE1	1:E:569:ARG:NH1	1.97	0.80
6:E:5203:O:O	7:E:5204:4MO:MO	1.53	0.77
6:C:5103:O:O	7:C:5104:4MO:MO	1.59	0.73
1:A:475:GLN:HG3	11:A:7620:HOH:O	1.89	0.73
2:H:100:ALA:HB3	11:H:6124:HOH:O	1.97	0.64
1:G:157:GLN:HG2	11:G:7364:HOH:O	1.98	0.64
1:C:651:SER:HB3	11:C:7804:HOH:O	1.97	0.63
1:G:204:CYS:SG	3:G:6008:HG:HG	2.16	0.63
1:E:569:ARG:NE	11:E:7857:HOH:O	2.21	0.62
1:G:475:GLN:HG3	11:G:7579:HOH:O	1.99	0.61
1:C:698:LEU:HB2	1:C:800:THR:HG23	1.83	0.60
1:G:575:ARG:HD3	11:G:7714:HOH:O	2.01	0.59
1:G:397:GLN:HG3	11:G:7068:HOH:O	2.03	0.57
2:D:10:ALA:HB1	11:D:6110:HOH:O	2.04	0.57
1:A:397:GLN:HG3	11:A:7072:HOH:O	2.05	0.56
1:C:404:VAL:HG11	1:C:417:CYS:HB2	1.88	0.56
1:G:404:VAL:HG11	1:G:417:CYS:HB2	1.87	0.56
1:A:575:ARG:HD3	11:A:7664:HOH:O	2.04	0.56
1:C:397:GLN:HG3	11:C:7023:HOH:O	2.05	0.55
1:C:207:THR:HG22	1:C:397:GLN:HE22	1.73	0.54
1:C:569:ARG:HH11	1:C:569:ARG:HG3	1.72	0.53
2:B:104:ARG:N	2:B:104:ARG:HD3	2.24	0.53
1:E:561:MET:CE	1:E:569:ARG:HH11	2.08	0.53
1:E:475:GLN:HG3	11:G:7585:HOH:O	2.09	0.51
1:G:533:PRO:HG3	1:G:538:LEU:HD13	1.92	0.50
1:E:732:PRO:O	1:E:736:LYS:HG3	2.12	0.50
1:E:532:HIS:HB2	1:E:533:PRO:CD	2.41	0.50
1:C:204:CYS:HB3	1:C:207:THR:CG2	2.41	0.50
2:D:61:THR:CG2	2:D:103:PRO:HD3	2.41	0.49
1:A:204:CYS:HB3	1:A:207:THR:HG22	1.95	0.49
1:C:248:LEU:O	1:C:252:GLN:HG3	2.12	0.49
2:H:100:ALA:CB	11:H:6124:HOH:O	2.58	0.49
1:A:204:CYS:HB3	1:A:207:THR:CG2	2.44	0.48
1:G:532:HIS:HB2	1:G:533:PRO:CD	2.43	0.47
1:E:698:LEU:HB2	1:E:800:THR:HG23	1.96	0.47
2:D:104:ARG:N	2:D:104:ARG:HD3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:VAL:HG11	1:A:417:CYS:HB2	1.95	0.47
1:C:204:CYS:HB3	1:C:207:THR:HG22	1.95	0.47
1:C:385:LYS:HE2	5:C:5101:MGD:S13	2.55	0.47
2:B:1:ARG:CA	11:B:6129:HOH:O	2.58	0.46
2:H:100:ALA:N	11:H:6124:HOH:O	2.48	0.46
1:E:385:LYS:HE2	5:E:5201:MGD:S13	2.55	0.46
1:C:532:HIS:HB2	1:C:533:PRO:CD	2.46	0.46
1:E:297:LEU:HG	1:E:366:TRP:CH2	2.50	0.46
1:E:561:MET:CE	1:E:569:ARG:NH1	2.74	0.46
2:F:104:ARG:N	2:F:104:ARG:HD3	2.31	0.46
1:A:66:THR:HG21	11:B:6126:HOH:O	2.14	0.46
1:G:459:ASN:HB3	1:G:463:SER:OG	2.15	0.46
1:E:297:LEU:HD21	1:E:362:ARG:HD2	1.97	0.45
1:C:459:ASN:HB3	1:C:463:SER:OG	2.17	0.45
2:B:100:ALA:HB3	11:B:6126:HOH:O	2.17	0.45
1:E:25:ILE:O	1:E:542:ASN:HB2	2.16	0.45
1:G:385:LYS:HE2	5:G:5301:MGD:S13	2.56	0.45
1:C:297:LEU:HD21	1:C:362:ARG:HD2	1.97	0.45
2:H:111:ALA:CB	11:H:6132:HOH:O	2.65	0.45
1:A:186:ALA:HB1	1:A:590:PHE:CD1	2.52	0.44
1:C:359:MET:HE2	1:C:359:MET:HB3	1.79	0.44
1:G:299:LEU:HD23	1:G:359:MET:CE	2.47	0.44
1:A:698:LEU:HB2	1:A:800:THR:HG23	1.99	0.44
1:G:252:GLN:OE1	11:G:7755:HOH:O	2.21	0.44
1:C:699:ASN:HB3	1:C:770:THR:O	2.16	0.44
1:G:698:LEU:HB2	1:G:800:THR:HG23	2.00	0.44
1:A:532:HIS:HB2	1:A:533:PRO:CD	2.47	0.44
1:E:297:LEU:HG	1:E:366:TRP:CZ3	2.52	0.44
2:F:61:THR:CG2	2:F:103:PRO:HD3	2.48	0.44
1:C:89:LYS:NZ	11:C:7545:HOH:O	2.45	0.43
1:C:25:ILE:O	1:C:542:ASN:HB2	2.17	0.43
1:G:576:ASP:OD1	1:G:580:LYS:HE3	2.18	0.43
1:E:162:SER:HB2	1:E:452:MET:HE1	2.01	0.43
1:A:297:LEU:HG	1:A:366:TRP:CZ3	2.53	0.43
1:A:385:LYS:HE2	5:A:5001:MGD:S13	2.58	0.43
1:E:186:ALA:HB1	1:E:590:PHE:CD1	2.54	0.43
1:A:533:PRO:HG3	1:A:538:LEU:HD13	2.00	0.43
1:C:729:GLU:HA	1:C:760:TYR:O	2.19	0.43
1:G:699:ASN:HB3	1:G:770:THR:O	2.18	0.43
1:E:512:SER:O	1:E:527:MET:HA	2.19	0.43
1:A:297:LEU:HG	1:A:366:TRP:CH2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:ASN:HB3	1:A:770:THR:O	2.19	0.42
1:E:121:SER:HB2	1:E:558:GLY:HA3	2.00	0.42
1:E:729:GLU:HA	1:E:760:TYR:O	2.19	0.42
1:C:299:LEU:HD23	1:C:359:MET:CE	2.48	0.42
1:A:481:LYS:O	1:A:485:GLN:HG3	2.20	0.42
1:E:170:GLY:HA2	5:E:5201:MGD:C6	2.50	0.42
1:G:512:SER:O	1:G:527:MET:HA	2.19	0.42
1:C:186:ALA:HB1	1:C:590:PHE:CD1	2.55	0.42
1:E:467:GLN:O	1:E:471:GLU:HG3	2.20	0.42
1:G:162:SER:HA	1:G:193:ARG:HG3	2.01	0.42
1:A:25:ILE:O	1:A:542:ASN:HB2	2.19	0.42
1:G:428:THR:HG23	1:G:619:SER:HB2	2.02	0.42
1:C:297:LEU:HG	1:C:366:TRP:CZ3	2.55	0.41
2:H:90:ALA:O	2:H:104:ARG:HD2	2.20	0.41
1:C:569:ARG:NE	11:C:7783:HOH:O	2.25	0.41
1:G:574:LEU:HD13	1:G:590:PHE:CE1	2.55	0.41
1:G:721:GLU:OE1	11:G:7852:HOH:O	2.21	0.41
1:G:402:ASP:OD2	1:G:676:LYS:O	2.38	0.41
1:G:680:TRP:CZ2	1:G:682:GLY:HA2	2.55	0.41
1:A:699:ASN:OD1	5:A:5002:MGD:H8	2.20	0.41
1:E:459:ASN:HB3	1:E:463:SER:OG	2.20	0.41
1:G:297:LEU:HD21	1:G:362:ARG:HD2	2.03	0.41
1:E:575:ARG:HD3	11:E:7382:HOH:O	2.20	0.41
2:H:104:ARG:N	2:H:104:ARG:HD3	2.36	0.41
1:C:162:SER:HB2	1:C:452:MET:HE1	2.03	0.41
1:E:735:CYS:HB3	1:E:740:VAL:O	2.20	0.41
1:A:297:LEU:HD21	1:A:362:ARG:HD2	2.02	0.41
1:A:450:ARG:HD2	1:A:503:THR:OG1	2.21	0.41
1:E:450:ARG:HD2	1:E:503:THR:OG1	2.21	0.41
1:E:561:MET:HE2	11:E:7219:HOH:O	2.21	0.40
1:C:170:GLY:HA2	5:C:5101:MGD:C6	2.51	0.40
1:E:680:TRP:CZ2	1:E:682:GLY:HA2	2.57	0.40
1:E:401:LEU:HD13	1:E:401:LEU:HA	1.96	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	820/825 (99%)	790 (96%)	29 (4%)	1 (0%)	48	29
1	C	820/825 (99%)	792 (97%)	27 (3%)	1 (0%)	48	29
1	E	820/825 (99%)	790 (96%)	29 (4%)	1 (0%)	48	29
1	G	820/825 (99%)	792 (97%)	28 (3%)	0	100	100
2	B	131/133 (98%)	125 (95%)	6 (5%)	0	100	100
2	D	131/133 (98%)	130 (99%)	1 (1%)	0	100	100
2	F	131/133 (98%)	127 (97%)	4 (3%)	0	100	100
2	H	131/133 (98%)	127 (97%)	4 (3%)	0	100	100
All	All	3804/3832 (99%)	3673 (97%)	128 (3%)	3 (0%)	48	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	793	ILE
1	E	793	ILE
1	A	793	ILE

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	674/676 (100%)	669 (99%)	5 (1%)	76	62
1	C	674/676 (100%)	666 (99%)	8 (1%)	63	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	674/676 (100%)	669 (99%)	5 (1%)	76	62
1	G	674/676 (100%)	671 (100%)	3 (0%)	84	76
2	B	105/105 (100%)	105 (100%)	0	100	100
2	D	105/105 (100%)	105 (100%)	0	100	100
2	F	105/105 (100%)	104 (99%)	1 (1%)	68	49
2	H	105/105 (100%)	105 (100%)	0	100	100
All	All	3116/3124 (100%)	3094 (99%)	22 (1%)	76	62

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	198	PRO
1	A	249	PRO
1	A	282	PRO
1	A	437	LYS
1	C	24	CYS
1	C	157	GLN
1	C	198	PRO
1	C	282	PRO
1	C	410	VAL
1	C	435	ASP
1	C	501	GLU
1	C	569	ARG
1	E	7	ILE
1	E	24	CYS
1	E	249	PRO
1	E	282	PRO
1	E	433	PRO
2	F	28	PRO
1	G	24	CYS
1	G	282	PRO
1	G	410	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	ASN
1	A	234	ASN

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Mol	Chain	Res	Type
1	A	579	GLN
1	A	589	GLN
1	C	216	ASN
1	C	223	GLN
1	C	234	ASN
1	C	270	GLN
1	C	482	GLN
1	C	579	GLN
1	E	216	ASN
1	E	223	GLN
1	E	234	ASN
1	E	482	GLN
1	E	579	GLN
1	E	688	GLN
1	E	689	GLN
1	G	216	ASN
1	G	234	ASN
1	G	270	GLN
1	G	475	GLN
1	G	589	GLN
1	G	688	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 53 ligands modelled in this entry, 28 are monoatomic - leaving 25 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
9	EDO	A	7005	-	3,3,3	0.43	0	2,2,2	0.18	0
5	MGD	C	5101	7	47,52,52	1.35	7 (14%)	58,81,81	1.32	5 (8%)
5	MGD	C	5102	7	47,52,52	1.21	5 (10%)	58,81,81	1.29	4 (6%)
9	EDO	G	7008	-	3,3,3	0.69	0	2,2,2	0.18	0
5	MGD	A	5001	7	47,52,52	1.15	6 (12%)	58,81,81	1.39	5 (8%)
8	F3S	G	5305	1	0,9,9	-	-	-	-	-
8	F3S	C	5105	1	0,9,9	-	-	-	-	-
10	FES	B	5006	2	0,4,4	-	-	-	-	-
9	EDO	E	7003	-	3,3,3	0.67	0	2,2,2	0.17	0
5	MGD	E	5202	7	47,52,52	1.41	10 (21%)	58,81,81	1.38	9 (15%)
10	FES	H	5306	2	0,4,4	-	-	-	-	-
9	EDO	G	7004	-	3,3,3	0.94	0	2,2,2	0.23	0
5	MGD	G	5302	7	47,52,52	1.17	6 (12%)	58,81,81	1.44	7 (12%)
10	FES	F	5206	2	0,4,4	-	-	-	-	-
5	MGD	E	5201	7	47,52,52	1.27	4 (8%)	58,81,81	1.24	3 (5%)
5	MGD	G	5301	7	47,52,52	1.44	6 (12%)	58,81,81	1.47	5 (8%)
9	EDO	C	7002	-	3,3,3	0.99	0	2,2,2	0.34	0
9	EDO	E	7009	-	3,3,3	0.79	0	2,2,2	0.15	0
8	F3S	E	5205	1	0,9,9	-	-	-	-	-
8	F3S	A	5005	1	0,9,9	-	-	-	-	-
9	EDO	A	7001	-	3,3,3	0.96	0	2,2,2	0.23	0
9	EDO	C	7006	-	3,3,3	0.59	0	2,2,2	0.14	0
10	FES	D	5106	2	0,4,4	-	-	-	-	-
5	MGD	A	5002	7	47,52,52	1.35	7 (14%)	58,81,81	1.45	7 (12%)
9	EDO	E	7007	-	3,3,3	0.50	0	2,2,2	0.30	0

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
9	EDO	A	7005	-	-	0/1/1/1	-
5	MGD	C	5101	7	-	5/22/66/66	0/6/6/6
5	MGD	C	5102	7	-	4/22/66/66	0/6/6/6
9	EDO	G	7008	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MGD	A	5001	7	-	5/22/66/66	0/6/6/6
8	F3S	G	5305	1	-	-	0/3/3/3
8	F3S	C	5105	1	-	-	0/3/3/3
10	FES	B	5006	2	-	-	0/1/1/1
9	EDO	E	7003	-	-	0/1/1/1	-
5	MGD	E	5202	7	-	4/22/66/66	0/6/6/6
10	FES	H	5306	2	-	-	0/1/1/1
9	EDO	G	7004	-	-	0/1/1/1	-
5	MGD	G	5302	7	-	5/22/66/66	0/6/6/6
10	FES	F	5206	2	-	-	0/1/1/1
5	MGD	E	5201	7	-	3/22/66/66	0/6/6/6
5	MGD	G	5301	7	-	4/22/66/66	0/6/6/6
9	EDO	C	7002	-	-	0/1/1/1	-
9	EDO	E	7009	-	-	0/1/1/1	-
8	F3S	E	5205	1	-	-	0/3/3/3
9	EDO	A	7001	-	-	0/1/1/1	-
9	EDO	C	7006	-	-	0/1/1/1	-
8	F3S	A	5005	1	-	-	0/3/3/3
10	FES	D	5106	2	-	-	0/1/1/1
5	MGD	A	5002	7	-	5/22/66/66	0/6/6/6
9	EDO	E	7007	-	-	0/1/1/1	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	5301	MGD	C23-C14	6.00	1.58	1.53
5	E	5201	MGD	C23-C14	5.00	1.57	1.53
5	C	5101	MGD	C23-C14	4.04	1.56	1.53
5	A	5002	MGD	C14-N15	3.94	1.50	1.46
5	A	5002	MGD	C23-C14	3.91	1.56	1.53
5	C	5101	MGD	C21-N22	3.57	1.39	1.35
5	E	5202	MGD	C23-C14	3.43	1.56	1.53
5	A	5002	MGD	C16-C21	3.38	1.44	1.38
5	C	5101	MGD	C16-C21	3.22	1.44	1.38
5	G	5302	MGD	PA-O3B	3.18	1.62	1.59
5	C	5102	MGD	C16-C21	3.17	1.44	1.38
5	G	5301	MGD	C16-C21	3.11	1.44	1.38
5	C	5102	MGD	PB-O3B	3.08	1.62	1.59
5	G	5302	MGD	C16-N15	3.00	1.44	1.37
5	E	5201	MGD	C16-C21	3.00	1.43	1.38
5	E	5201	MGD	O17-C17	3.00	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	5102	MGD	O11-C11	-2.86	1.38	1.43
5	C	5101	MGD	C14-N15	2.78	1.49	1.46
5	C	5102	MGD	C14-N15	2.77	1.49	1.46
5	A	5001	MGD	O11-C23	-2.73	1.39	1.43
5	E	5202	MGD	PB-O1B	-2.73	1.41	1.50
5	G	5301	MGD	O11-C11	-2.69	1.38	1.43
5	E	5202	MGD	C16-C21	2.68	1.43	1.38
5	A	5001	MGD	C23-C14	2.67	1.55	1.53
5	E	5202	MGD	O11-C11	-2.59	1.38	1.43
5	A	5001	MGD	C21-N22	2.54	1.38	1.35
5	E	5202	MGD	C23-N22	-2.50	1.41	1.45
5	E	5202	MGD	C2-N2	2.49	1.40	1.34
5	G	5302	MGD	C16-C21	2.39	1.42	1.38
5	E	5202	MGD	PB-O3B	2.36	1.62	1.59
5	A	5002	MGD	C16-C17	2.31	1.48	1.41
5	A	5002	MGD	C17-N18	2.30	1.43	1.38
5	A	5002	MGD	C21-N22	2.28	1.38	1.35
5	G	5302	MGD	C14-N15	2.26	1.49	1.46
5	E	5202	MGD	C21-N20	-2.25	1.32	1.36
5	G	5302	MGD	C17-N18	2.25	1.43	1.38
5	A	5001	MGD	C14-N15	2.24	1.49	1.46
5	A	5001	MGD	PA-O2A	-2.24	1.44	1.55
5	E	5202	MGD	PA-O3B	2.24	1.61	1.59
5	G	5301	MGD	C21-N22	2.22	1.37	1.35
5	C	5101	MGD	C2-N2	2.21	1.39	1.34
5	A	5002	MGD	C19-N20	2.18	1.38	1.33
5	C	5101	MGD	PB-O3B	2.17	1.61	1.59
5	E	5201	MGD	O11-C11	-2.17	1.39	1.43
5	C	5101	MGD	C16-C17	2.14	1.48	1.41
5	G	5301	MGD	PB-O2B	-2.10	1.45	1.55
5	A	5001	MGD	PB-O2B	-2.08	1.45	1.55
5	G	5302	MGD	C19-N18	2.07	1.42	1.37
5	C	5102	MGD	C23-C14	2.07	1.55	1.53
5	E	5202	MGD	C14-N15	2.05	1.48	1.46
5	G	5301	MGD	PA-O3B	2.04	1.61	1.59

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	5301	MGD	C23-C14-N15	6.75	114.50	107.87
5	G	5302	MGD	C19-N20-C21	6.42	124.69	113.36
5	A	5002	MGD	C23-C14-N15	5.84	113.61	107.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	5202	MGD	C19-N20-C21	5.60	123.24	113.36
5	E	5201	MGD	C19-N20-C21	5.58	123.21	113.36
5	G	5301	MGD	C19-N20-C21	5.46	123.00	113.36
5	A	5002	MGD	C19-N20-C21	5.43	122.95	113.36
5	C	5101	MGD	C23-C14-N15	5.10	112.87	107.87
5	A	5001	MGD	C19-N20-C21	5.02	122.22	113.36
5	C	5102	MGD	C19-N20-C21	4.89	121.99	113.36
5	A	5001	MGD	O11-C23-C14	4.85	112.20	108.96
5	C	5101	MGD	C19-N20-C21	4.74	121.73	113.36
5	C	5102	MGD	C23-C14-N15	4.69	112.47	107.87
5	G	5302	MGD	C23-C14-N15	4.46	112.25	107.87
5	A	5001	MGD	C23-C14-N15	4.36	112.16	107.87
5	E	5201	MGD	C23-C14-N15	3.68	111.48	107.87
5	E	5202	MGD	C23-C14-N15	3.38	111.19	107.87
5	C	5101	MGD	O11-C23-C14	2.93	110.92	108.96
5	G	5302	MGD	C19-N18-C17	-2.84	119.95	125.11
5	A	5001	MGD	O2B-PB-O3B	2.80	114.84	107.27
5	E	5202	MGD	N18-C19-N20	-2.71	118.36	123.32
5	E	5202	MGD	O17-C17-C16	-2.64	120.90	127.26
5	C	5102	MGD	C17-C16-N15	2.58	123.29	116.27
5	E	5201	MGD	C17-C16-N15	2.57	123.27	116.27
5	G	5301	MGD	O2B-PB-O3B	2.55	114.18	107.27
5	A	5001	MGD	C17-C16-N15	2.51	123.12	116.27
5	E	5202	MGD	C17-C16-N15	2.51	123.11	116.27
5	G	5301	MGD	C17-C16-N15	2.50	123.09	116.27
5	A	5002	MGD	C19-N18-C17	-2.50	120.58	125.11
5	G	5302	MGD	C17-C16-N15	2.49	123.05	116.27
5	C	5101	MGD	C17-C16-N15	2.48	123.02	116.27
5	A	5002	MGD	O11-C23-N22	2.43	110.81	108.61
5	G	5302	MGD	C16-C17-N18	2.26	118.33	112.13
5	E	5202	MGD	O2A-PA-O1A	2.21	122.74	112.44
5	A	5002	MGD	C17-C16-N15	2.20	122.28	116.27
5	G	5302	MGD	N18-C19-N20	-2.20	119.29	123.32
5	E	5202	MGD	C4'-O4'-C1'	-2.20	104.61	109.47
5	G	5301	MGD	N18-C19-N20	-2.18	119.33	123.32
5	E	5202	MGD	O4'-C1'-C2'	-2.17	101.96	106.62
5	A	5002	MGD	C16-C17-N18	2.16	118.07	112.13
5	C	5101	MGD	O11-C23-N22	-2.11	106.69	108.61
5	E	5202	MGD	C16-C17-N18	2.09	117.87	112.13
5	A	5002	MGD	O4'-C1'-C2'	-2.06	102.20	106.62
5	C	5102	MGD	C4'-O4'-C1'	-2.01	105.02	109.47
5	G	5302	MGD	O2A-PA-O1A	2.01	121.78	112.44

There are no chirality outliers.

All (35) torsion outliers are listed below:

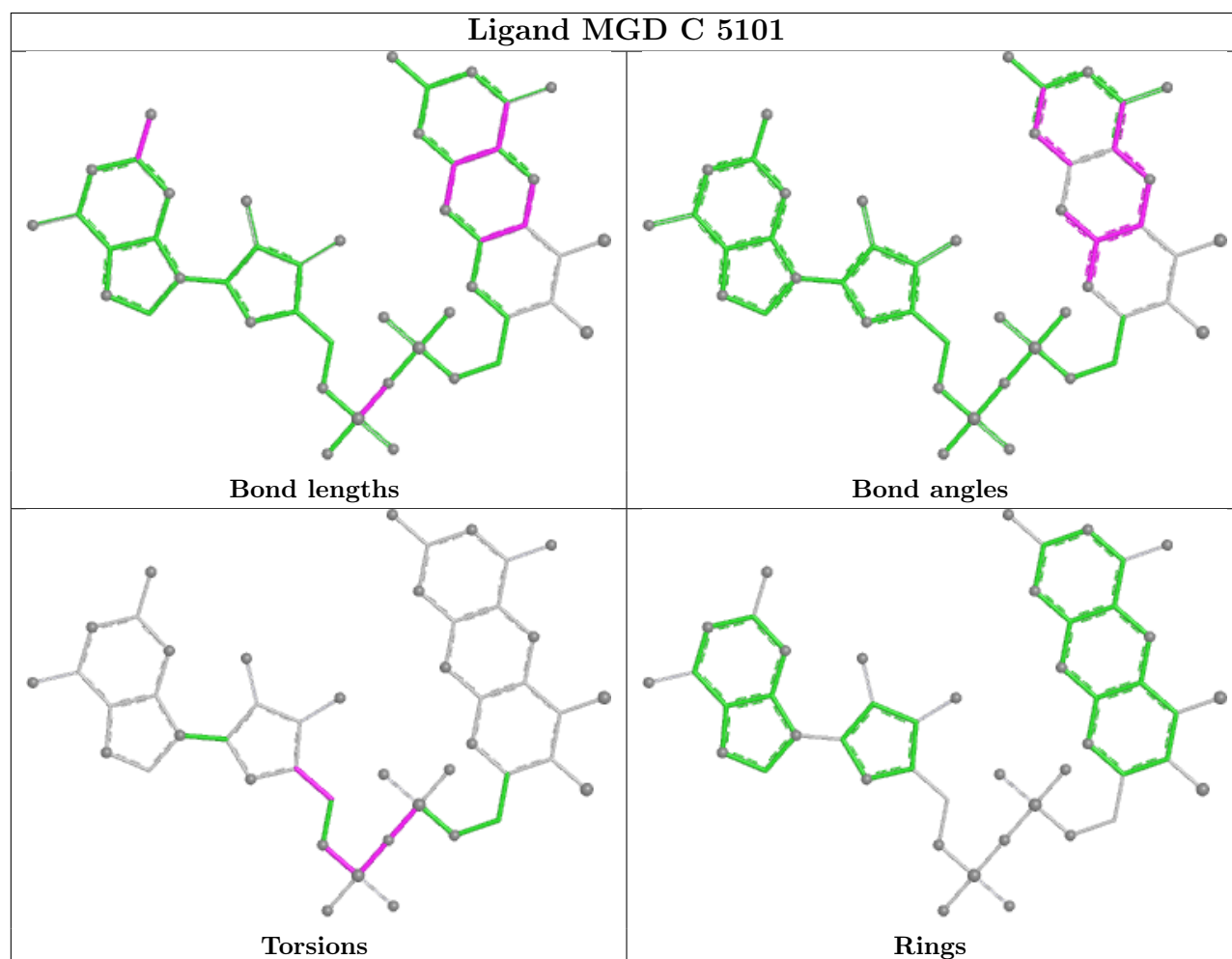
Mol	Chain	Res	Type	Atoms
5	A	5001	MGD	C5'-O5'-PB-O1B
5	A	5002	MGD	PA-O3B-PB-O5'
5	A	5002	MGD	C5'-O5'-PB-O1B
5	C	5101	MGD	PA-O3B-PB-O5'
5	C	5101	MGD	C5'-O5'-PB-O1B
5	C	5102	MGD	C5'-O5'-PB-O1B
5	C	5102	MGD	C5'-O5'-PB-O3B
5	E	5201	MGD	PA-O3B-PB-O5'
5	E	5201	MGD	C5'-O5'-PB-O1B
5	E	5202	MGD	C5'-O5'-PB-O1B
5	E	5202	MGD	C5'-O5'-PB-O3B
5	G	5301	MGD	PA-O3B-PB-O5'
5	G	5301	MGD	C5'-O5'-PB-O1B
5	G	5302	MGD	C5'-O5'-PB-O1B
5	G	5302	MGD	C5'-O5'-PB-O3B
5	A	5001	MGD	O4'-C4'-C5'-O5'
5	A	5001	MGD	PA-O3B-PB-O5'
5	C	5102	MGD	PA-O3B-PB-O5'
5	E	5202	MGD	PA-O3B-PB-O5'
5	G	5302	MGD	PA-O3B-PB-O5'
5	G	5301	MGD	O4'-C4'-C5'-O5'
5	C	5101	MGD	O4'-C4'-C5'-O5'
5	A	5002	MGD	C5'-O5'-PB-O2B
5	A	5002	MGD	C5'-O5'-PB-O3B
5	G	5302	MGD	C5'-O5'-PB-O2B
5	C	5101	MGD	C3'-C4'-C5'-O5'
5	A	5001	MGD	C3'-C4'-C5'-O5'
5	E	5201	MGD	O4'-C4'-C5'-O5'
5	G	5301	MGD	C3'-C4'-C5'-O5'
5	A	5001	MGD	PB-O3B-PA-O2A
5	C	5101	MGD	PB-O3B-PA-O2A
5	A	5002	MGD	PB-O3B-PA-O2A
5	C	5102	MGD	PB-O3B-PA-O2A
5	E	5202	MGD	PB-O3B-PA-O2A
5	G	5302	MGD	PB-O3B-PA-O2A

There are no ring outliers.

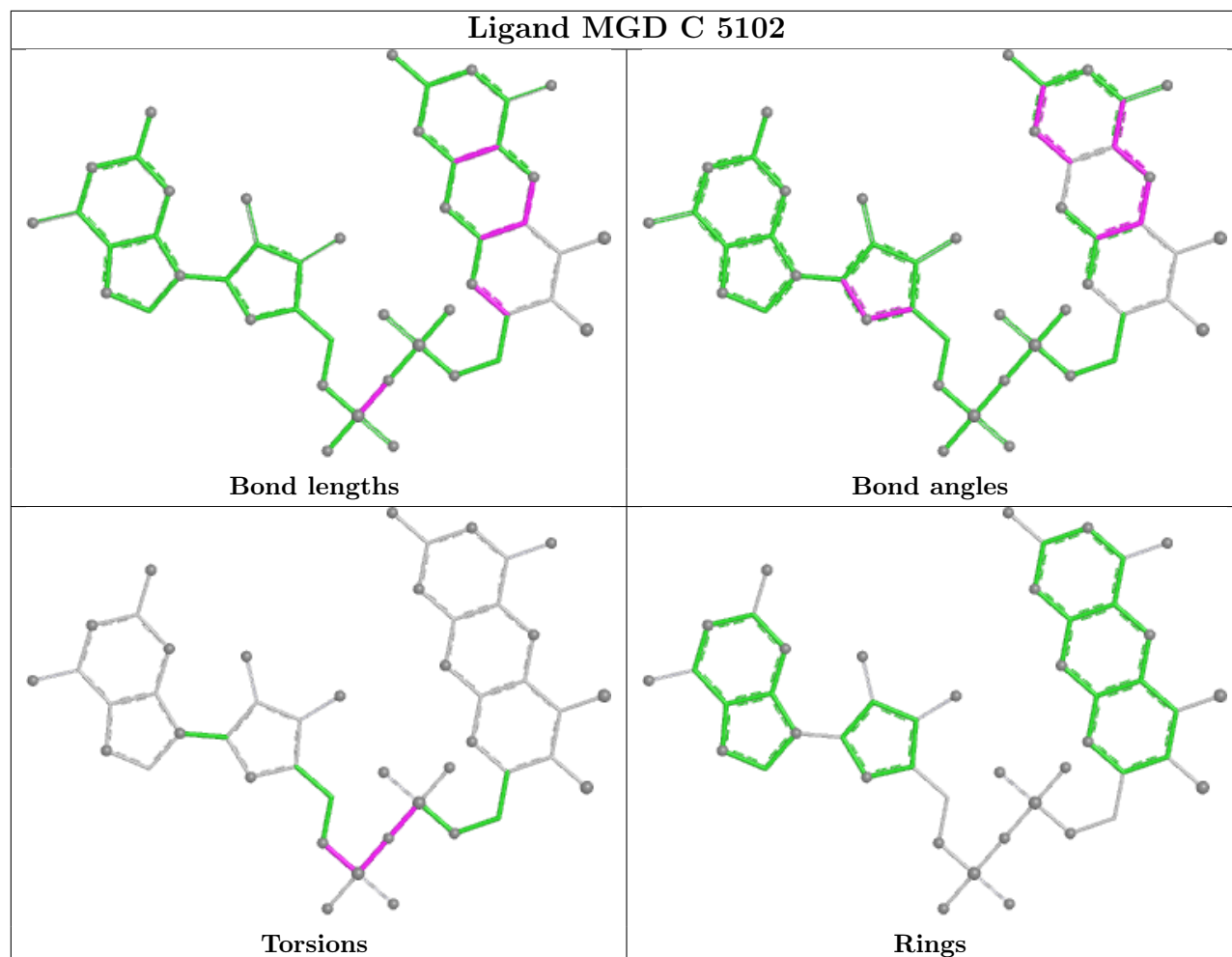
5 monomers are involved in 7 short contacts:

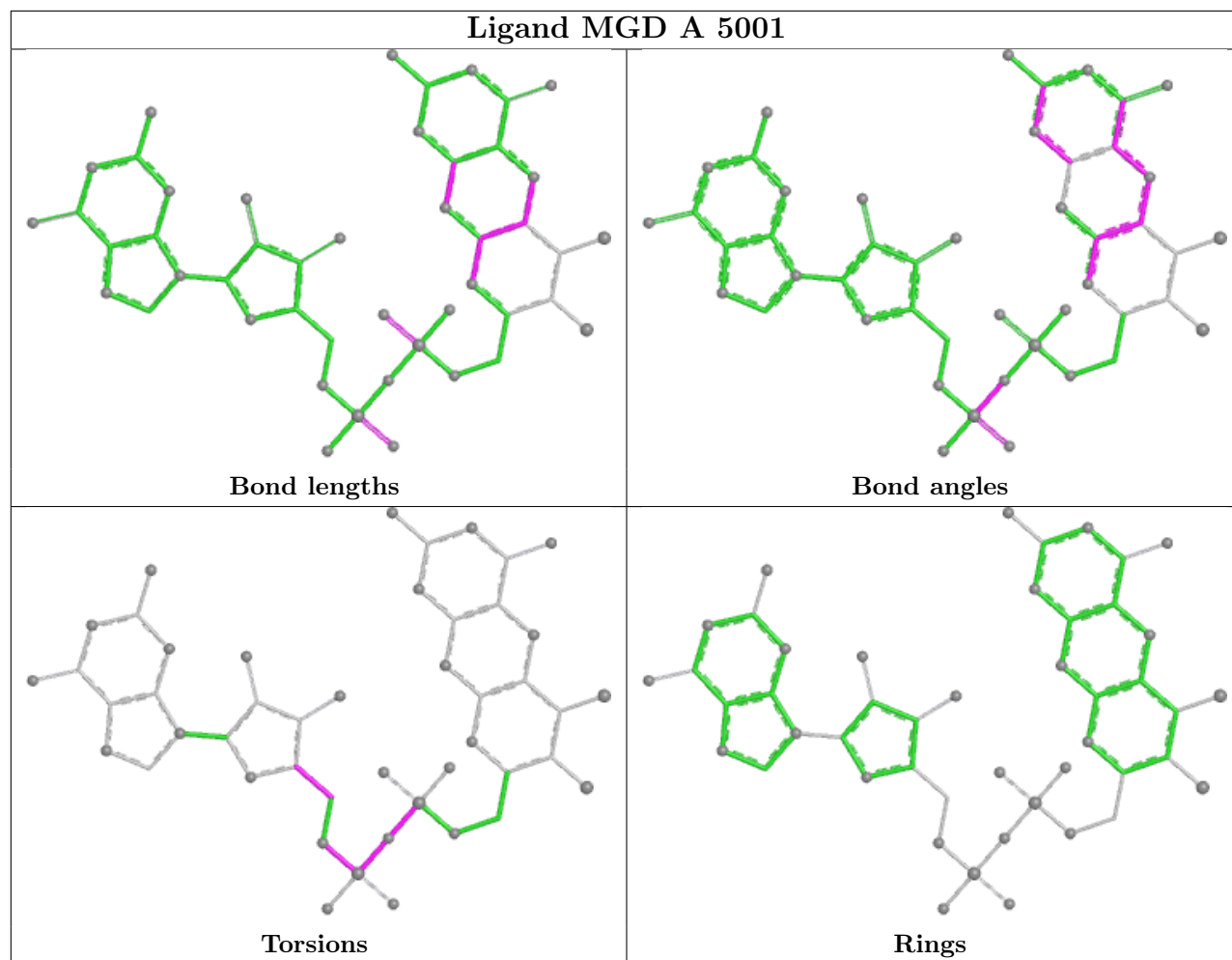
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	5101	MGD	2	0
5	A	5001	MGD	1	0
5	E	5201	MGD	2	0
5	G	5301	MGD	1	0
5	A	5002	MGD	1	0

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

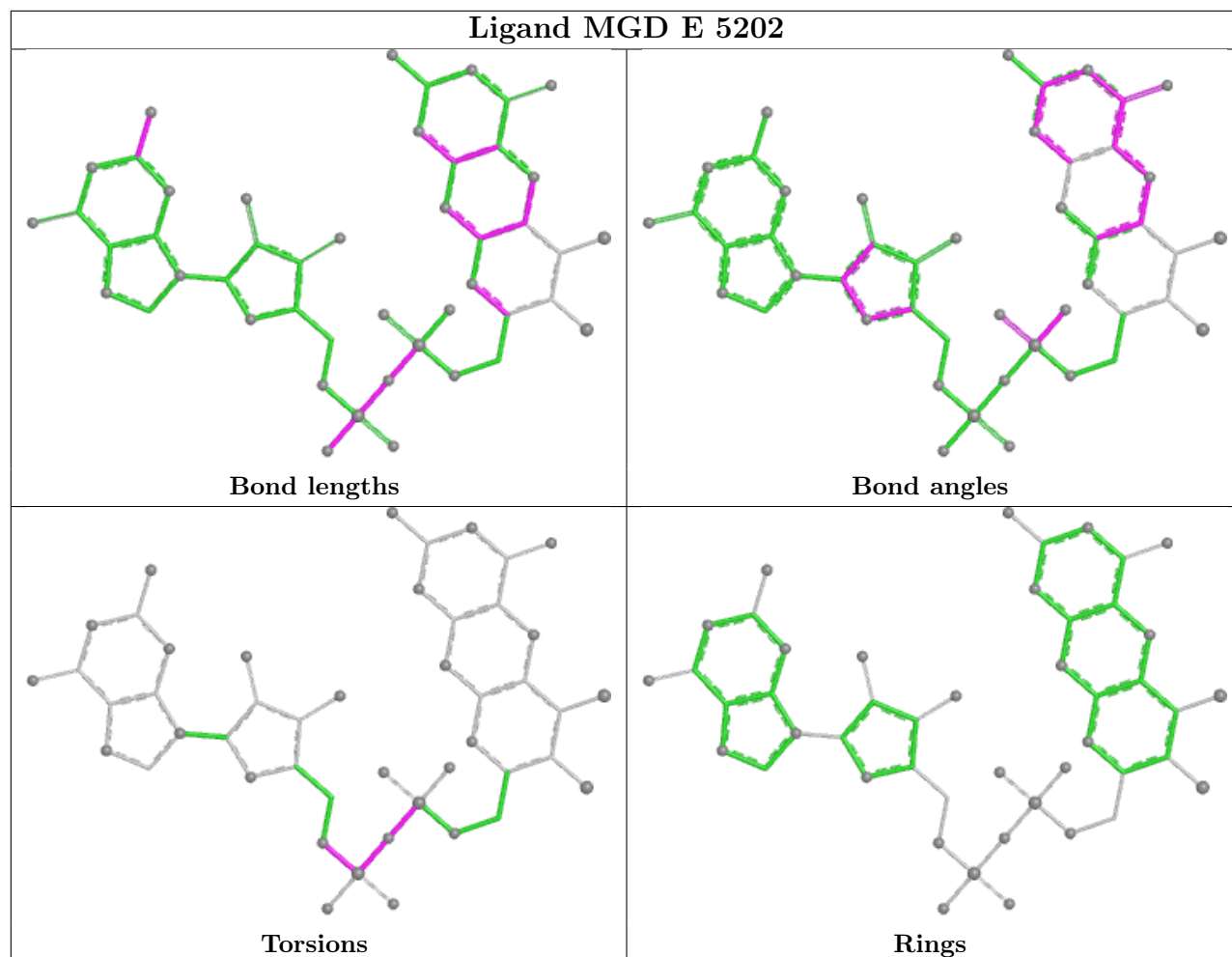


Ligand MGD C 5102

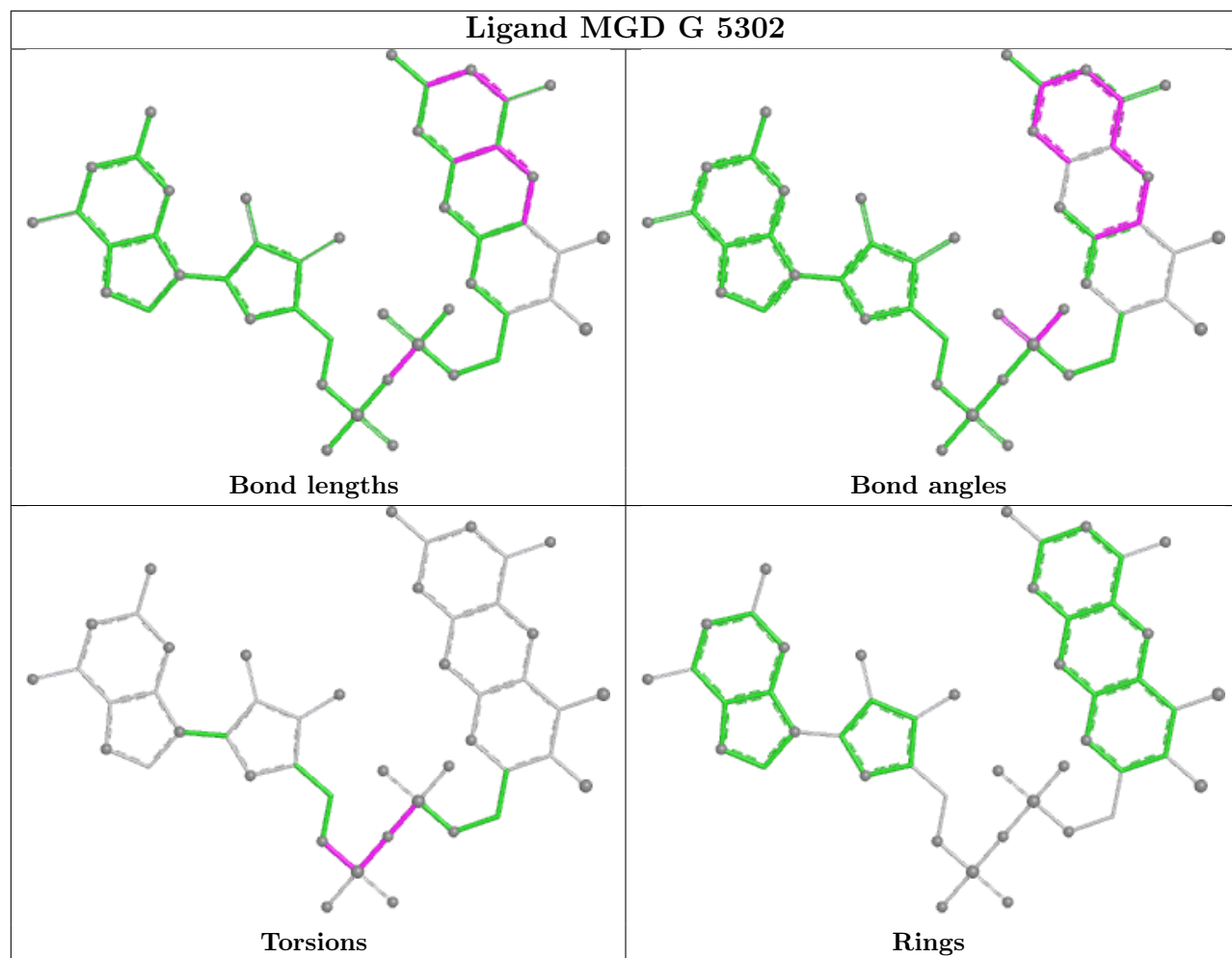




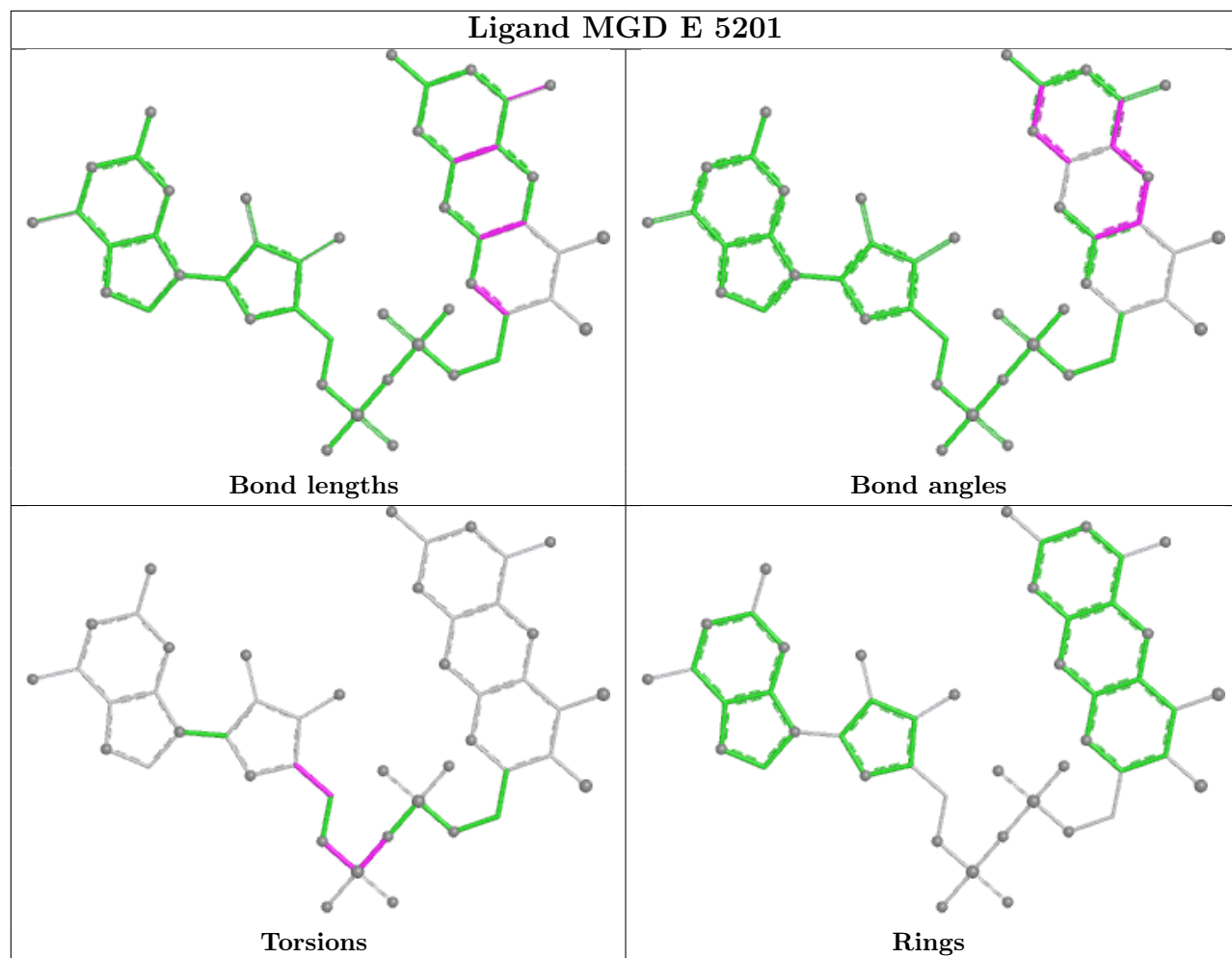
Ligand MGD E 5202



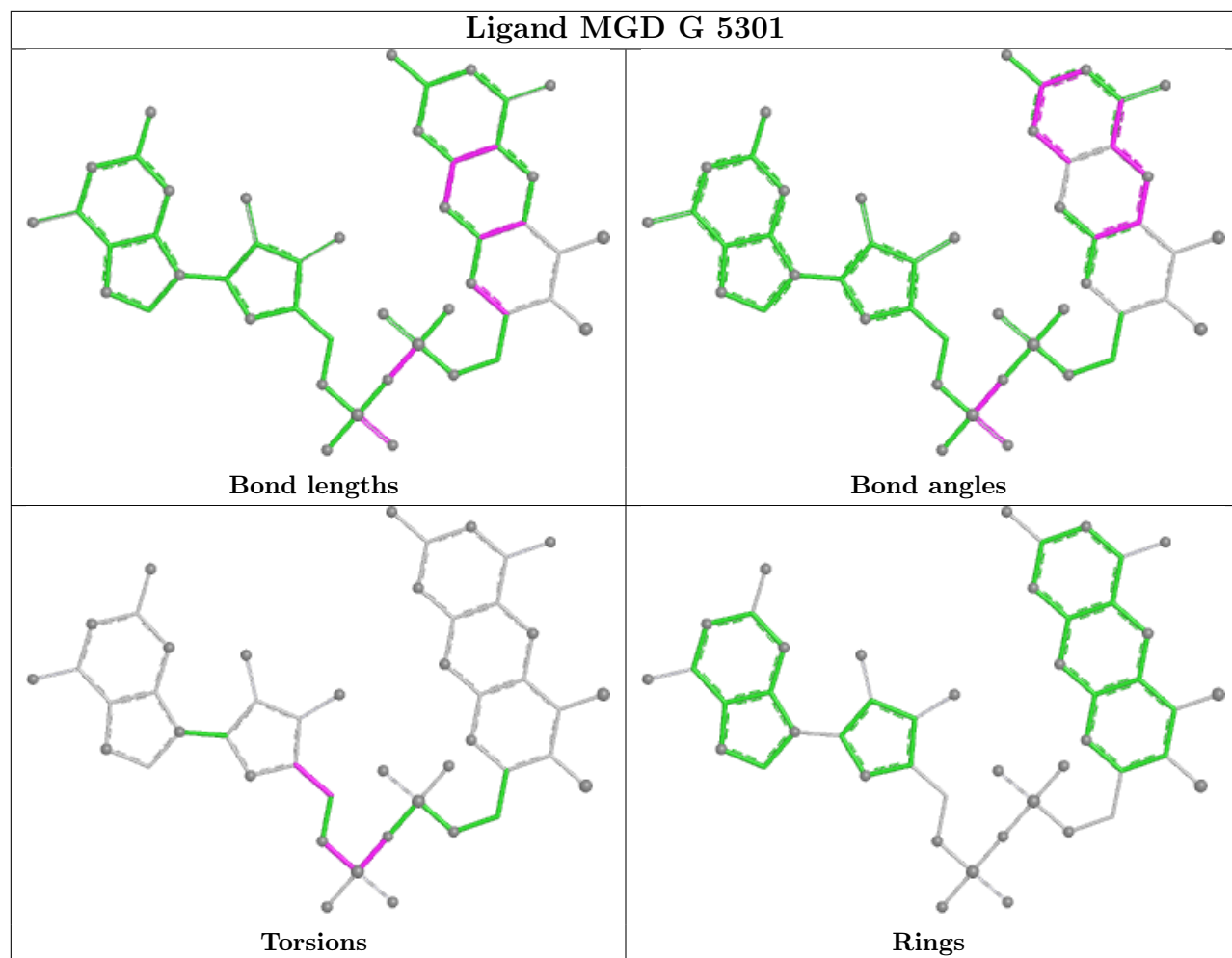
Ligand MGD G 5302

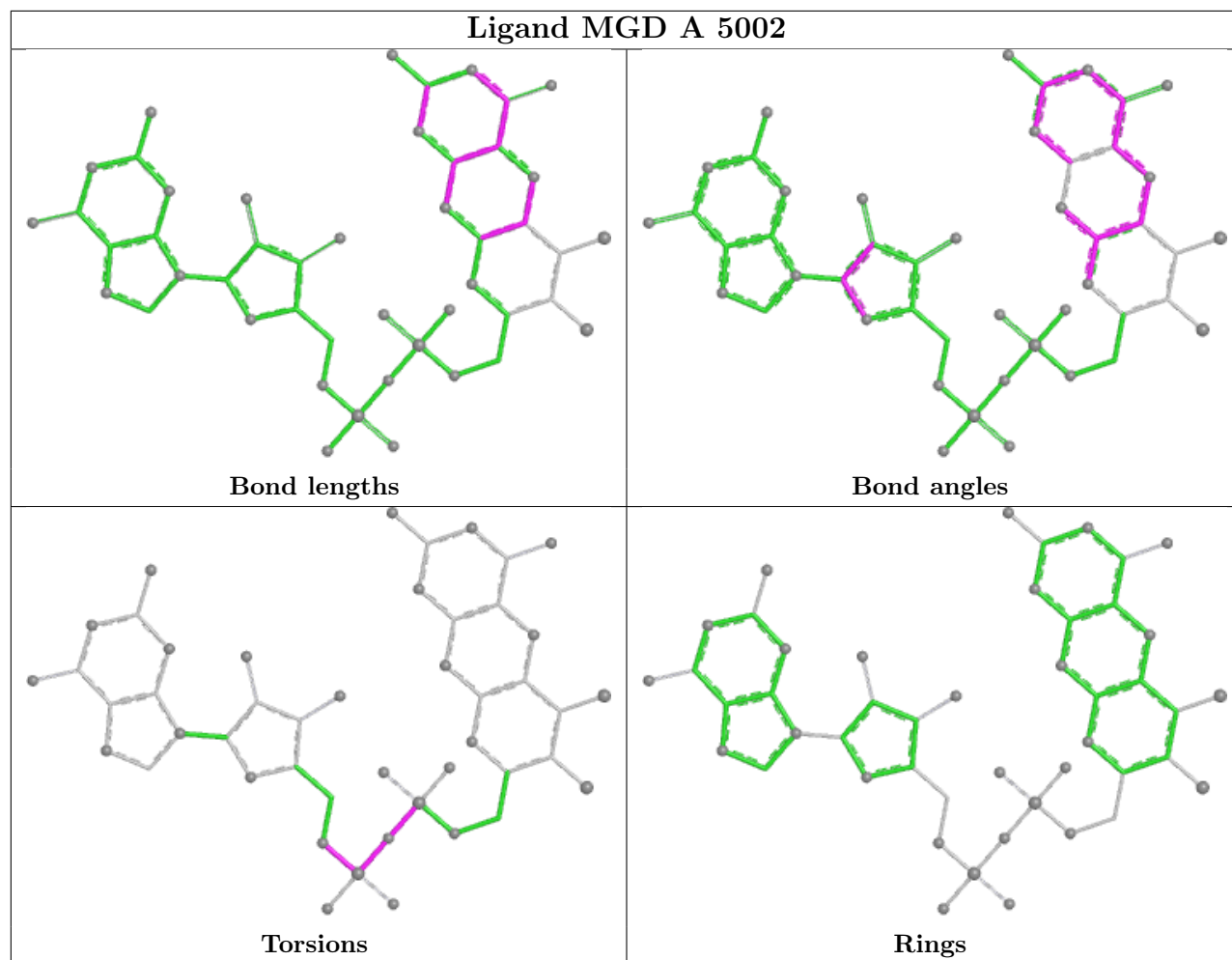


Ligand MGD E 5201



Ligand MGD G 5301





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	822/825 (99%)	-0.51	1 (0%) 92 92	9, 15, 24, 36	26 (3%)
1	C	822/825 (99%)	-0.66	1 (0%) 92 92	8, 13, 22, 30	23 (2%)
1	E	822/825 (99%)	-0.68	0 100 100	8, 13, 21, 31	28 (3%)
1	G	822/825 (99%)	-0.58	1 (0%) 92 92	9, 15, 23, 32	29 (3%)
2	B	133/133 (100%)	-0.60	0 100 100	10, 14, 20, 27	0
2	D	133/133 (100%)	-0.50	0 100 100	10, 14, 22, 28	1 (0%)
2	F	133/133 (100%)	-0.51	0 100 100	10, 14, 21, 27	1 (0%)
2	H	133/133 (100%)	-0.59	1 (0%) 82 86	10, 14, 20, 27	1 (0%)
All	All	3820/3832 (99%)	-0.60	4 (0%) 92 92	8, 14, 23, 36	109 (2%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	4	ASN	2.9
1	G	4	ASN	2.6
2	H	45	GLY	2.3
1	A	4	ASN	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 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(Å ²)	Q<0.9
3	HG	A	6009	1/1	0.95	0.09	29,29,29,29	1
9	EDO	A	7001	4/4	0.95	0.07	13,15,15,16	0
9	EDO	E	7009	4/4	0.95	0.07	14,16,17,18	0
3	HG	E	6011	1/1	0.96	0.08	29,29,29,29	1
9	EDO	E	7003	4/4	0.97	0.06	11,12,12,14	0
9	EDO	G	7004	4/4	0.97	0.06	12,13,13,15	0
6	O	E	5203	1/1	0.98	0.04	9,9,9,9	0
3	HG	C	6006	1/1	0.98	0.07	15,15,15,15	1
9	EDO	A	7005	4/4	0.98	0.04	12,14,14,15	0
9	EDO	C	7002	4/4	0.98	0.05	9,10,11,12	0
3	HG	C	6010	1/1	0.98	0.07	32,32,32,32	1
9	EDO	E	7007	4/4	0.98	0.04	11,12,12,14	0
3	HG	A	6005	1/1	0.98	0.07	18,18,18,18	1
6	O	A	5003	1/1	0.98	0.06	15,15,15,15	0
9	EDO	G	7008	4/4	0.98	0.04	13,14,14,15	0
5	MGD	A	5002	47/47	0.99	0.03	9,10,12,12	0
5	MGD	C	5101	47/47	0.99	0.04	8,10,12,12	0
5	MGD	C	5102	47/47	0.99	0.04	7,9,10,11	0
5	MGD	E	5201	47/47	0.99	0.03	8,9,10,11	0
5	MGD	E	5202	47/47	0.99	0.03	6,8,9,10	0
5	MGD	G	5301	47/47	0.99	0.03	7,10,12,12	0
5	MGD	G	5302	47/47	0.99	0.03	7,10,11,12	0
3	HG	E	6007	1/1	0.99	0.08	15,15,15,15	1
6	O	C	5103	1/1	0.99	0.04	10,10,10,10	0
3	HG	B	6001	1/1	0.99	0.06	14,14,14,14	1
3	HG	F	6003	1/1	0.99	0.06	13,13,13,13	1
3	HG	G	6008	1/1	0.99	0.07	17,17,17,17	1
3	HG	G	6012	1/1	0.99	0.08	30,30,30,30	1
9	EDO	C	7006	4/4	0.99	0.04	9,10,11,11	0
4	CA	C	5107	1/1	0.99	0.05	19,19,19,19	0
4	CA	C	5108	1/1	0.99	0.04	14,14,14,14	0
4	CA	G	5307	1/1	0.99	0.05	18,18,18,18	0
4	CA	G	5308	1/1	0.99	0.03	13,13,13,13	0
5	MGD	A	5001	47/47	0.99	0.04	10,11,13,13	0
7	4MO	E	5204	1/1	1.00	0.02	10,10,10,10	0
7	4MO	G	5304	1/1	1.00	0.02	12,12,12,12	0
8	F3S	A	5005	7/7	1.00	0.02	9,10,11,11	0

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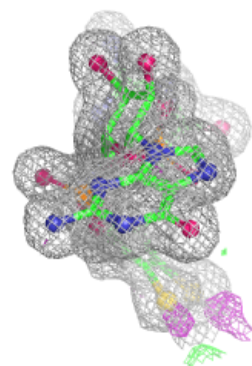
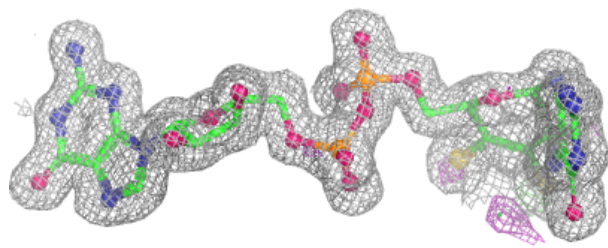
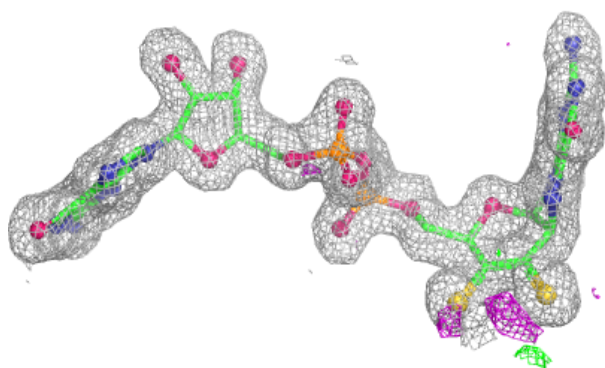
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	F3S	C	5105	7/7	1.00	0.01	6,8,9,10	0
8	F3S	E	5205	7/7	1.00	0.01	8,8,8,9	0
8	F3S	G	5305	7/7	1.00	0.02	9,10,10,10	0
4	CA	A	5008	1/1	1.00	0.04	12,12,12,12	0
3	HG	D	6002	1/1	1.00	0.07	14,14,14,14	1
3	HG	H	6004	1/1	1.00	0.06	13,13,13,13	1
4	CA	E	5207	1/1	1.00	0.04	18,18,18,18	0
4	CA	E	5208	1/1	1.00	0.03	12,12,12,12	0
4	CA	A	5007	1/1	1.00	0.04	18,18,18,18	0
6	O	G	5303	1/1	1.00	0.03	12,12,12,12	0
7	4MO	A	5004	1/1	1.00	0.01	12,12,12,12	0
7	4MO	C	5104	1/1	1.00	0.01	10,10,10,10	0
10	FES	B	5006	4/4	1.00	0.02	11,11,12,12	0
10	FES	D	5106	4/4	1.00	0.01	11,11,12,12	0
10	FES	F	5206	4/4	1.00	0.01	11,11,11,11	0
10	FES	H	5306	4/4	1.00	0.02	11,12,12,13	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.

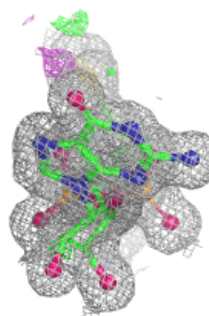
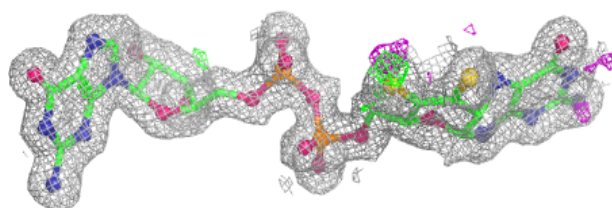
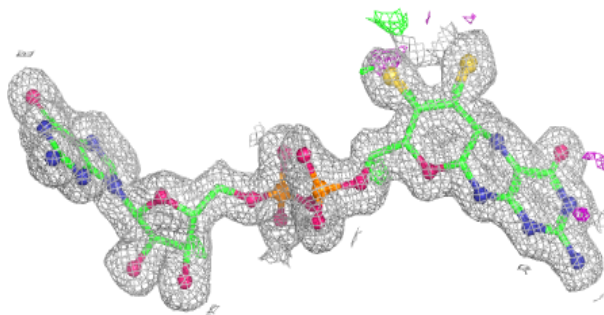
Electron density around MGD A 5002:

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

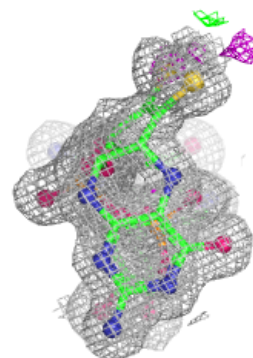
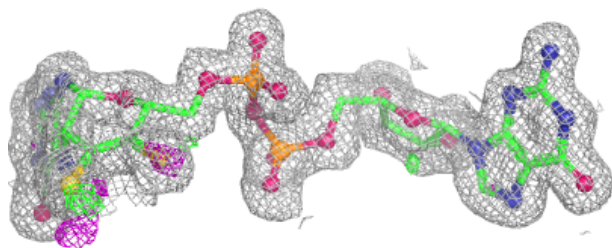
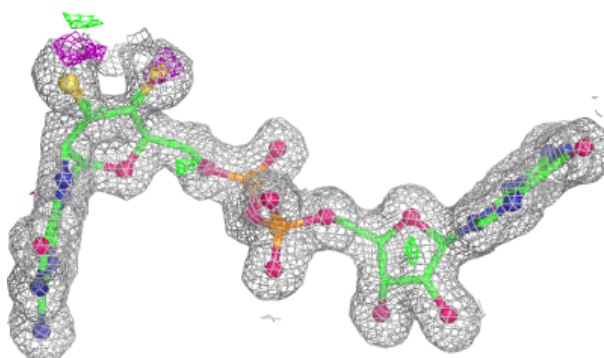


Electron density around MGD C 5101:

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

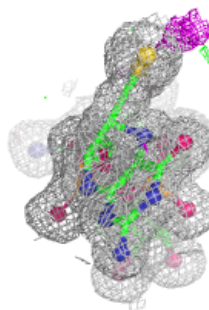
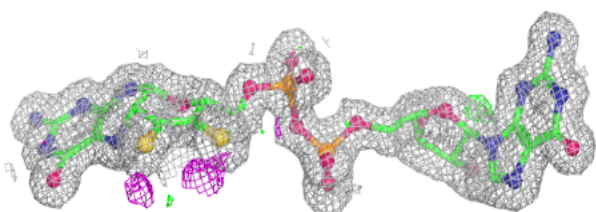
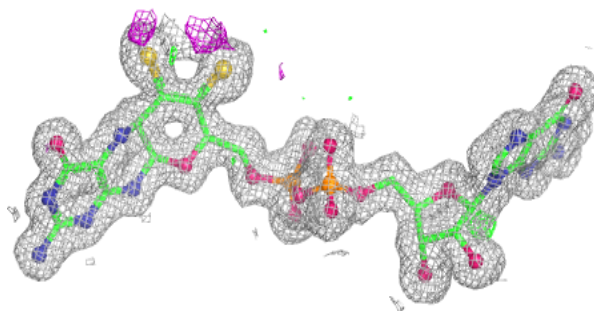
**Electron density around MGD C 5102:**

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

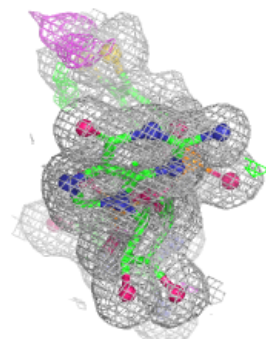
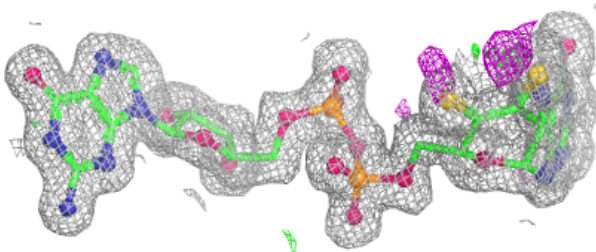
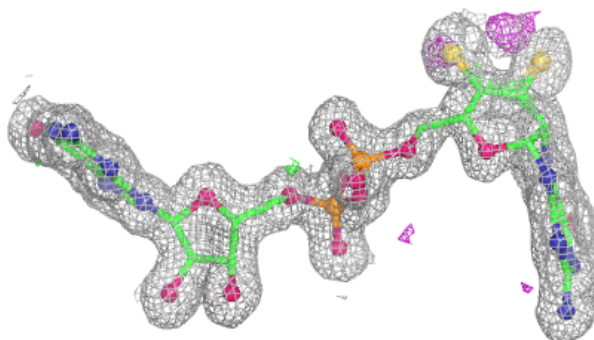


Electron density around MGD E 5201:

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

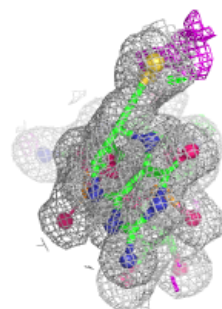
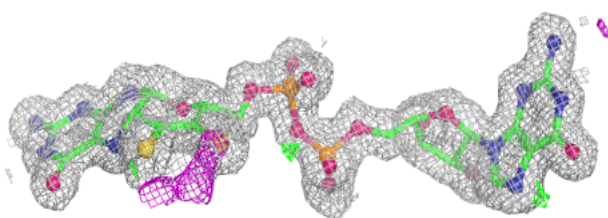
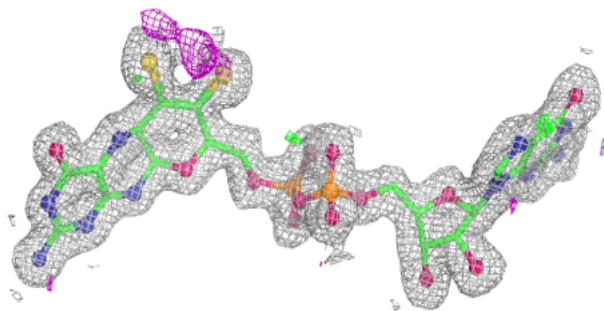
**Electron density around MGD E 5202:**

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

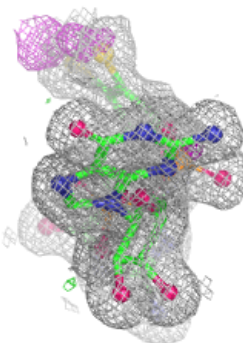
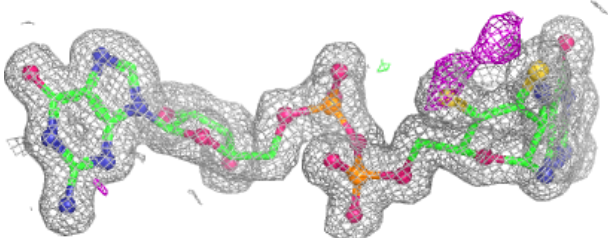
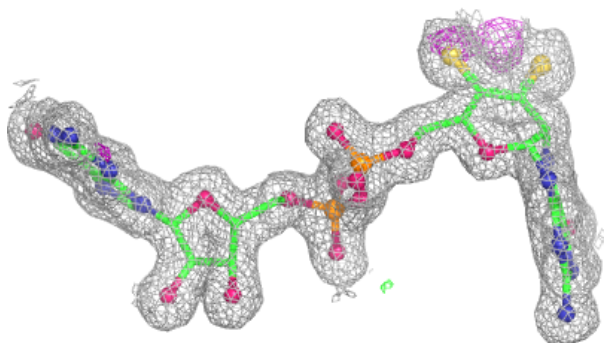


Electron density around MGD G 5301:

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

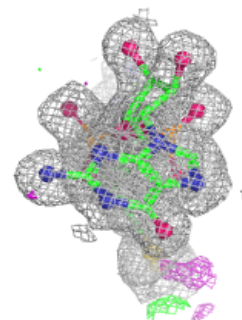
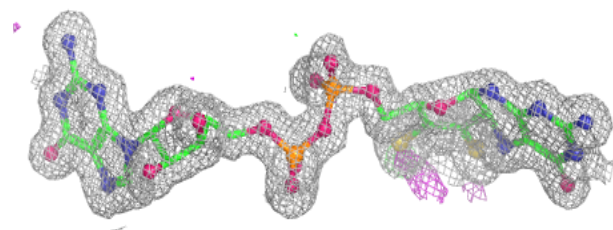
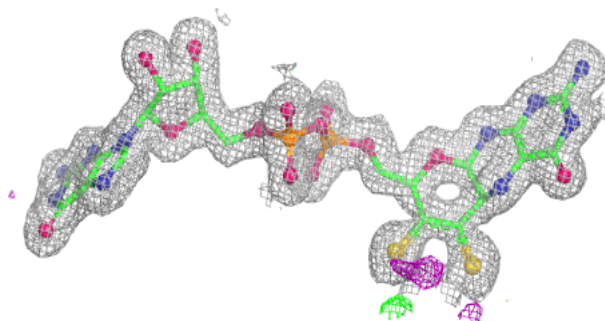
**Electron density around MGD G 5302:**

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



Electron density around MGD A 5001:

$2mF_o-DF_c$ (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.