



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:01 PM UTC

PDB ID : 5NQD / pdb_00005nqd
Title : Arsenite oxidase AioAB from Rhizobium sp. str. NT-26 mutant AioBF108A
Authors : Santos-Silva, T.; Romao, M.; Vieira, M.; Marques, A.T.
Deposited on : 2017-04-20
Resolution : 2.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

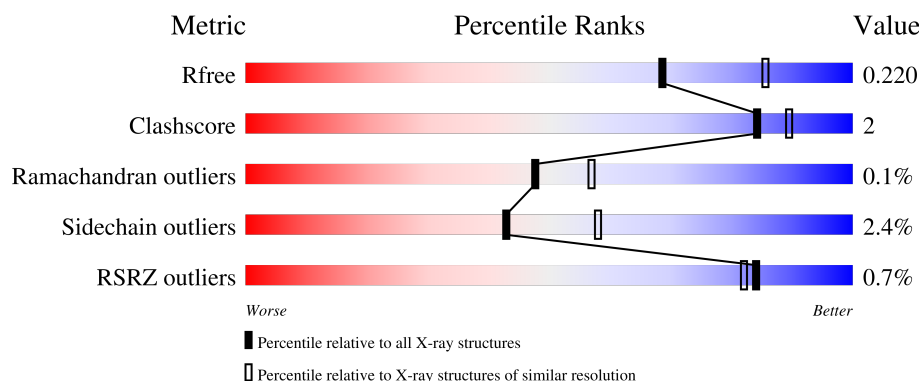
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.



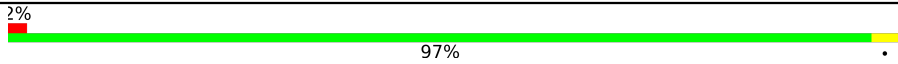
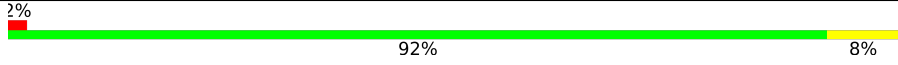
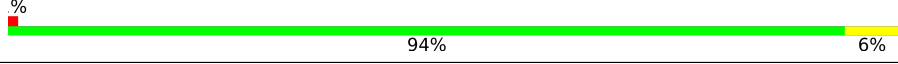
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	843	92% 7%
1	C	843	93% 6%
1	E	843	93% 6%
1	G	843	92% 7%
2	B	132	97%

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Mol	Chain	Length	Quality of chain
2	D	132	
2	F	132	
2	H	132	

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
11	EDO	G	2012	-	-	-	X
9	GOL	A	2011	-	X	-	-
9	GOL	G	2010	-	X	-	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 32195 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 AroA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	843	Total	C	N	O	S	0	0	0
			6545	4088	1167	1253	37			
1	C	843	Total	C	N	O	S	0	0	0
			6545	4088	1167	1253	37			
1	E	843	Total	C	N	O	S	0	0	0
			6545	4088	1167	1253	37			
1	G	843	Total	C	N	O	S	0	0	0
			6545	4088	1167	1253	37			

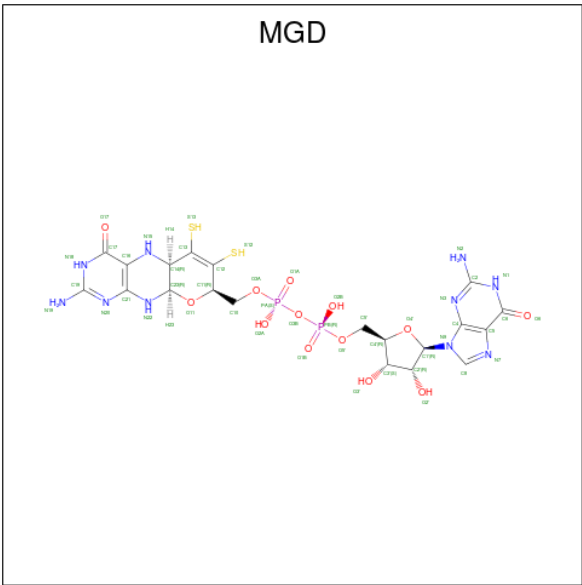
- Molecule 2 is a protein called Arsenite oxidase small subunit AioB Rieske [2Fe-2S] cluster.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	132	Total	C	N	O	S	0	0	0
			989	623	166	198	2			
2	D	132	Total	C	N	O	S	0	0	0
			989	623	166	198	2			
2	F	132	Total	C	N	O	S	0	0	0
			989	623	166	198	2			
2	H	132	Total	C	N	O	S	0	0	0
			989	623	166	198	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	108	ALA	PHE	conflict	UNP L0NMC5
D	108	ALA	PHE	conflict	UNP L0NMC5
F	108	ALA	PHE	conflict	UNP L0NMC5
H	108	ALA	PHE	conflict	UNP L0NMC5

- Molecule 3 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
3	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
3	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
3	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
3	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
3	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
3	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
3	G	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
3	G	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

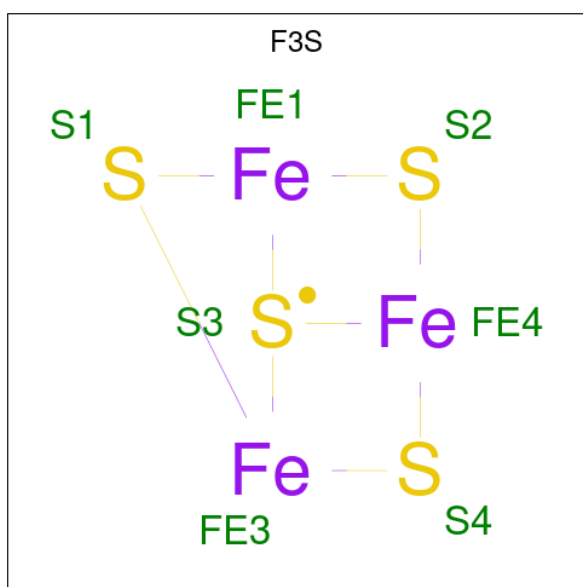
- Molecule 4 is OXYGEN ATOM (CCD ID: O) (formula: O).

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

- Molecule 5 is MOLYBDENUM(IV) ION (CCD ID: 4MO) (formula: Mo).

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

- Molecule 6 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe₃S₄).



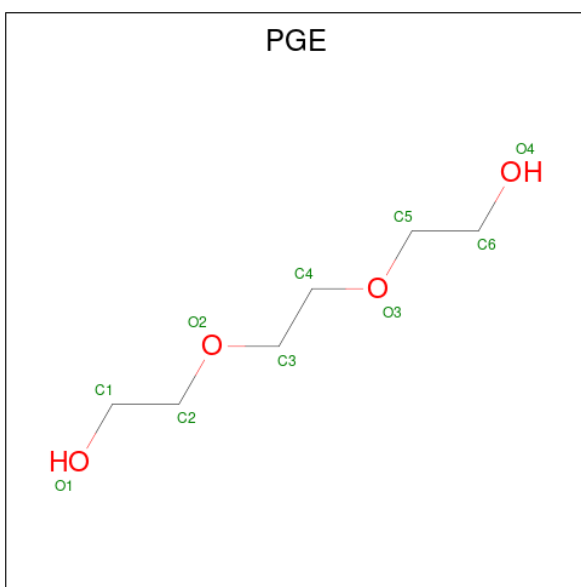
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 7	Fe 3	S 4	0	0
6	C	1	Total 7	Fe 3	S 4	0	0
6	E	1	Total 7	Fe 3	S 4	0	0
6	G	1	Total 7	Fe 3	S 4	0	0

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



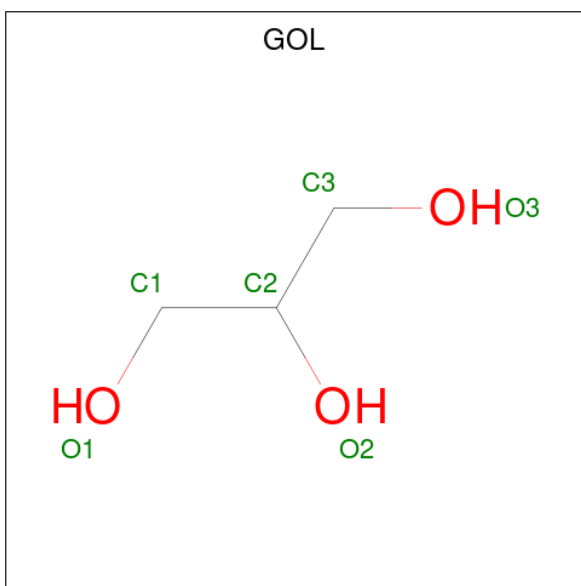
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	G	1	Total	O	S	0	0
			5	4	1		
7	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



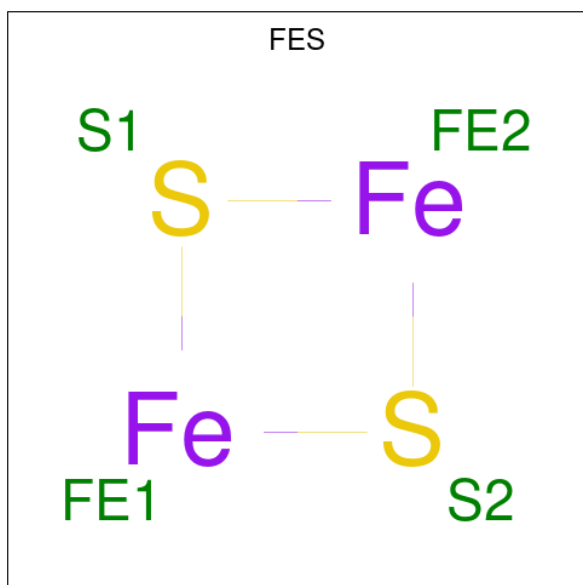
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		
9	C	1	Total	C	O	0	0
			6	3	3		
9	E	1	Total	C	O	0	0
			6	3	3		

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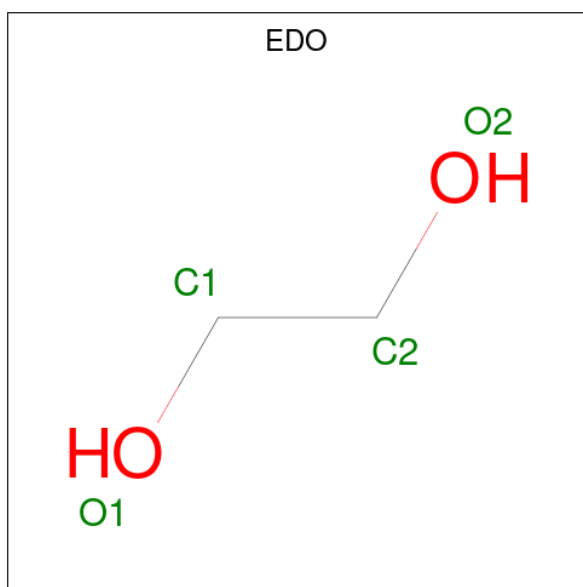
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	G	1	Total	C	O	0	0
			6	3	3		
9	G	1	Total	C	O	0	0
			6	3	3		

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



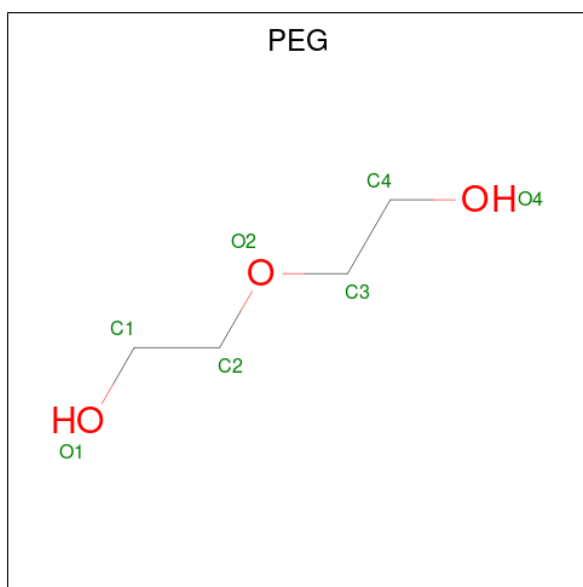
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	0
			4	2	2		
10	D	1	Total	Fe	S	0	0
			4	2	2		
10	F	1	Total	Fe	S	0	0
			4	2	2		
10	H	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 11 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



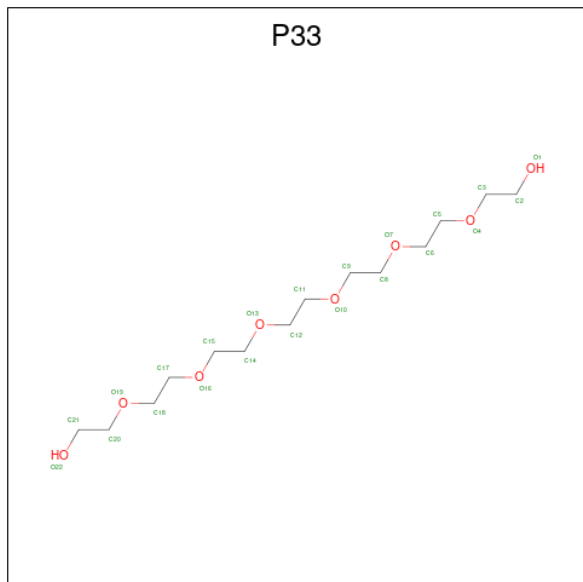
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			4	2	2		
11	C	1	Total	C	O	0	0
			4	2	2		
11	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 12 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 13 is 3,6,9,12,15,18-HEXAOXAICOSANE-1,20-DIOL (CCD ID: P33) (formula: $C_{14}H_{30}O_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	G	1	Total	C	O	0	0
			22	14	8		
13	G	1	Total	C	O	0	0
			22	14	8		

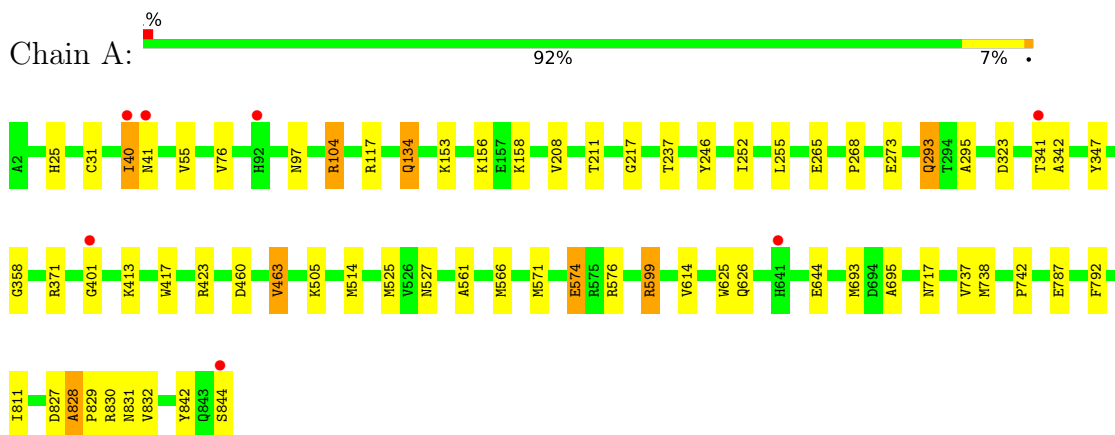
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	383	Total	O	0	0
			383	383		
14	B	25	Total	O	0	0
			25	25		
14	C	308	Total	O	0	0
			308	308		
14	D	33	Total	O	0	0
			33	33		
14	E	284	Total	O	0	0
			284	284		
14	F	25	Total	O	0	0
			25	25		
14	G	374	Total	O	0	0
			374	374		
14	H	36	Total	O	0	0
			36	36		

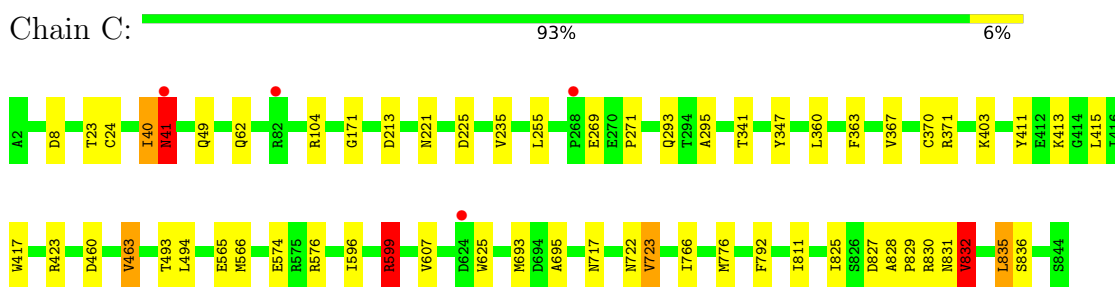
3 Residue-property plots

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.

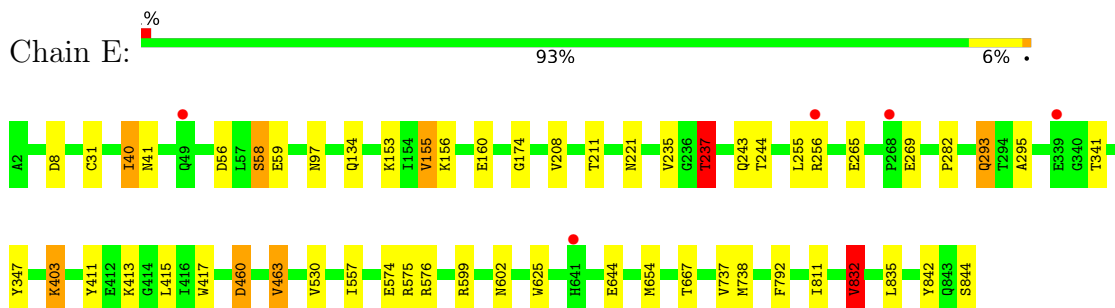
• Molecule 1: AroA



• Molecule 1: AroA

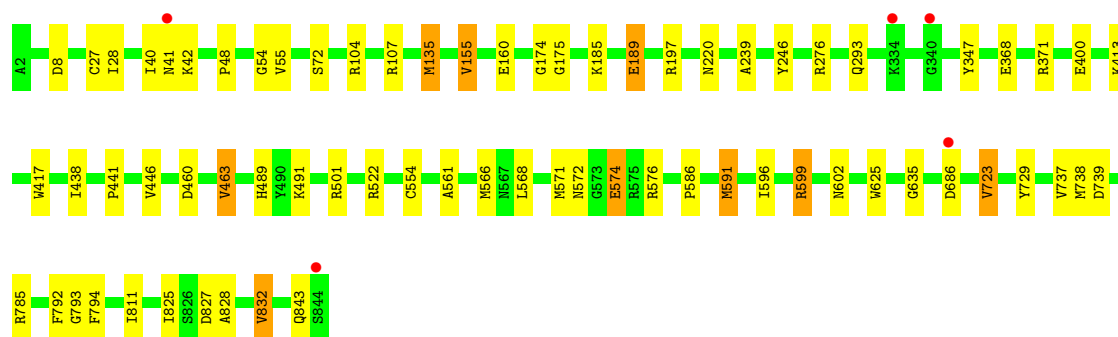


• Molecule 1: AroA



• Molecule 1: AroA





- Molecule 2: Arsenite oxidase small subunit AioB Rieske [2Fe-2S] cluster

Chain B: 97% .



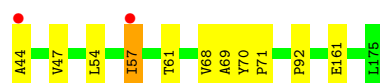
- Molecule 2: Arsenite oxidase small subunit AioB Rieske [2Fe-2S] cluster

Chain D: 97% .



- Molecule 2: Arsenite oxidase small subunit AioB Rieske [2Fe-2S] cluster

Chain F: 92% 8% .



- Molecule 2: Arsenite oxidase small subunit AioB Rieske [2Fe-2S] cluster

Chain H: 94% 6% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	141.41Å 148.66Å 232.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.55 – 2.20 49.55 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.55-2.20) 100.0 (49.55-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.172 , 0.217 0.179 , 0.220	Depositor DCC
R_{free} test set	12218 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 27.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	32195	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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: SO4, FES, 4MO, O, EDO, PGE, F3S, P33, MGD, PEG, 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	1.07	1/6693 (0.0%)	1.05	13/9068 (0.1%)
1	C	1.08	3/6693 (0.0%)	1.09	13/9068 (0.1%)
1	E	1.06	2/6693 (0.0%)	1.06	6/9068 (0.1%)
1	G	1.05	3/6693 (0.0%)	1.06	12/9068 (0.1%)
2	B	0.94	0/1011	0.93	0/1378
2	D	0.97	0/1011	0.95	0/1378
2	F	0.97	0/1011	0.99	0/1378
2	H	0.99	0/1011	0.97	1/1378 (0.1%)
All	All	1.06	9/30816 (0.0%)	1.05	45/41784 (0.1%)

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	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	41	ASN	N-CA	8.05	1.55	1.46
1	G	175	GLY	C-O	6.92	1.28	1.23
1	A	252	ILE	CA-C	6.30	1.59	1.52
1	C	171	GLY	N-CA	6.15	1.50	1.44
1	G	591	MET	N-CA	-5.83	1.41	1.45
1	E	460	ASP	C-O	-5.29	1.17	1.24
1	C	271	PRO	CA-C	5.21	1.59	1.52
1	E	40	ILE	CA-CB	5.07	1.59	1.54
1	G	41	ASN	N-CA	5.03	1.53	1.46

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	723	VAL	CB-CA-C	-7.89	99.47	112.26
1	E	237	THR	CB-CA-C	-7.59	94.33	109.35
1	G	723	VAL	CB-CA-C	-7.49	100.13	112.26
1	C	40	ILE	CA-C-N	-7.47	113.24	126.45
1	C	40	ILE	C-N-CA	-7.47	113.24	126.45
1	A	828	ALA	CA-C-N	-7.28	112.82	120.03
1	A	828	ALA	C-N-CA	-7.28	112.82	120.03
1	G	832	VAL	N-CA-CB	-6.99	103.28	112.36
1	C	599	ARG	NE-CZ-NH2	-6.87	113.02	119.20
1	G	40	ILE	CA-C-N	-6.54	112.77	123.05
1	G	40	ILE	C-N-CA	-6.54	112.77	123.05
1	G	635	GLY	N-CA-C	6.46	116.09	110.21
1	A	268	PRO	N-CA-C	-6.46	102.18	111.22
1	A	104	ARG	NE-CZ-NH2	-6.24	113.59	119.20
1	C	40	ILE	N-CA-C	-6.23	99.93	109.78
1	A	574	GLU	N-CA-CB	-6.12	100.89	110.98
2	H	139	GLY	N-CA-C	5.91	119.37	110.75
1	C	40	ILE	O-C-N	-5.86	116.59	122.62
1	C	565	GLU	N-CA-C	-5.73	106.29	113.28
1	G	41	ASN	N-CA-C	5.65	119.75	112.86
1	G	246	TYR	N-CA-C	-5.60	105.09	111.14
1	G	104	ARG	NE-CZ-NH2	-5.54	114.21	119.20
1	G	239	ALA	N-CA-C	5.51	118.05	111.71
1	A	217	GLY	N-CA-C	-5.48	104.95	111.36
1	C	835	LEU	N-CA-C	5.45	118.35	110.28
1	C	825	ILE	CB-CA-C	-5.44	105.30	111.55
1	A	40	ILE	CA-C-N	-5.39	115.68	125.66
1	A	40	ILE	C-N-CA	-5.39	115.68	125.66
1	A	599	ARG	CG-CD-NE	-5.38	100.16	112.00
1	A	134	GLN	CB-CA-C	-5.36	100.67	111.17
1	C	599	ARG	NE-CZ-NH1	5.33	126.83	121.50
1	E	282	PRO	CB-CA-C	-5.32	104.29	111.85
1	E	832	VAL	N-CA-CB	-5.29	105.48	112.36
1	G	825	ILE	CB-CA-C	-5.21	105.10	111.92
1	C	832	VAL	N-CA-CB	-5.16	105.45	112.16
1	E	40	ILE	CA-C-N	-5.14	116.16	125.66
1	E	40	ILE	C-N-CA	-5.14	116.16	125.66
1	A	246	TYR	N-CA-C	-5.12	105.78	111.36
1	G	135	MET	CG-SD-CE	-5.11	89.67	100.90
1	G	574	GLU	N-CA-CB	-5.10	102.57	110.98
1	A	614	VAL	N-CA-C	5.08	115.85	110.72
1	C	8	ASP	CB-CA-C	-5.06	99.42	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	ILE	N-CA-C	-5.04	101.82	109.78
1	E	244	THR	N-CA-C	5.01	117.13	111.02
1	C	596	ILE	N-CA-C	-5.00	105.62	110.42

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	401	GLY	Peptide

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	6545	0	6296	35	0
1	C	6545	0	6296	30	0
1	E	6545	0	6296	24	0
1	G	6545	0	6296	32	1
2	B	989	0	943	1	0
2	D	989	0	943	3	0
2	F	989	0	943	6	0
2	H	989	0	943	4	0
3	A	94	0	44	1	0
3	C	94	0	44	1	0
3	E	94	0	44	1	0
3	G	94	0	44	2	0
4	A	1	0	0	1	0
4	C	1	0	0	1	0
4	E	1	0	0	0	0
4	G	1	0	0	1	0
5	A	1	0	0	1	0
5	C	1	0	0	1	0
5	E	1	0	0	0	0
5	G	1	0	0	1	0
6	A	7	0	0	0	0
6	C	7	0	0	0	0
6	E	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	7	0	0	0	0
7	A	20	0	0	1	0
7	C	20	0	0	0	0
7	E	10	0	0	0	0
7	G	10	0	0	0	0
8	A	10	0	14	0	0
9	A	6	0	8	0	0
9	C	6	0	8	0	0
9	E	6	0	8	0	0
9	G	12	0	16	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	B	4	0	6	0	0
11	C	4	0	6	0	0
11	G	4	0	6	0	0
12	C	7	0	10	0	0
13	G	44	0	60	3	0
14	A	383	0	0	6	0
14	B	25	0	0	0	0
14	C	308	0	0	3	0
14	D	33	0	0	1	0
14	E	284	0	0	0	0
14	F	25	0	0	1	0
14	G	374	0	0	6	1
14	H	36	0	0	0	0
All	All	32195	0	29274	136	2

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 (136) 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:574:GLU:OE1	1:E:576:ARG:NH1	1.95	1.00
4:G:2003:O:O	5:G:2004:4MO:MO	1.35	0.97
1:A:566:MET:HE1	14:A:2104:HOH:O	1.75	0.87
1:G:574:GLU:OE1	1:G:576:ARG:NH1	2.08	0.86
1:G:599:ARG:NH1	1:G:602:ASN:OD1	2.10	0.85
1:G:566:MET:HE1	14:G:2118:HOH:O	1.75	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:574:GLU:OE1	1:C:576:ARG:NH1	2.09	0.84
1:A:265:GLU:OE1	14:A:2101:HOH:O	1.96	0.82
1:A:358:GLY:HA3	1:A:693:MET:HE3	1.62	0.82
1:G:522:ARG:NH1	14:G:2101:HOH:O	2.11	0.81
1:C:423:ARG:HA	1:C:693:MET:HE1	1.62	0.79
1:A:574:GLU:OE1	1:A:576:ARG:NH1	2.19	0.75
1:C:832:VAL:HG22	1:C:835:LEU:HD22	1.68	0.74
1:A:413:LYS:HD2	1:A:417:TRP:NE1	2.04	0.73
4:C:2003:O:O	5:C:2004:4MO:MO	1.61	0.71
1:G:135:MET:HE1	1:G:554:CYS:O	1.90	0.70
4:A:2003:O:O	5:A:2004:4MO:MO	1.63	0.70
1:C:413:LYS:HD2	1:C:417:TRP:NE1	2.07	0.69
1:A:787:GLU:OE1	14:A:2102:HOH:O	2.10	0.69
1:C:693:MET:HE2	1:C:695:ALA:HB2	1.77	0.66
1:A:599:ARG:NH2	1:A:625:TRP:O	2.25	0.66
1:G:413:LYS:HD2	1:G:417:TRP:NE1	2.11	0.65
1:G:739:ASP:OD1	14:G:2102:HOH:O	2.14	0.65
1:G:599:ARG:NH2	1:G:625:TRP:O	2.32	0.63
13:G:2008:P33:H91	14:G:2433:HOH:O	1.99	0.61
1:E:56:ASP:OD1	1:E:58:SER:OG	2.17	0.60
1:C:423:ARG:HA	1:C:693:MET:CE	2.30	0.60
2:F:70:TYR:CD1	2:F:71:PRO:HA	2.36	0.60
1:A:40:ILE:O	1:A:41:ASN:HB2	2.02	0.60
1:A:423:ARG:HA	1:A:693:MET:HE1	1.83	0.60
1:C:566:MET:HE1	14:C:2103:HOH:O	2.02	0.59
1:C:776:MET:SD	1:C:832:VAL:HG21	2.42	0.59
1:C:829:PRO:HB2	1:C:831:ASN:OD1	2.04	0.58
1:A:413:LYS:HD2	1:A:417:TRP:CE2	2.39	0.57
1:E:40:ILE:O	1:E:41:ASN:HB2	2.05	0.56
1:G:8:ASP:HB3	2:H:47:VAL:HG21	1.87	0.55
2:H:54:LEU:HD11	2:H:160:ALA:HB2	1.87	0.55
1:A:25:HIS:HD2	14:A:2108:HOH:O	1.88	0.55
1:A:323:ASP:OD2	1:A:371:ARG:NH2	2.39	0.54
1:C:413:LYS:HD2	1:C:417:TRP:CE2	2.42	0.54
1:C:40:ILE:O	1:C:41:ASN:CG	2.50	0.54
1:G:501:ARG:NH2	14:G:2107:HOH:O	2.41	0.53
1:E:832:VAL:HG22	1:E:835:LEU:HD22	1.90	0.53
1:E:415:LEU:HD23	1:E:415:LEU:C	2.33	0.53
1:G:571:MET:HE1	13:G:2008:P33:H112	1.91	0.53
1:A:423:ARG:HA	1:A:693:MET:CE	2.38	0.53
1:A:574:GLU:OE2	14:A:2103:HOH:O	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:ASP:O	1:A:828:ALA:C	2.52	0.53
2:F:57:ILE:HD11	2:F:92:PRO:HD2	1.91	0.52
1:E:599:ARG:NH1	1:E:602:ASN:OD1	2.42	0.52
2:H:70:TYR:CD1	2:H:71:PRO:HA	2.44	0.52
1:G:561:ALA:O	1:G:566:MET:CE	2.58	0.51
1:G:155:VAL:HG22	1:G:160:GLU:HA	1.91	0.51
1:A:40:ILE:O	1:A:41:ASN:CB	2.56	0.51
1:G:561:ALA:O	1:G:566:MET:HE3	2.09	0.51
1:A:830:ARG:NH1	7:A:2008:SO4:O4	2.44	0.51
2:F:68:VAL:HG12	2:F:69:ALA:N	2.26	0.51
1:E:8:ASP:HB3	2:F:47:VAL:HG21	1.93	0.50
1:E:599:ARG:NH2	1:E:625:TRP:O	2.43	0.50
1:G:737:VAL:HG12	1:G:738:MET:HE2	1.94	0.50
2:D:70:TYR:CD1	2:D:71:PRO:HA	2.47	0.50
1:G:174:GLY:HA2	3:G:2001:MGD:C6	2.42	0.50
1:E:153:LYS:HE3	1:E:530:VAL:HG21	1.93	0.50
1:G:413:LYS:HD2	1:G:417:TRP:CE2	2.47	0.50
1:A:829:PRO:HB2	1:A:831:ASN:OD1	2.12	0.49
1:E:255:LEU:HB3	1:E:295:ALA:HB2	1.93	0.49
1:C:370:CYS:O	1:C:371:ARG:C	2.56	0.49
1:C:235:VAL:O	1:C:411:TYR:HA	2.12	0.48
1:C:460:ASP:O	1:C:463:VAL:HB	2.13	0.48
1:G:591:MET:HG3	1:G:596:ILE:HG13	1.95	0.48
1:A:561:ALA:O	1:A:566:MET:CE	2.62	0.48
1:E:31:CYS:SG	1:E:97:ASN:HB3	2.54	0.48
1:C:213:ASP:HB3	1:C:360:LEU:HD11	1.96	0.47
1:E:221:ASN:O	1:E:575:ARG:NH2	2.47	0.47
1:C:566:MET:HE1	14:C:2333:HOH:O	2.14	0.47
2:B:70:TYR:CD1	2:B:71:PRO:HA	2.50	0.47
1:E:737:VAL:HG12	1:E:738:MET:HE2	1.95	0.47
1:A:341:THR:HG22	14:A:2112:HOH:O	2.15	0.46
1:A:341:THR:OG1	1:A:342:ALA:N	2.49	0.46
1:A:255:LEU:HB3	1:A:295:ALA:HB2	1.97	0.45
1:C:827:ASP:O	1:C:828:ALA:C	2.59	0.45
1:C:255:LEU:HB3	1:C:295:ALA:HB2	1.98	0.45
1:E:293:GLN:HG2	1:E:842:TYR:HE2	1.82	0.45
1:G:197:ARG:CZ	1:G:489:HIS:CE1	3.00	0.45
1:C:104:ARG:NH2	1:C:722:ASN:OD1	2.50	0.45
2:F:54:LEU:HD13	2:F:68:VAL:HG11	1.98	0.45
1:E:413:LYS:HD2	1:E:417:TRP:NE1	2.32	0.44
13:G:2008:P33:C9	14:G:2433:HOH:O	2.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:MET:O	1:A:525:MET:HE1	2.17	0.44
1:A:717:ASN:OD1	3:A:2002:MGD:H8	2.18	0.44
1:C:363:PHE:O	1:C:367:VAL:HG23	2.18	0.44
1:C:415:LEU:C	1:C:415:LEU:HD23	2.43	0.44
1:E:460:ASP:O	1:E:463:VAL:HB	2.18	0.44
1:G:738:MET:HE1	1:G:794:PHE:CZ	2.53	0.44
1:C:493:THR:HG23	1:C:494:LEU:O	2.18	0.43
2:F:44:ALA:N	14:F:303:HOH:O	2.50	0.43
1:G:72:SER:HB2	1:G:107:ARG:HA	1.99	0.43
1:E:208:VAL:HB	1:E:211:THR:HG22	2.00	0.43
1:G:561:ALA:HB2	1:G:586:PRO:HB3	2.00	0.43
1:E:293:GLN:HG2	1:E:842:TYR:CE2	2.53	0.43
1:G:491:LYS:O	1:G:793:GLY:HA2	2.18	0.43
1:C:566:MET:CE	14:C:2333:HOH:O	2.66	0.43
1:E:174:GLY:HA2	3:E:2001:MGD:C6	2.48	0.43
1:A:208:VAL:HB	1:A:211:THR:HG22	2.01	0.43
1:A:571:MET:HA	1:A:576:ARG:O	2.19	0.43
1:C:40:ILE:O	1:C:41:ASN:CB	2.63	0.43
1:E:269:GLU:O	1:E:403:LYS:HD2	2.19	0.43
1:A:460:ASP:O	1:A:463:VAL:HB	2.18	0.43
1:A:693:MET:HE2	1:A:695:ALA:HB2	2.01	0.43
1:C:221:ASN:HB2	1:C:225:ASP:OD2	2.19	0.43
1:G:28:ILE:O	1:G:572:ASN:HB2	2.18	0.43
1:E:237:THR:CG2	1:E:243:GLN:OE1	2.67	0.43
1:A:737:VAL:HG12	1:A:738:MET:HE2	2.01	0.42
1:C:599:ARG:HD3	1:C:599:ARG:HA	1.75	0.42
1:E:40:ILE:O	1:E:41:ASN:CB	2.65	0.42
1:C:23:THR:O	1:C:24:CYS:C	2.62	0.42
1:C:717:ASN:OD1	3:C:2002:MGD:H8	2.20	0.42
1:A:76:VAL:HG23	1:A:117:ARG:HD2	2.01	0.42
1:E:155:VAL:HG22	1:E:160:GLU:HA	2.02	0.42
1:G:843:GLN:OE1	2:H:116:ASN:HB2	2.20	0.42
2:D:44:ALA:HB3	14:D:320:HOH:O	2.18	0.41
1:E:235:VAL:O	1:E:411:TYR:HA	2.21	0.41
1:G:460:ASP:O	1:G:463:VAL:HB	2.19	0.41
1:A:153:LYS:HE2	1:A:527:ASN:OD1	2.20	0.41
1:A:742:PRO:HG2	1:A:832:VAL:HG12	2.03	0.41
1:A:31:CYS:SG	1:A:97:ASN:HB3	2.61	0.41
1:G:827:ASP:O	1:G:828:ALA:C	2.64	0.41
1:A:599:ARG:HA	1:A:599:ARG:HD3	1.83	0.41
1:A:293:GLN:HG2	1:A:842:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:836:SER:OG	2:D:129:ASP:OD2	2.26	0.41
1:G:220:ASN:H	1:G:446:VAL:HG12	1.86	0.41
1:G:185:LYS:O	1:G:189:GLU:HB3	2.21	0.41
1:G:729:TYR:CD1	3:G:2001:MGD:H2'	2.56	0.40
1:C:599:ARG:NH2	1:C:625:TRP:O	2.37	0.40
1:G:48:PRO:O	1:G:54:GLY:HA2	2.21	0.40
1:G:368:GLU:OE1	1:G:371:ARG:NH1	2.55	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:2463:HOH:O	14:G:2463:HOH:O[2_545]	1.27	0.93
1:G:686:ASP:O	1:G:686:ASP:O[2_545]	1.98	0.22

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	841/843 (100%)	808 (96%)	32 (4%)	1 (0%)	48	57
1	C	841/843 (100%)	805 (96%)	35 (4%)	1 (0%)	48	57
1	E	841/843 (100%)	807 (96%)	33 (4%)	1 (0%)	48	57
1	G	841/843 (100%)	804 (96%)	36 (4%)	1 (0%)	48	57
2	B	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
2	D	130/132 (98%)	123 (95%)	7 (5%)	0	100	100
2	F	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
2	H	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
All	All	3884/3900 (100%)	3715 (96%)	165 (4%)	4 (0%)	48	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	811	ILE
1	C	811	ILE
1	E	811	ILE
1	A	811	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	677/677 (100%)	662 (98%)	15 (2%)	45	61
1	C	677/677 (100%)	661 (98%)	16 (2%)	43	58
1	E	677/677 (100%)	657 (97%)	20 (3%)	36	49
1	G	677/677 (100%)	659 (97%)	18 (3%)	39	53
2	B	104/104 (100%)	102 (98%)	2 (2%)	50	66
2	D	104/104 (100%)	104 (100%)	0	100	100
2	F	104/104 (100%)	101 (97%)	3 (3%)	37	51
2	H	104/104 (100%)	103 (99%)	1 (1%)	68	81
All	All	3124/3124 (100%)	3049 (98%)	75 (2%)	43	58

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	VAL
1	A	104	ARG
1	A	134	GLN
1	A	156	LYS
1	A	158	LYS
1	A	237	THR
1	A	273	GLU
1	A	293	GLN
1	A	347	TYR
1	A	463	VAL

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Mol	Chain	Res	Type
1	A	505	LYS
1	A	626	GLN
1	A	644	GLU
1	A	792	PHE
1	A	844	SER
2	B	53	ARG
2	B	57	ILE
1	C	41	ASN
1	C	49	GLN
1	C	62	GLN
1	C	269	GLU
1	C	293	GLN
1	C	341	THR
1	C	347	TYR
1	C	403	LYS
1	C	463	VAL
1	C	599	ARG
1	C	607	VAL
1	C	723	VAL
1	C	766	ILE
1	C	792	PHE
1	C	830	ARG
1	C	832	VAL
1	E	58	SER
1	E	59	GLU
1	E	134	GLN
1	E	155	VAL
1	E	156	LYS
1	E	237	THR
1	E	256	ARG
1	E	265	GLU
1	E	293	GLN
1	E	341	THR
1	E	347	TYR
1	E	403	LYS
1	E	463	VAL
1	E	557	ILE
1	E	644	GLU
1	E	654	MET
1	E	667	THR
1	E	792	PHE
1	E	832	VAL

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Mol	Chain	Res	Type
1	E	844	SER
2	F	57	ILE
2	F	61	THR
2	F	161	GLU
1	G	27	CYS
1	G	42	LYS
1	G	55	VAL
1	G	155	VAL
1	G	189	GLU
1	G	276	ARG
1	G	293	GLN
1	G	347	TYR
1	G	400	GLU
1	G	438	ILE
1	G	441	PRO
1	G	463	VAL
1	G	568	LEU
1	G	599	ARG
1	G	723	VAL
1	G	785	ARG
1	G	792	PHE
1	G	832	VAL
2	H	154	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	41	ASN
1	A	293	GLN
1	A	425	ASN
1	A	535	GLN
1	A	589	GLN
1	A	619	GLN
2	B	143	GLN
1	C	79	GLN
1	C	195	ASN
1	C	220	ASN
1	C	293	GLN
1	C	472	GLN
1	C	535	GLN
1	C	589	GLN

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Mol	Chain	Res	Type
1	C	814	ASN
1	E	6	HIS
1	E	21	ASN
1	E	34	HIS
1	E	122	GLN
1	E	293	GLN
1	E	425	ASN
1	E	675	GLN
1	E	732	GLN
2	F	116	ASN
2	F	143	GLN
1	G	49	GLN
1	G	249	ASN
1	G	293	GLN
1	G	478	GLN
1	G	814	ASN
2	H	116	ASN
2	H	143	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 48 ligands modelled in this entry, 8 are monoatomic - leaving 40 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	$\# Z > 2$
6	F3S	C	2005	1	0,9,9	-	-	-		
3	MGD	G	2001	5	47,52,52	1.42	7 (14%)	58,81,81	1.89	15 (25%)
9	GOL	A	2011	-	5,5,5	1.12	0	5,5,5	1.51	2 (40%)
3	MGD	A	2001	5	47,52,52	1.51	8 (17%)	58,81,81	1.66	13 (22%)
3	MGD	G	2002	5	47,52,52	1.92	11 (23%)	58,81,81	1.78	13 (22%)
7	SO4	A	2008	-	4,4,4	0.84	0	6,6,6	1.02	0
7	SO4	A	2006	-	4,4,4	0.54	0	6,6,6	0.87	0
3	MGD	A	2002	5	47,52,52	1.75	7 (14%)	58,81,81	1.88	15 (25%)
6	F3S	G	2005	1	0,9,9	-	-	-		
10	FES	H	201	2	0,4,4	-	-	-		
7	SO4	C	2009	-	4,4,4	0.74	0	6,6,6	0.56	0
10	FES	D	201	2	0,4,4	-	-	-		
11	EDO	C	2012	-	3,3,3	0.46	0	2,2,2	0.49	0
7	SO4	C	2006	-	4,4,4	0.66	0	6,6,6	0.70	0
7	SO4	C	2007	-	4,4,4	0.64	0	6,6,6	0.83	0
9	GOL	E	2008	-	5,5,5	0.51	0	5,5,5	0.40	0
12	PEG	C	2010	-	6,6,6	0.65	0	5,5,5	0.62	0
7	SO4	A	2009	-	4,4,4	0.56	0	6,6,6	0.83	0
3	MGD	E	2002	5	47,52,52	1.47	8 (17%)	58,81,81	2.03	18 (31%)
9	GOL	G	2010	-	5,5,5	1.33	1 (20%)	5,5,5	1.85	2 (40%)
8	PGE	A	2010	-	9,9,9	1.14	0	8,8,8	1.29	0
7	SO4	A	2007	-	4,4,4	0.50	0	6,6,6	0.85	0
13	P33	G	2009	-	21,21,21	0.69	0	20,20,20	0.82	1 (5%)
3	MGD	C	2002	5	47,52,52	1.72	10 (21%)	58,81,81	1.94	17 (29%)
6	F3S	A	2005	1	0,9,9	-	-	-		
11	EDO	G	2012	-	3,3,3	0.59	0	2,2,2	0.36	0
7	SO4	G	2006	-	4,4,4	0.51	0	6,6,6	0.75	0
7	SO4	G	2007	-	4,4,4	0.63	0	6,6,6	0.55	0
13	P33	G	2008	-	21,21,21	1.04	0	20,20,20	1.53	4 (20%)
9	GOL	C	2011	-	5,5,5	0.73	0	5,5,5	1.07	0
10	FES	F	201	2	0,4,4	-	-	-		
3	MGD	C	2001	5	47,52,52	1.53	9 (19%)	58,81,81	2.01	15 (25%)
7	SO4	E	2007	-	4,4,4	0.56	0	6,6,6	0.52	0
9	GOL	G	2011	-	5,5,5	1.15	0	5,5,5	1.95	2 (40%)
11	EDO	B	202	-	3,3,3	0.37	0	2,2,2	0.85	0
7	SO4	E	2006	-	4,4,4	0.42	0	6,6,6	0.46	0
3	MGD	E	2001	5	47,52,52	1.62	7 (14%)	58,81,81	1.94	12 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	FES	B	201	2	0,4,4	-	-	-		
7	SO4	C	2008	-	4,4,4	0.54	0	6,6,6	0.28	0
6	F3S	E	2005	1	0,9,9	-	-	-		

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
6	F3S	C	2005	1	-	-	0/3/3/3
3	MGD	G	2001	5	-	5/22/66/66	0/6/6/6
9	GOL	A	2011	-	-	4/4/4/4	-
3	MGD	A	2001	5	-	5/22/66/66	0/6/6/6
3	MGD	G	2002	5	-	4/22/66/66	0/6/6/6
3	MGD	A	2002	5	-	4/22/66/66	0/6/6/6
6	F3S	G	2005	1	-	-	0/3/3/3
10	FES	H	201	2	-	-	0/1/1/1
10	FES	D	201	2	-	-	0/1/1/1
11	EDO	C	2012	-	-	1/1/1/1	-
12	PEG	C	2010	-	-	3/4/4/4	-
9	GOL	E	2008	-	-	4/4/4/4	-
3	MGD	E	2002	5	-	6/22/66/66	0/6/6/6
9	GOL	G	2010	-	-	3/4/4/4	-
8	PGE	A	2010	-	-	4/7/7/7	-
13	P33	G	2009	-	-	9/19/19/19	-
3	MGD	C	2002	5	-	3/22/66/66	0/6/6/6
6	F3S	A	2005	1	-	-	0/3/3/3
11	EDO	G	2012	-	-	1/1/1/1	-
13	P33	G	2008	-	-	9/19/19/19	-
9	GOL	C	2011	-	-	3/4/4/4	-
10	FES	F	201	2	-	-	0/1/1/1
3	MGD	C	2001	5	-	4/22/66/66	0/6/6/6
9	GOL	G	2011	-	-	2/4/4/4	-
11	EDO	B	202	-	-	1/1/1/1	-
3	MGD	E	2001	5	-	4/22/66/66	0/6/6/6
10	FES	B	201	2	-	-	0/1/1/1
6	F3S	E	2005	1	-	-	0/3/3/3

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2001	MGD	C16-C21	6.55	1.49	1.38
3	C	2002	MGD	C16-C21	5.58	1.48	1.38
3	C	2001	MGD	C16-C21	5.56	1.48	1.38
3	G	2002	MGD	C16-C21	5.46	1.48	1.38
3	G	2002	MGD	PA-O3B	5.44	1.65	1.59
3	A	2002	MGD	C16-C21	5.09	1.47	1.38
3	G	2001	MGD	C16-C21	5.06	1.47	1.38
3	C	2002	MGD	C21-N22	-5.01	1.30	1.35
3	E	2002	MGD	C16-C21	5.00	1.47	1.38
3	A	2002	MGD	PA-O3B	4.87	1.64	1.59
3	A	2001	MGD	C16-C21	4.57	1.46	1.38
3	A	2002	MGD	PB-O3B	4.20	1.64	1.59
3	G	2002	MGD	C14-N15	-4.11	1.41	1.46
3	G	2002	MGD	PB-O3B	4.11	1.63	1.59
3	G	2002	MGD	C21-N22	-3.93	1.31	1.35
3	E	2002	MGD	PA-O3B	3.91	1.63	1.59
3	A	2002	MGD	C5-C4	3.64	1.48	1.38
3	A	2001	MGD	C17-N18	-3.57	1.32	1.38
3	E	2001	MGD	C4-N9	-3.52	1.29	1.38
3	C	2002	MGD	C17-N18	-3.49	1.32	1.38
3	C	2001	MGD	PB-O3B	3.48	1.63	1.59
3	E	2002	MGD	PB-O3B	3.27	1.63	1.59
3	G	2001	MGD	C5-C4	3.24	1.47	1.38
3	A	2001	MGD	C5-C4	3.24	1.47	1.38
3	G	2002	MGD	C5-N7	-3.23	1.32	1.39
3	G	2002	MGD	C4-N9	-3.21	1.29	1.38
3	C	2001	MGD	C6-N1	-3.13	1.33	1.38
3	E	2001	MGD	C5-C4	3.02	1.47	1.38
3	A	2002	MGD	C21-N22	-2.91	1.32	1.35
3	C	2002	MGD	C5-C4	2.88	1.46	1.38
3	G	2001	MGD	PB-O3B	2.85	1.62	1.59
3	C	2002	MGD	C4-N9	-2.85	1.30	1.38
3	E	2001	MGD	C21-N22	-2.80	1.32	1.35
3	G	2002	MGD	C5-C4	2.80	1.46	1.38
3	C	2002	MGD	C6-N1	-2.77	1.33	1.38
3	C	2001	MGD	C5-C4	2.76	1.46	1.38
3	A	2001	MGD	C6-N1	-2.69	1.33	1.38
3	A	2001	MGD	C4-N9	-2.68	1.31	1.38
3	C	2001	MGD	C4-N9	-2.65	1.31	1.38
3	E	2001	MGD	PA-O3B	2.61	1.62	1.59
3	C	2001	MGD	C5-N7	-2.48	1.34	1.39
3	C	2001	MGD	O11-C23	-2.45	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2002	MGD	C5-N7	-2.43	1.34	1.39
3	E	2001	MGD	C6-N1	-2.39	1.34	1.38
3	G	2001	MGD	C5-N7	-2.34	1.34	1.39
3	A	2002	MGD	O11-C23	-2.33	1.40	1.43
3	E	2002	MGD	C5-C4	2.33	1.45	1.38
3	A	2001	MGD	C5-N7	-2.33	1.34	1.39
3	C	2001	MGD	C14-N15	-2.30	1.43	1.46
3	G	2002	MGD	C17-N18	-2.30	1.34	1.38
3	C	2001	MGD	C16-C17	2.28	1.48	1.41
3	G	2001	MGD	C16-C17	2.26	1.48	1.41
9	G	2010	GOL	O1-C1	2.23	1.51	1.42
3	G	2002	MGD	C6-N1	-2.22	1.34	1.38
3	G	2001	MGD	C16-N15	-2.19	1.32	1.37
3	G	2002	MGD	O11-C23	-2.19	1.40	1.43
3	A	2001	MGD	C23-C14	-2.18	1.51	1.53
3	G	2001	MGD	C17-N18	-2.15	1.34	1.38
3	E	2002	MGD	C4-N9	-2.14	1.32	1.38
3	C	2002	MGD	C21-N20	-2.13	1.32	1.36
3	E	2002	MGD	C16-C17	2.11	1.48	1.41
3	A	2002	MGD	O6-C6	2.09	1.27	1.23
3	E	2002	MGD	C6-N1	-2.07	1.35	1.38
3	A	2001	MGD	C16-N15	-2.07	1.33	1.37
3	C	2002	MGD	O11-C11	-2.06	1.39	1.43
3	E	2001	MGD	C16-C17	2.03	1.48	1.41
3	E	2002	MGD	C17-N18	-2.00	1.35	1.38
3	C	2002	MGD	C19-N20	2.00	1.38	1.33

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2001	MGD	C23-C14-N15	6.61	114.36	107.87
3	E	2001	MGD	C23-C14-N15	6.01	113.78	107.87
3	E	2002	MGD	C23-C14-N15	5.35	113.12	107.87
3	A	2002	MGD	C23-C14-N15	5.24	113.01	107.87
3	C	2001	MGD	C23-C14-N15	5.09	112.87	107.87
3	C	2002	MGD	C23-C14-N15	5.07	112.85	107.87
3	E	2001	MGD	C19-N20-C21	4.95	122.10	113.36
3	G	2001	MGD	C19-N20-C21	4.92	122.04	113.36
3	C	2002	MGD	O11-C23-N22	-4.85	104.20	108.61
3	A	2001	MGD	C23-C14-N15	4.85	112.63	107.87
3	C	2001	MGD	C19-N20-C21	4.82	121.86	113.36
3	C	2002	MGD	C5-C4-N3	-4.59	121.09	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2002	MGD	O11-C23-N22	-4.54	104.48	108.61
3	C	2001	MGD	C5-C4-N3	-4.45	121.31	128.39
3	E	2001	MGD	C2-N3-C4	4.37	119.82	112.30
3	E	2002	MGD	C2-N3-C4	4.29	119.69	112.30
3	G	2002	MGD	C5-C4-N3	-4.25	121.62	128.39
3	G	2001	MGD	C5-C4-N3	-4.24	121.65	128.39
3	E	2002	MGD	C4'-O4'-C1'	-4.19	100.21	109.47
3	E	2002	MGD	C5-C4-N3	-4.18	121.73	128.39
3	G	2002	MGD	C19-N20-C21	4.16	120.70	113.36
3	A	2002	MGD	C5-C4-N3	-4.09	121.88	128.39
3	C	2001	MGD	C6-C5-N7	4.01	137.58	130.29
3	C	2001	MGD	O17-C17-C16	-3.98	117.67	127.26
3	E	2001	MGD	C5-C4-N3	-3.97	122.08	128.39
3	A	2002	MGD	C19-N20-C21	3.96	120.35	113.36
3	C	2001	MGD	C2-N3-C4	3.90	119.02	112.30
3	A	2002	MGD	N9-C4-N3	3.82	133.58	125.95
3	E	2002	MGD	C19-N20-C21	3.81	120.09	113.36
3	C	2001	MGD	N9-C4-N3	3.80	133.56	125.95
3	C	2002	MGD	C2-N3-C4	3.74	118.74	112.30
3	E	2002	MGD	N9-C4-N3	3.73	133.42	125.95
3	C	2002	MGD	C6-C5-N7	3.72	137.06	130.29
3	G	2002	MGD	N9-C4-N3	3.71	133.38	125.95
3	E	2002	MGD	C6-C5-N7	3.70	137.01	130.29
3	G	2001	MGD	C2-N3-C4	3.65	118.59	112.30
3	G	2002	MGD	O11-C23-N22	-3.64	105.31	108.61
3	A	2001	MGD	C5-C4-N3	-3.54	122.75	128.39
3	A	2001	MGD	C19-N20-C21	3.51	119.55	113.36
3	A	2001	MGD	N9-C4-N3	3.50	132.95	125.95
3	A	2002	MGD	O17-C17-C16	-3.41	119.04	127.26
3	G	2002	MGD	C23-C14-N15	3.35	111.15	107.87
3	G	2001	MGD	N9-C4-N3	3.29	132.53	125.95
3	E	2001	MGD	N9-C4-N3	3.27	132.50	125.95
3	E	2001	MGD	C6-C5-N7	3.27	136.25	130.29
3	C	2002	MGD	O2A-PA-O1A	3.24	127.54	112.44
3	E	2001	MGD	C17-C16-N15	3.10	124.72	116.27
3	E	2002	MGD	O3B-PB-O1B	-3.10	101.39	110.70
3	G	2002	MGD	O3B-PB-O1B	-3.06	101.50	110.70
13	G	2008	P33	O10-C9-C8	3.05	124.25	110.35
3	E	2002	MGD	O2B-PB-O3B	3.03	115.47	107.27
3	G	2002	MGD	C4'-O4'-C1'	-3.01	102.82	109.47
3	G	2001	MGD	C6-C5-N7	2.99	135.74	130.29
3	C	2002	MGD	C19-N20-C21	2.98	118.62	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	MGD	O3B-PB-O1B	-2.92	101.92	110.70
3	E	2001	MGD	O17-C17-C16	-2.89	120.29	127.26
3	G	2002	MGD	C2-N3-C4	2.84	117.18	112.30
13	G	2008	P33	C15-O16-C17	2.83	125.65	113.26
3	G	2002	MGD	O17-C17-C16	-2.77	120.58	127.26
3	E	2002	MGD	O11-C23-C14	-2.77	107.12	108.96
3	G	2002	MGD	O6-C6-C5	-2.76	119.23	126.53
3	C	2002	MGD	C4-C5-N7	-2.75	106.31	110.67
9	G	2011	GOL	O2-C2-C1	2.75	120.57	109.18
3	C	2002	MGD	O2A-PA-O3B	-2.72	99.92	107.27
3	C	2002	MGD	O11-C23-C14	2.71	110.77	108.96
3	G	2002	MGD	O2A-PA-O1A	2.70	125.02	112.44
3	E	2001	MGD	N19-C19-N18	2.68	122.41	116.76
3	C	2002	MGD	C4'-O4'-C1'	-2.67	103.57	109.47
3	C	2001	MGD	C6-C5-C4	-2.62	114.88	118.83
3	E	2001	MGD	C6-C5-C4	-2.62	114.89	118.83
3	C	2002	MGD	N9-C4-N3	2.61	131.17	125.95
3	A	2002	MGD	C4'-O4'-C1'	-2.59	103.76	109.47
3	A	2001	MGD	C17-C16-N15	2.58	123.29	116.27
3	A	2002	MGD	O11-C23-C14	2.57	110.68	108.96
3	C	2001	MGD	C16-C17-N18	2.56	119.16	112.13
3	E	2002	MGD	O17-C17-C16	-2.54	121.13	127.26
3	A	2001	MGD	C1'-N9-C4	-2.53	119.00	126.49
3	A	2002	MGD	O6-C6-C5	-2.53	119.86	126.53
3	A	2002	MGD	C6-C5-N7	2.52	134.87	130.29
13	G	2008	P33	C6-O7-C8	2.48	124.10	113.26
9	G	2010	GOL	O1-C1-C2	2.44	121.34	110.38
3	C	2001	MGD	O2A-PA-O3B	2.42	113.82	107.27
3	C	2002	MGD	O17-C17-C16	-2.42	121.44	127.26
3	C	2001	MGD	C19-N18-C17	-2.41	120.74	125.11
3	C	2001	MGD	C1'-N9-C4	-2.39	119.42	126.49
3	E	2002	MGD	O2A-PA-O1A	2.39	123.55	112.44
3	C	2001	MGD	C17-C16-N15	2.37	122.74	116.27
3	C	2001	MGD	O11-C23-C14	2.37	110.55	108.96
3	A	2001	MGD	O2A-PA-O3B	2.37	113.68	107.27
3	G	2001	MGD	C17-C16-N15	2.36	122.70	116.27
3	E	2001	MGD	O11-C23-C14	2.36	110.54	108.96
3	A	2002	MGD	N2-C2-N3	-2.32	115.15	119.67
3	A	2002	MGD	C16-C17-N18	2.31	118.47	112.13
3	E	2002	MGD	O6-C6-C5	-2.30	120.45	126.53
3	A	2002	MGD	O3B-PB-O1B	-2.30	103.78	110.70
3	E	2002	MGD	O11-C23-N22	-2.29	106.53	108.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2001	MGD	O11-C23-N22	2.28	110.68	108.61
3	A	2001	MGD	O17-C17-C16	-2.28	121.76	127.26
9	A	2011	GOL	O3-C3-C2	2.27	120.61	110.38
3	G	2001	MGD	O3A-C10-C11	-2.27	102.97	108.58
3	G	2001	MGD	O17-C17-C16	-2.26	121.81	127.26
3	A	2001	MGD	O6-C6-C5	-2.26	120.57	126.53
3	G	2001	MGD	O6-C6-C5	-2.26	120.58	126.53
3	E	2002	MGD	C6-C5-C4	-2.24	115.45	118.83
3	C	2002	MGD	C16-C17-N18	2.22	118.24	112.13
9	G	2010	GOL	O2-C2-C3	-2.22	100.00	109.18
13	G	2008	P33	O19-C20-C21	2.21	119.87	110.11
3	G	2001	MGD	C1'-N9-C4	-2.20	119.98	126.49
3	C	2002	MGD	O3B-PB-O1B	-2.19	104.11	110.70
3	C	2001	MGD	C5-C6-N1	2.19	118.82	113.25
3	C	2002	MGD	O2B-PB-O3B	2.18	113.17	107.27
3	E	2002	MGD	C5-C6-N1	2.18	118.80	113.25
3	G	2002	MGD	O11-C23-C14	-2.18	107.51	108.96
3	A	2001	MGD	O6-C6-N1	2.18	124.21	120.11
3	G	2001	MGD	O2B-PB-O1B	2.15	122.47	112.44
3	A	2001	MGD	C8-N9-C4	2.11	109.99	106.03
9	G	2011	GOL	O3-C3-C2	2.09	119.78	110.38
3	G	2001	MGD	O3B-PB-O1B	-2.08	104.45	110.70
3	A	2001	MGD	C16-C17-N18	2.06	117.80	112.13
9	A	2011	GOL	O1-C1-C2	2.06	119.65	110.38
13	G	2009	P33	C18-O19-C20	2.06	122.27	113.26
3	A	2002	MGD	C2-N3-C4	2.06	115.84	112.30
3	C	2002	MGD	C1'-N9-C4	-2.03	120.48	126.49
3	E	2002	MGD	O2A-PA-O3A	-2.02	98.40	107.57
3	G	2002	MGD	C16-C17-N18	2.02	117.67	112.13
3	G	2001	MGD	O2A-PA-O1A	2.02	121.83	112.44
3	A	2002	MGD	O4'-C1'-N9	2.01	112.91	108.36
3	E	2001	MGD	O2B-PB-O1B	2.01	121.78	112.44
3	E	2002	MGD	C16-C17-N18	2.00	117.62	112.13

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001	MGD	PA-O3B-PB-O5'
3	A	2001	MGD	C5'-O5'-PB-O3B
3	A	2002	MGD	C5'-O5'-PB-O1B
3	C	2001	MGD	C5'-O5'-PB-O3B

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Mol	Chain	Res	Type	Atoms
3	E	2001	MGD	PA-O3B-PB-O5'
3	E	2001	MGD	C5'-O5'-PB-O3B
3	E	2002	MGD	C5'-O5'-PB-O1B
3	G	2001	MGD	PA-O3B-PB-O5'
3	G	2001	MGD	C5'-O5'-PB-O1B
3	G	2002	MGD	C5'-O5'-PB-O1B
3	G	2002	MGD	C5'-O5'-PB-O3B
9	A	2011	GOL	O1-C1-C2-C3
9	A	2011	GOL	C1-C2-C3-O3
9	E	2008	GOL	O1-C1-C2-C3
9	E	2008	GOL	O2-C2-C3-O3
13	G	2008	P33	C18-C17-O16-C15
13	G	2009	P33	C8-C9-O10-C11
13	G	2009	P33	O4-C5-C6-O7
8	A	2010	PGE	O2-C3-C4-O3
13	G	2009	P33	O7-C8-C9-O10
13	G	2008	P33	O19-C20-C21-O22
13	G	2009	P33	O1-C2-C3-O4
13	G	2008	P33	O1-C2-C3-O4
9	C	2011	GOL	C1-C2-C3-O3
9	E	2008	GOL	C1-C2-C3-O3
9	G	2010	GOL	O1-C1-C2-C3
9	G	2011	GOL	C1-C2-C3-O3
13	G	2008	P33	O10-C11-C12-O13
9	A	2011	GOL	O1-C1-C2-O2
9	C	2011	GOL	O2-C2-C3-O3
13	G	2009	P33	O19-C20-C21-O22
8	A	2010	PGE	O1-C1-C2-O2
9	A	2011	GOL	O2-C2-C3-O3
9	E	2008	GOL	O1-C1-C2-O2
13	G	2009	P33	O16-C17-C18-O19
13	G	2008	P33	O7-C8-C9-O10
3	A	2002	MGD	PA-O3B-PB-O5'
3	C	2001	MGD	PA-O3B-PB-O5'
3	C	2002	MGD	PA-O3B-PB-O5'
3	E	2002	MGD	PA-O3B-PB-O5'
3	G	2002	MGD	PA-O3B-PB-O5'
13	G	2008	P33	O4-C5-C6-O7
13	G	2009	P33	C15-C14-O13-C12
9	G	2010	GOL	C1-C2-C3-O3
13	G	2008	P33	C5-C6-O7-C8
12	C	2010	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
12	C	2010	PEG	C4-C3-O2-C2
8	A	2010	PGE	C1-C2-O2-C3
3	E	2002	MGD	PB-O3B-PA-O1A
13	G	2008	P33	O16-C17-C18-O19
13	G	2009	P33	C6-C5-O4-C3
11	C	2012	EDO	O1-C1-C2-O2
3	A	2001	MGD	C5'-O5'-PB-O1B
3	A	2002	MGD	C5'-O5'-PB-O3B
3	C	2001	MGD	C5'-O5'-PB-O1B
3	C	2002	MGD	C5'-O5'-PB-O1B
3	E	2001	MGD	C5'-O5'-PB-O1B
3	E	2001	MGD	C10-O3A-PA-O1A
3	E	2002	MGD	C5'-O5'-PB-O2B
3	E	2002	MGD	C5'-O5'-PB-O3B
9	C	2011	GOL	O1-C1-C2-O2
3	G	2001	MGD	O4'-C4'-C5'-O5'
3	C	2001	MGD	O4'-C4'-C5'-O5'
13	G	2009	P33	C11-C12-O13-C14
11	B	202	EDO	O1-C1-C2-O2
11	G	2012	EDO	O1-C1-C2-O2
3	G	2001	MGD	C3'-C4'-C5'-O5'
9	G	2011	GOL	O1-C1-C2-O2
8	A	2010	PGE	C4-C3-O2-C2
12	C	2010	PEG	O1-C1-C2-O2
13	G	2008	P33	C2-C3-O4-C5
3	A	2001	MGD	O4'-C4'-C5'-O5'
3	E	2002	MGD	PB-O3B-PA-O2A
9	G	2010	GOL	O2-C2-C3-O3
3	A	2001	MGD	PB-O3B-PA-O2A
3	A	2002	MGD	PB-O3B-PA-O2A
3	C	2002	MGD	PB-O3B-PA-O2A
3	G	2001	MGD	PB-O3B-PA-O2A
3	G	2002	MGD	PB-O3B-PA-O2A

There are no ring outliers.

6 monomers are involved in 9 short contacts:

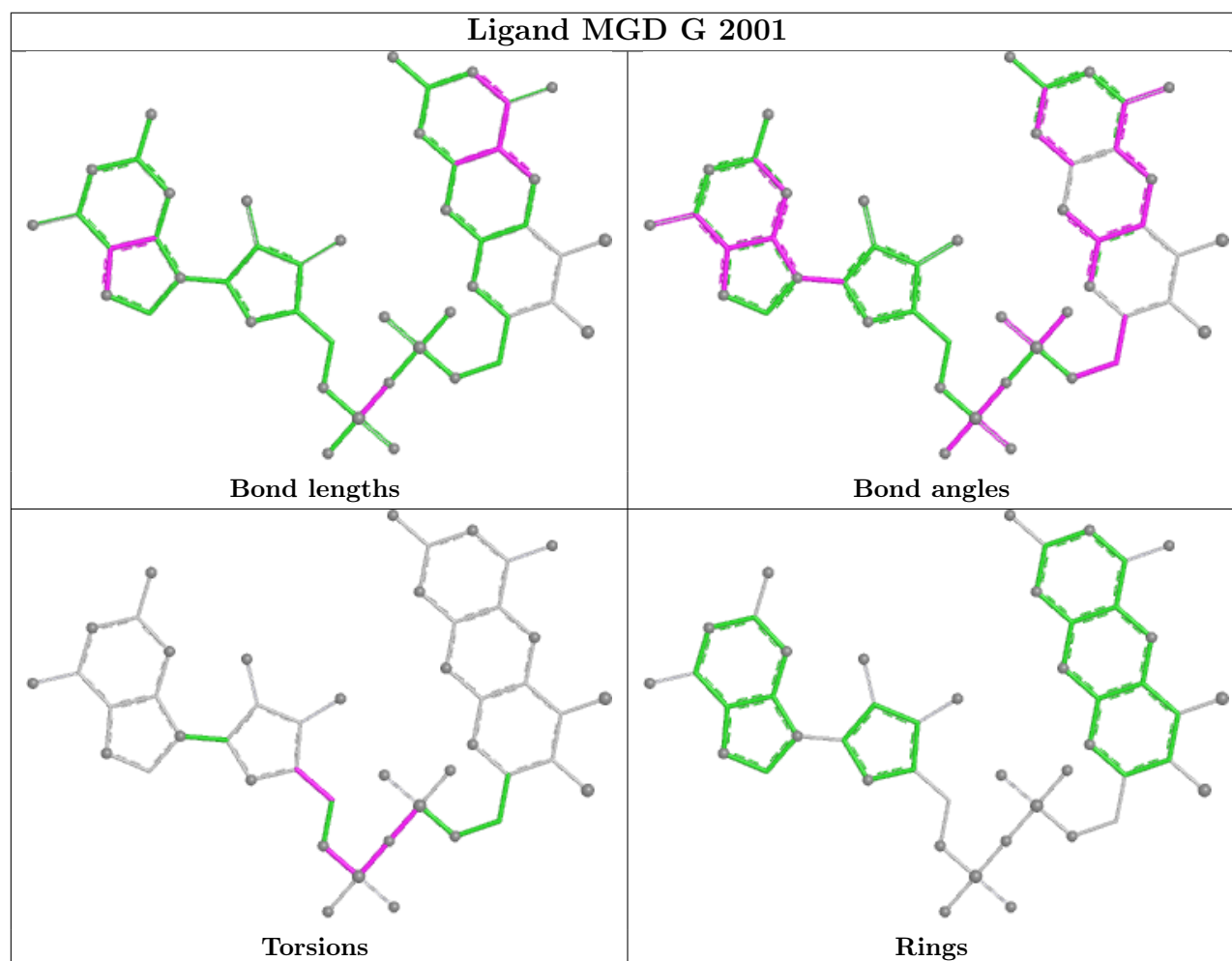
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2001	MGD	2	0
7	A	2008	SO4	1	0
3	A	2002	MGD	1	0
3	C	2002	MGD	1	0

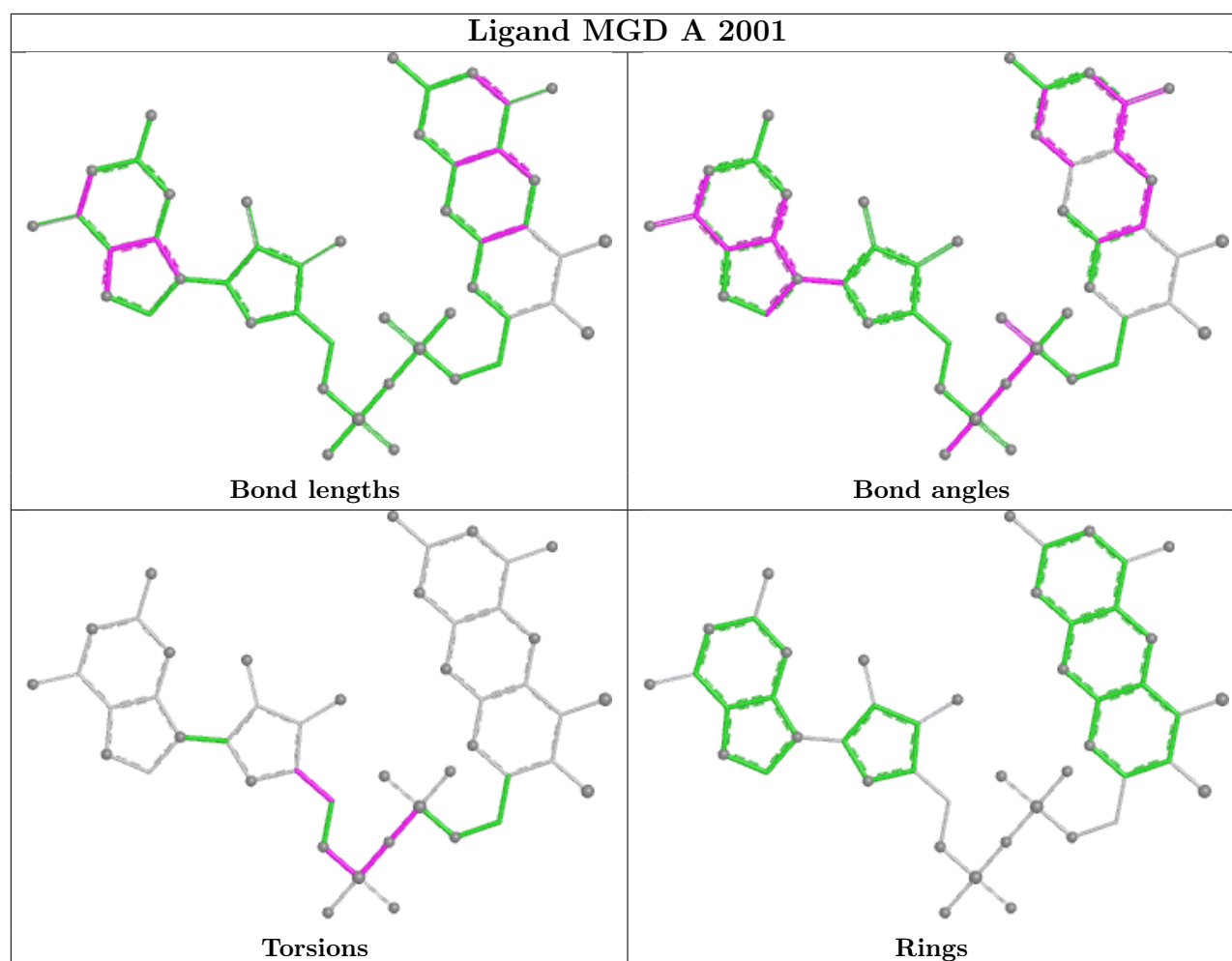
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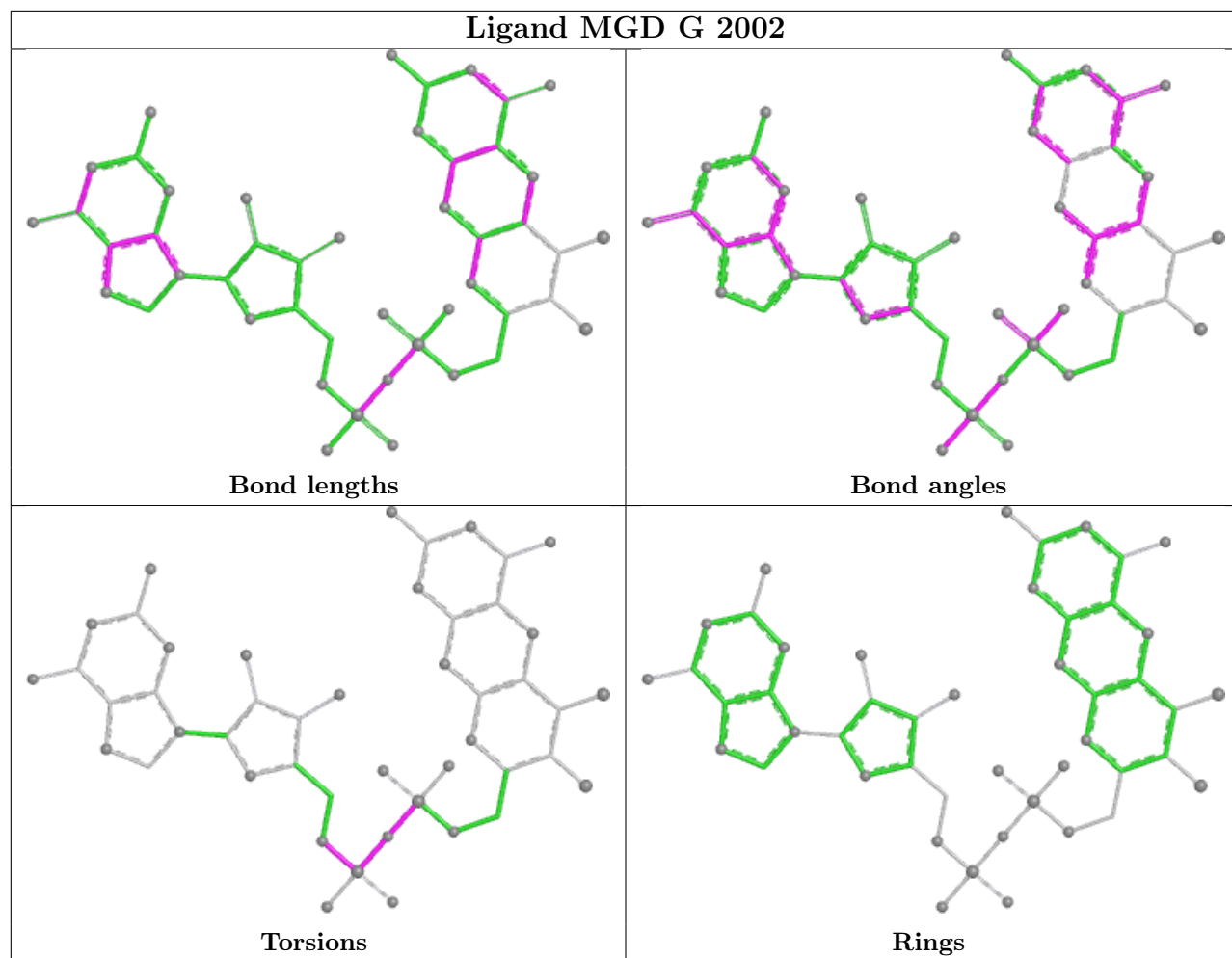
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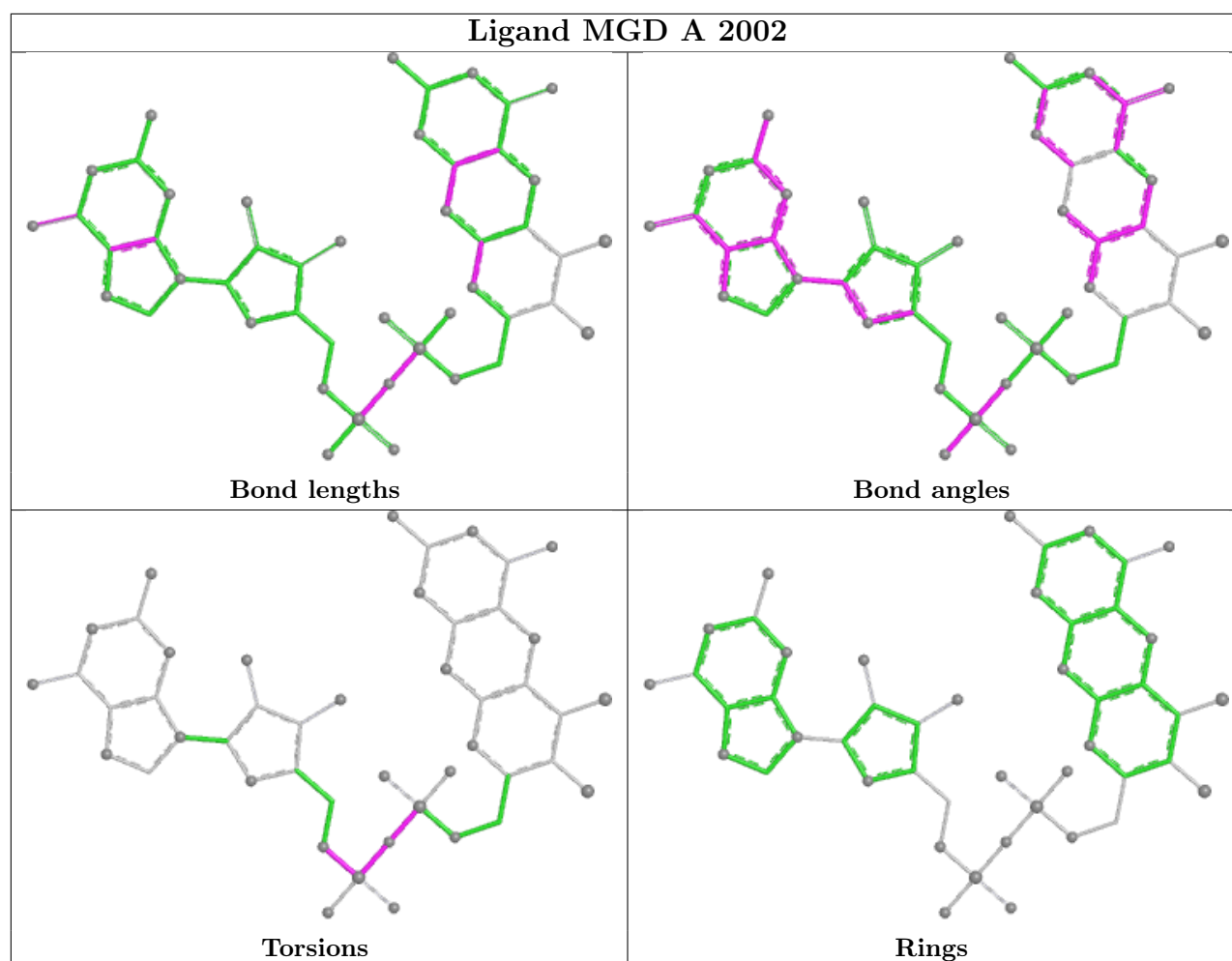
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	G	2008	P33	3	0
3	E	2001	MGD	1	0

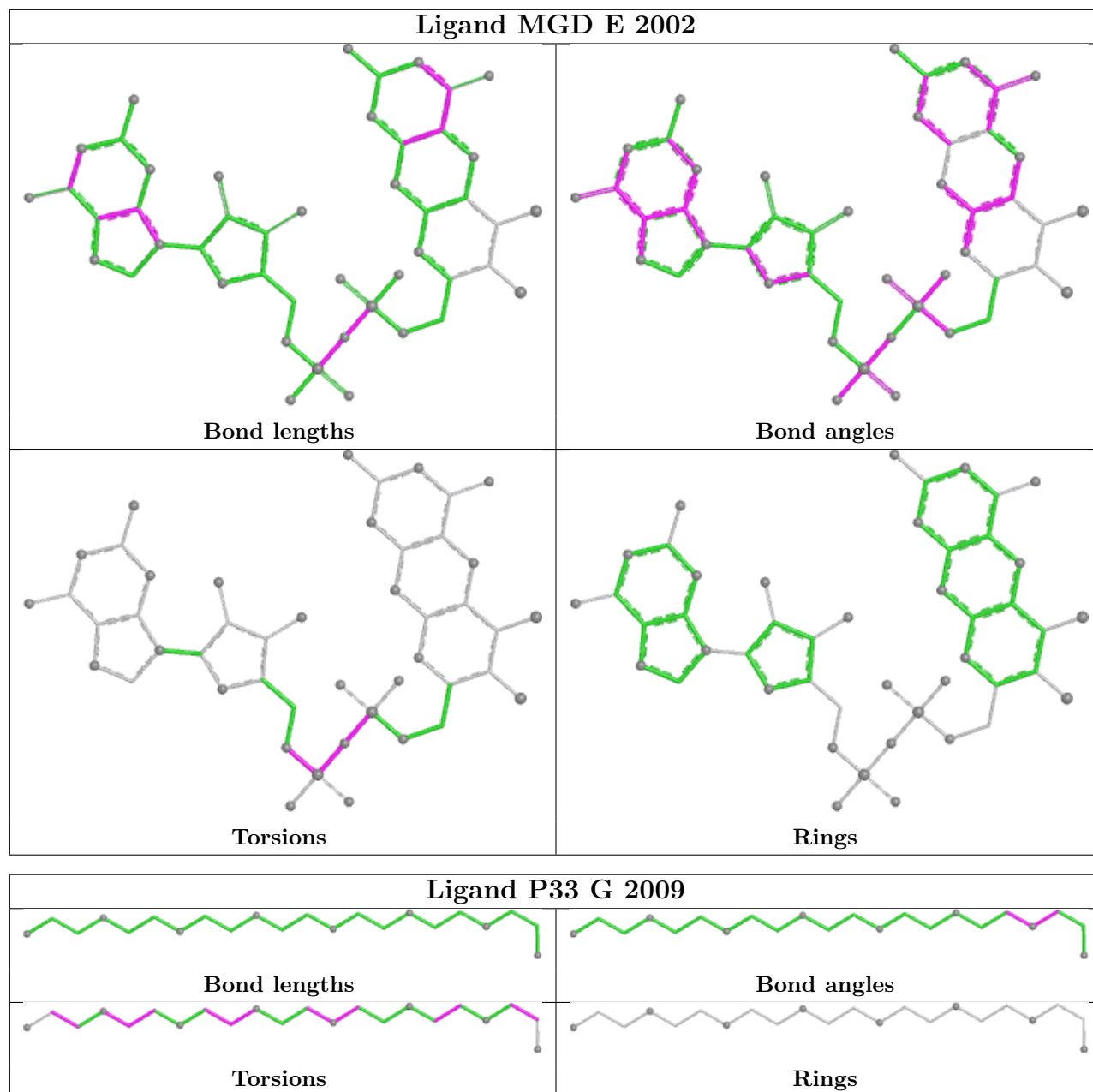
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

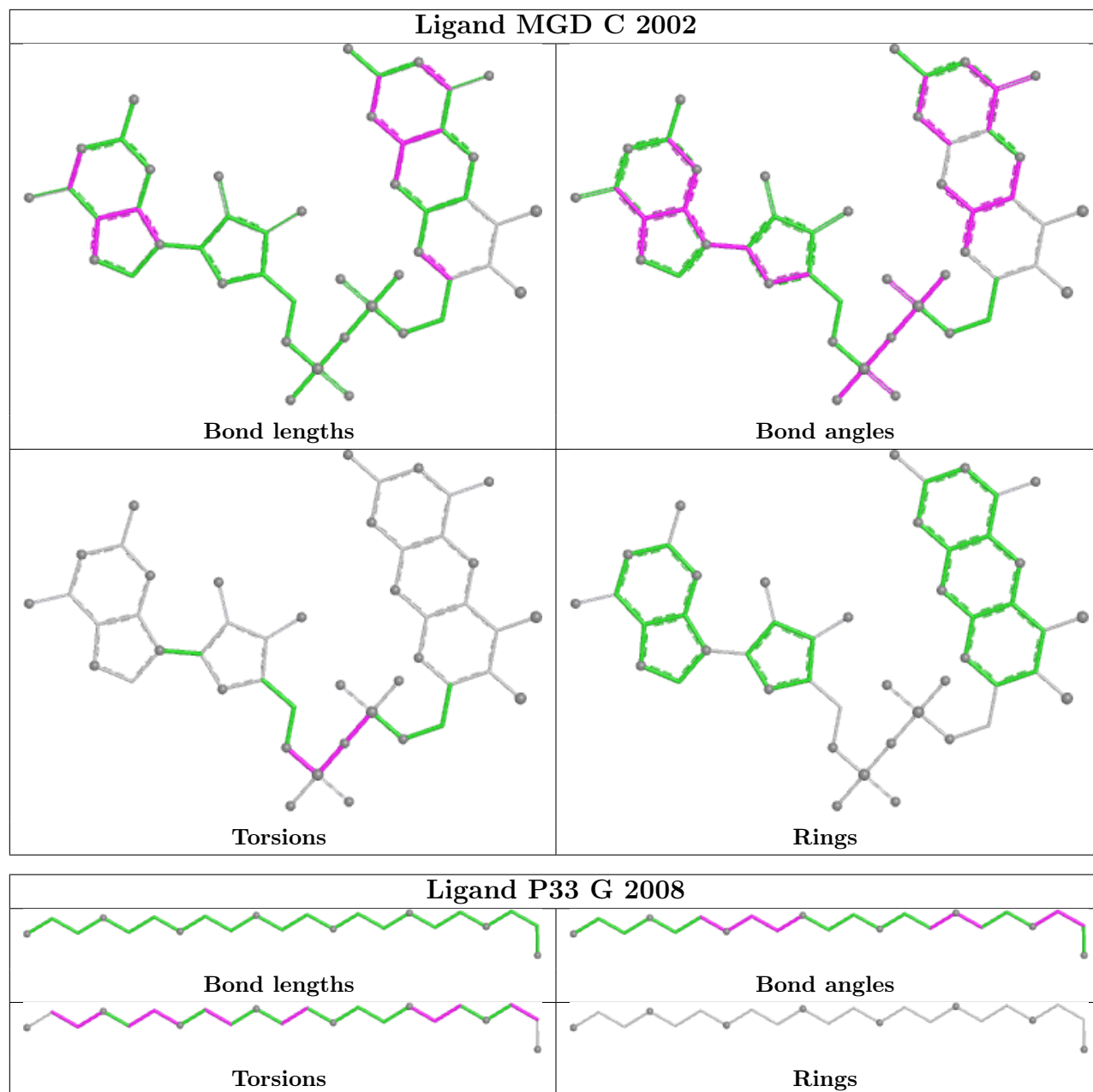


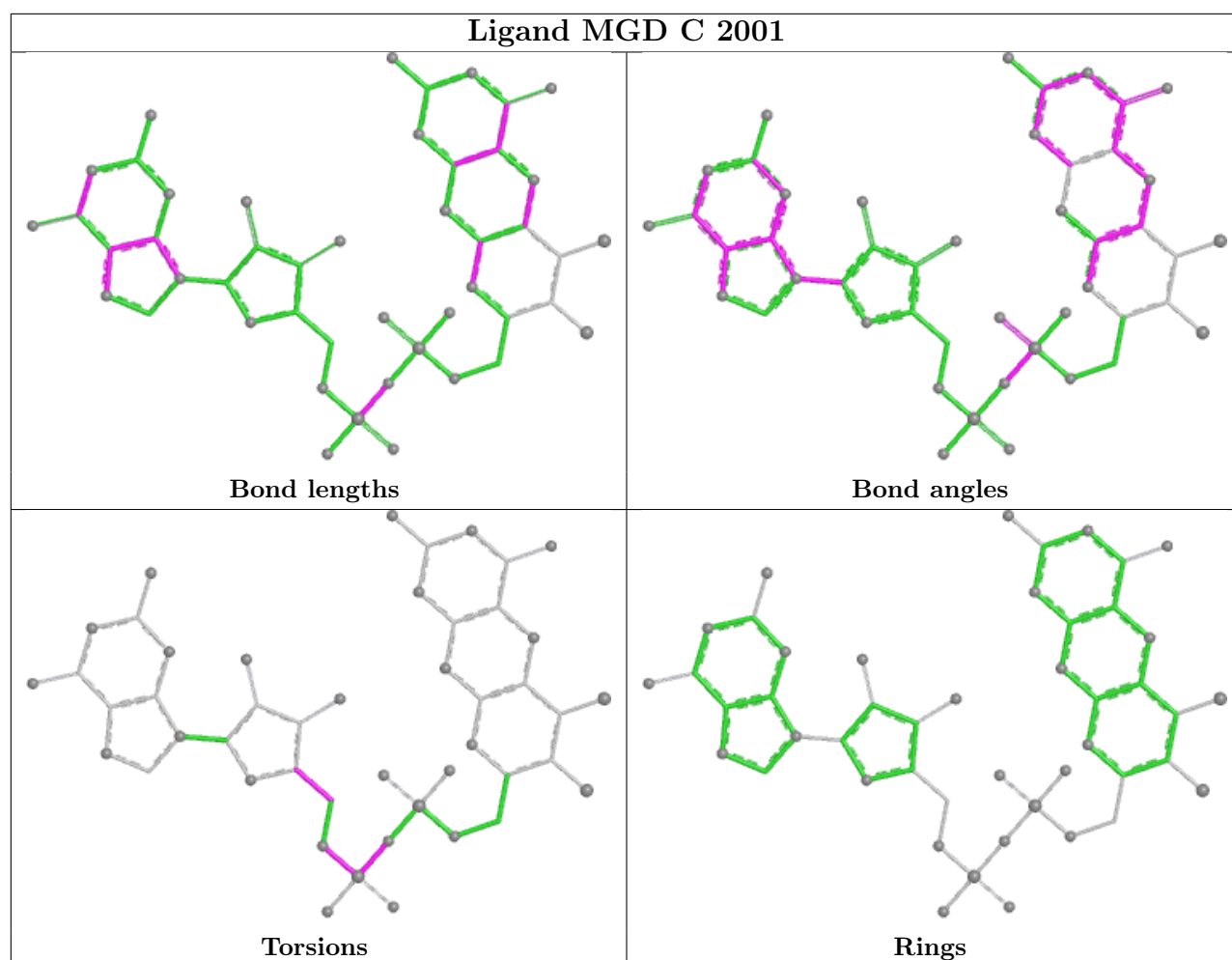


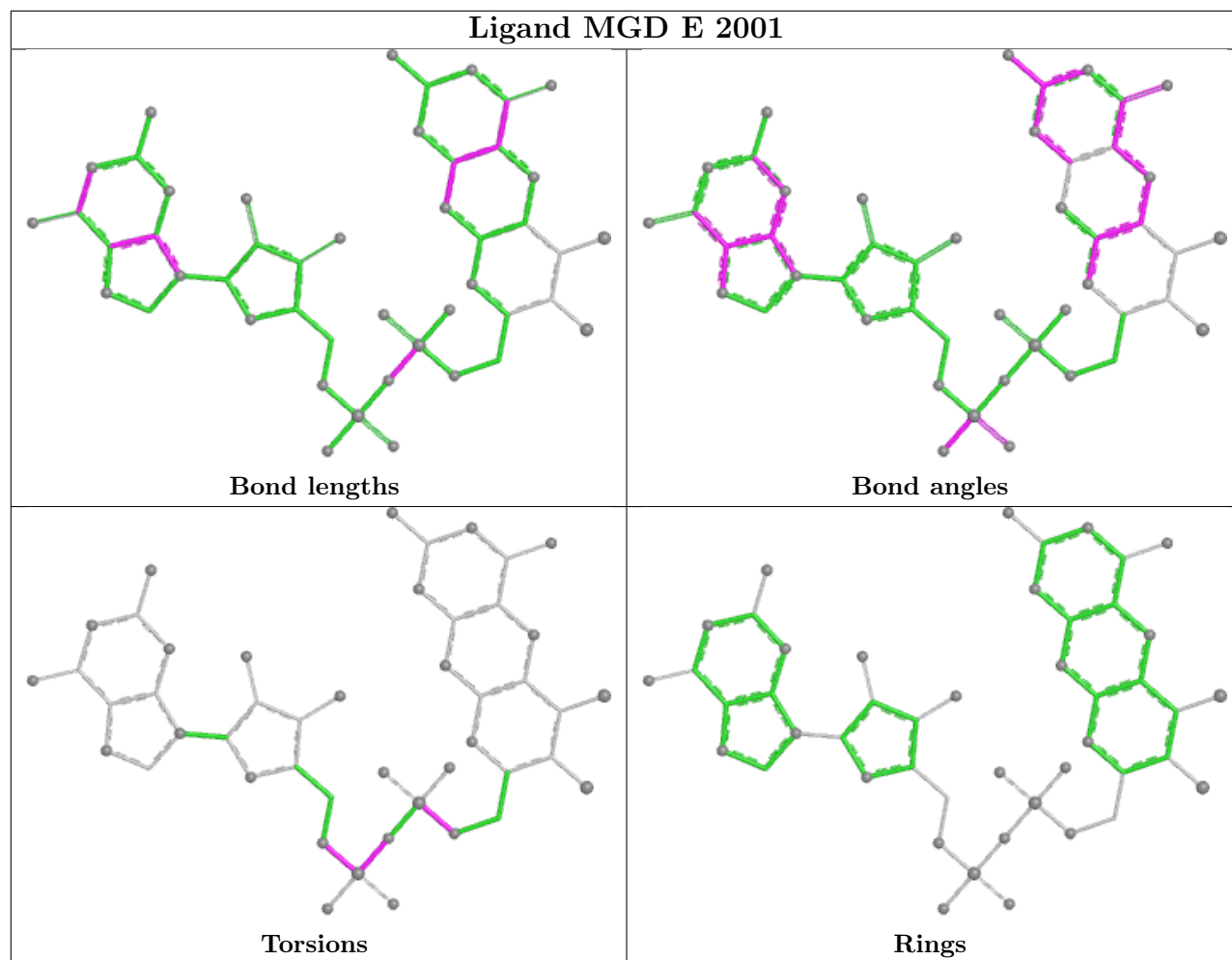












5.7 Other polymers [i](#)

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	843/843 (100%)	-0.55	7 (0%) 82 80	11, 21, 39, 65	0
1	C	843/843 (100%)	-0.40	4 (0%) 87 85	14, 24, 43, 73	0
1	E	843/843 (100%)	-0.38	5 (0%) 85 83	13, 24, 44, 72	0
1	G	843/843 (100%)	-0.52	5 (0%) 85 83	12, 22, 40, 72	0
2	B	132/132 (100%)	-0.11	0 100 100	19, 32, 51, 67	0
2	D	132/132 (100%)	-0.13	2 (1%) 72 69	20, 31, 50, 68	0
2	F	132/132 (100%)	0.29	2 (1%) 72 69	22, 36, 57, 65	0
2	H	132/132 (100%)	-0.23	1 (0%) 82 80	19, 29, 46, 60	0
All	All	3900/3900 (100%)	-0.40	26 (0%) 84 82	11, 24, 45, 73	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	340	GLY	3.9
1	E	49	GLN	3.1
1	G	41	ASN	3.0
1	C	41	ASN	2.9
2	F	44	ALA	2.9
1	A	401	GLY	2.8
1	C	268	PRO	2.7
1	A	92	HIS	2.6
1	E	339	GLU	2.6
1	A	41	ASN	2.6
1	G	844	SER	2.5
1	E	268	PRO	2.5
2	H	44	ALA	2.4
1	C	82	ARG	2.4
1	C	624	ASP	2.3
1	G	334	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	641	HIS	2.3
1	G	686	ASP	2.3
2	D	44	ALA	2.3
2	D	53	ARG	2.3
1	E	256	ARG	2.3
2	F	57	ILE	2.2
1	A	341	THR	2.1
1	A	844	SER	2.0
1	A	641	HIS	2.0
1	A	40	ILE	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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	EDO	G	2012	4/4	0.44	0.42	99,99,100,100	0
7	SO4	C	2009	5/5	0.64	0.18	64,72,76,87	0
9	GOL	A	2011	6/6	0.74	0.24	49,58,60,63	0
12	PEG	C	2010	7/7	0.77	0.24	49,53,60,65	0
9	GOL	C	2011	6/6	0.79	0.20	49,55,57,60	0
9	GOL	E	2008	6/6	0.80	0.20	47,55,61,62	0
9	GOL	G	2010	6/6	0.81	0.16	29,39,40,43	0
9	GOL	G	2011	6/6	0.81	0.16	35,43,47,48	0
7	SO4	E	2007	5/5	0.82	0.13	66,69,74,81	0
7	SO4	G	2007	5/5	0.85	0.11	54,64,68,72	0
7	SO4	C	2008	5/5	0.86	0.11	66,72,76,76	0
11	EDO	B	202	4/4	0.86	0.18	45,47,49,49	0
8	PGE	A	2010	10/10	0.87	0.14	29,35,36,38	0

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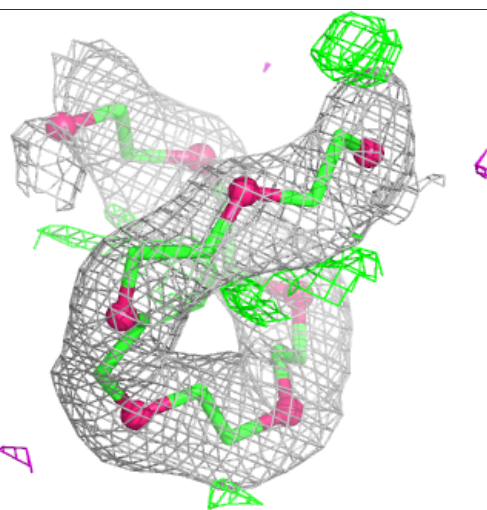
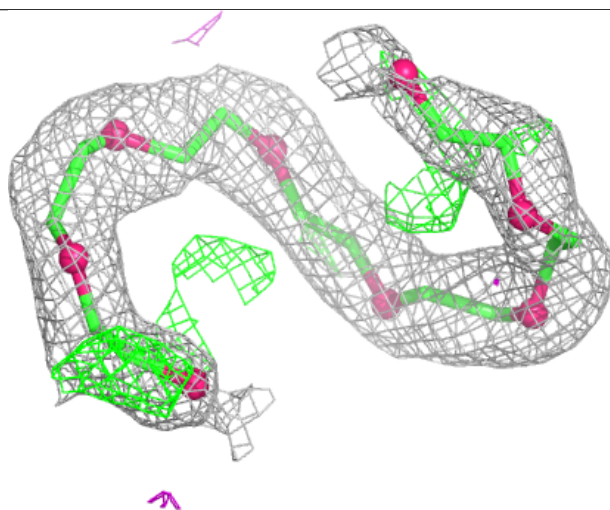
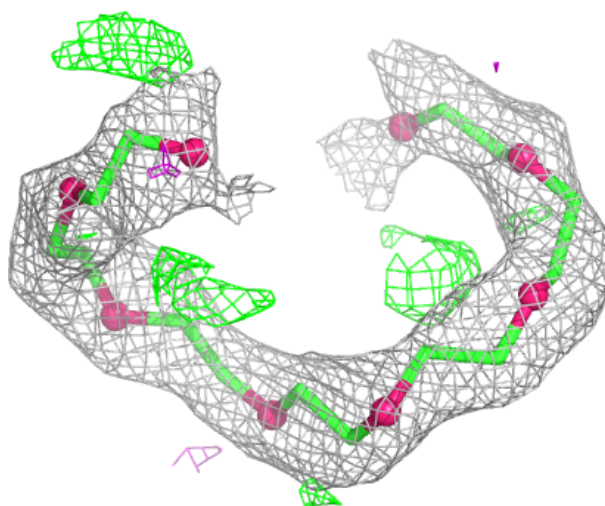
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	P33	G	2009	22/22	0.88	0.15	37,47,51,54	0
13	P33	G	2008	22/22	0.90	0.13	26,37,43,44	0
7	SO4	C	2007	5/5	0.90	0.13	57,57,64,67	0
7	SO4	A	2007	5/5	0.91	0.14	56,57,61,69	0
7	SO4	A	2006	5/5	0.92	0.14	50,57,66,66	0
11	EDO	C	2012	4/4	0.92	0.12	31,34,36,36	0
7	SO4	E	2006	5/5	0.93	0.08	61,65,68,73	0
7	SO4	A	2008	5/5	0.97	0.08	26,32,36,36	0
7	SO4	A	2009	5/5	0.98	0.06	29,32,34,35	0
7	SO4	C	2006	5/5	0.98	0.07	26,28,33,34	0
3	MGD	E	2001	47/47	0.98	0.04	14,17,20,22	0
3	MGD	E	2002	47/47	0.98	0.04	18,20,22,24	0
4	O	E	2003	1/1	0.98	0.08	32,32,32,32	0
7	SO4	G	2006	5/5	0.99	0.05	29,30,31,33	0
6	F3S	C	2005	7/7	0.99	0.03	21,22,24,24	0
6	F3S	E	2005	7/7	0.99	0.03	23,24,26,31	0
6	F3S	G	2005	7/7	0.99	0.03	20,22,25,25	0
3	MGD	C	2002	47/47	0.99	0.04	18,20,22,24	0
3	MGD	A	2001	47/47	0.99	0.04	13,16,17,18	0
3	MGD	A	2002	47/47	0.99	0.04	11,14,17,19	0
3	MGD	G	2001	47/47	0.99	0.04	14,18,19,21	0
10	FES	B	201	4/4	0.99	0.02	22,24,25,27	0
10	FES	D	201	4/4	0.99	0.03	27,28,29,31	0
10	FES	H	201	4/4	0.99	0.03	25,25,27,28	0
3	MGD	G	2002	47/47	0.99	0.04	14,17,19,20	0
4	O	A	2003	1/1	0.99	0.04	17,17,17,17	0
4	O	C	2003	1/1	0.99	0.07	22,22,22,22	0
3	MGD	C	2001	47/47	0.99	0.04	15,18,20,21	0
4	O	G	2003	1/1	0.99	0.05	23,23,23,23	0
6	F3S	A	2005	7/7	0.99	0.03	19,20,22,24	0
5	4MO	E	2004	1/1	1.00	0.01	23,23,23,23	0
5	4MO	G	2004	1/1	1.00	0.01	22,22,22,22	0
10	FES	F	201	4/4	1.00	0.02	29,30,31,31	0
5	4MO	A	2004	1/1	1.00	0.01	18,18,18,18	0
5	4MO	C	2004	1/1	1.00	0.01	23,23,23,23	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.

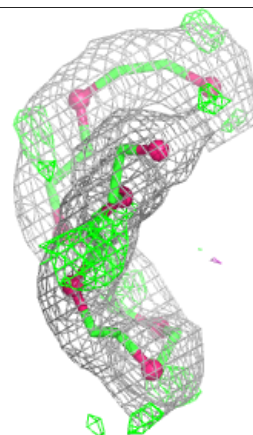
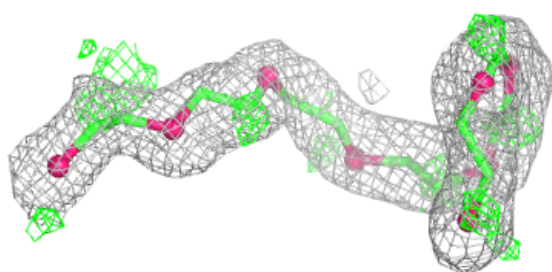
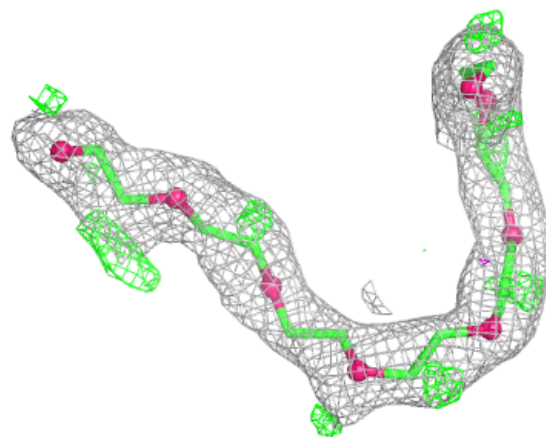
Electron density around P33 G 2009:

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

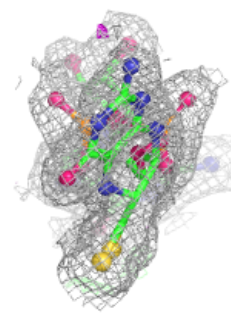
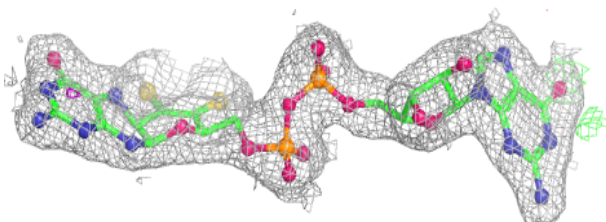
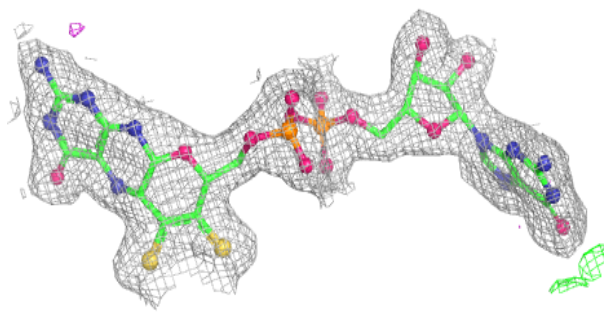


Electron density around P33 G 2008:

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

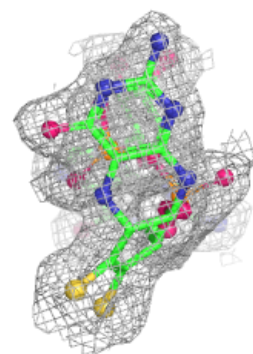
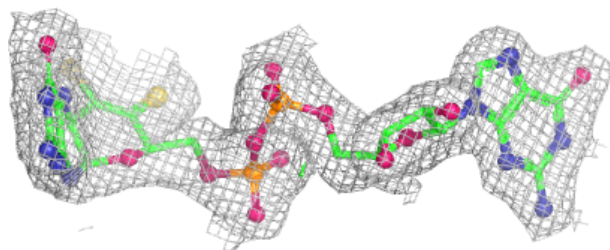
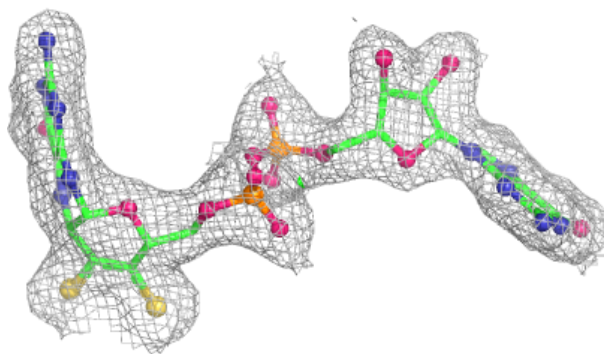
**Electron density around MGD E 2001:**

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

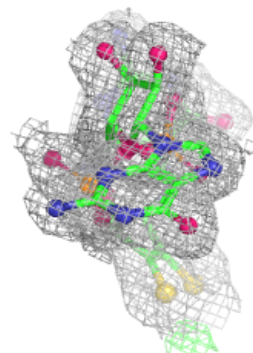
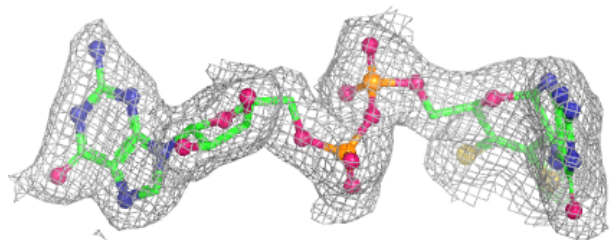
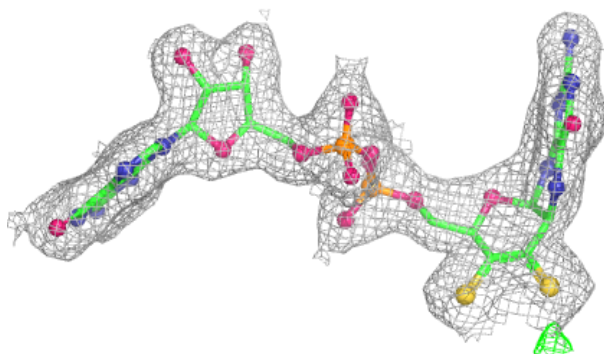


Electron density around MGD E 2002:

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

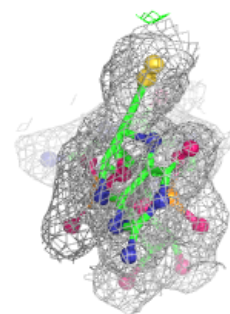
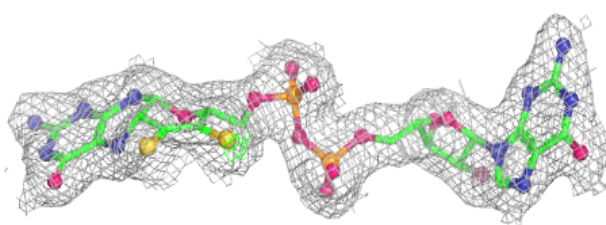
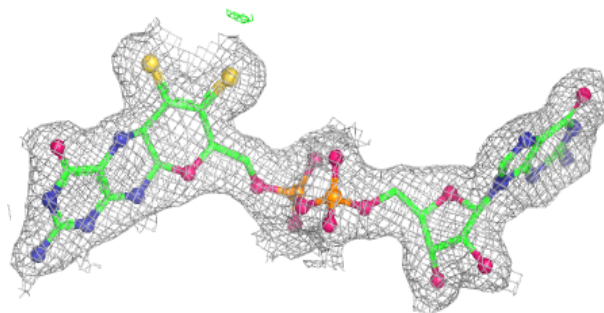
**Electron density around MGD C 2002:**

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

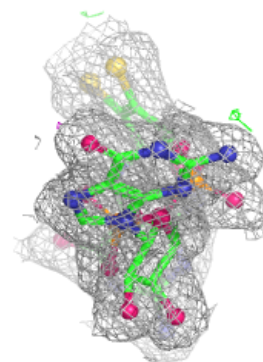
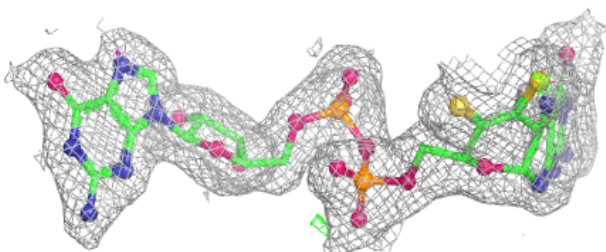
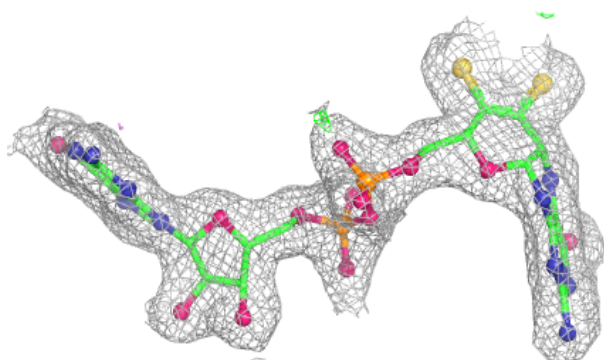


Electron density around MGD A 2001:

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

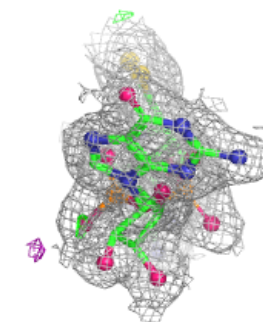
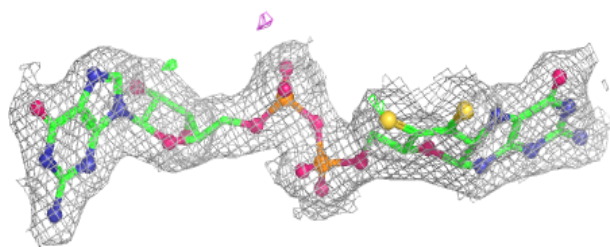
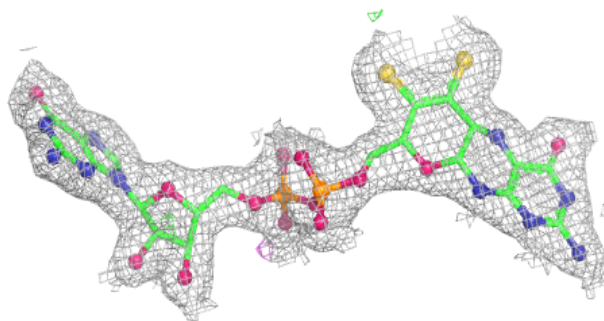
**Electron density around MGD A 2002:**

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

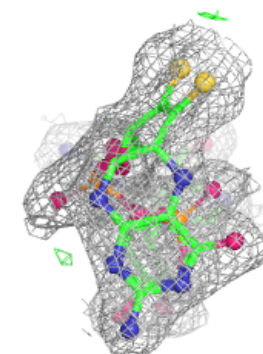
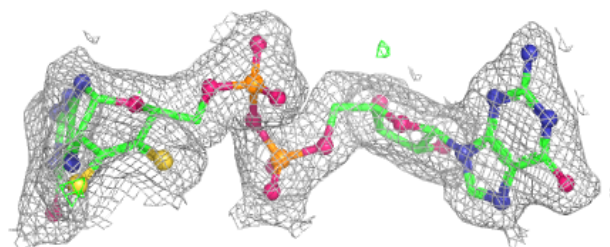
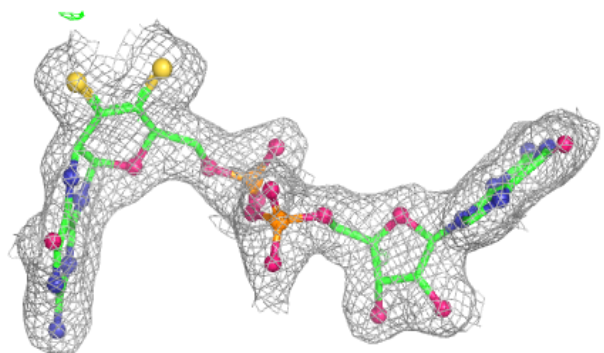


Electron density around MGD G 2001:

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

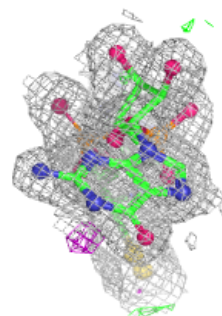
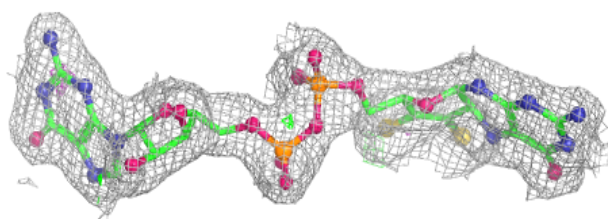
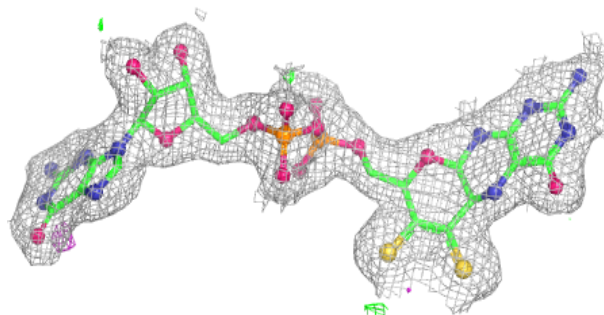
**Electron density around MGD G 2002:**

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



Electron density around MGD C 2001:

$2mF_o-DF_c$ (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.