



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 11:21 pm BST

PDB ID : 2NYA
Title : Crystal structure of the periplasmic nitrate reductase (NAP) from Escherichia coli
Authors : Jepson, B.J.N.; Richardson, D.J.; Hemmings, A.M.
Deposited on : 2006-11-20
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

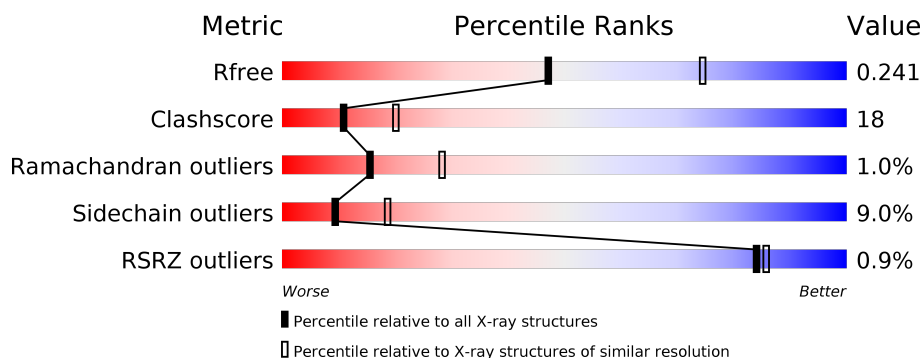
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	792	<div> <div></div> <div> <div></div> <div>68%</div> <div>27%</div> <div>5%</div> </div> </div>
1	F	792	<div> <div></div> <div> <div></div> <div>64%</div> <div>30%</div> <div>5%</div> </div> </div>

2 Entry composition [i](#)

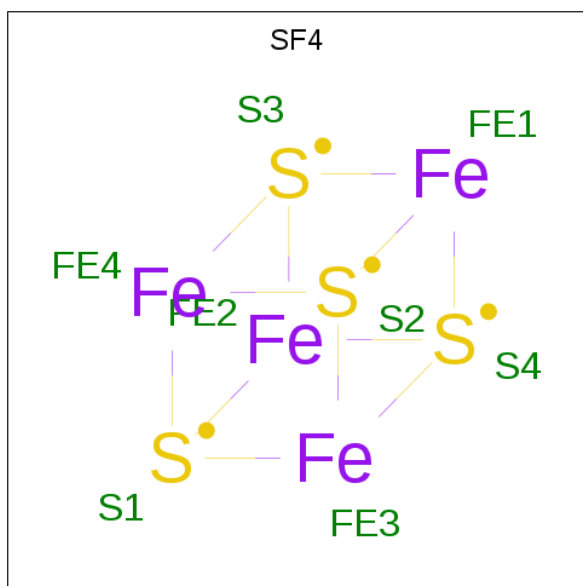
There are 5 unique types of molecules in this entry. The entry contains 13733 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Periplasmic nitrate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	791	Total	C	N	O	S	0	0	0
			6301	4012	1100	1157	32			
1	F	791	Total	C	N	O	S	0	0	0
			6301	4012	1100	1157	32			

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

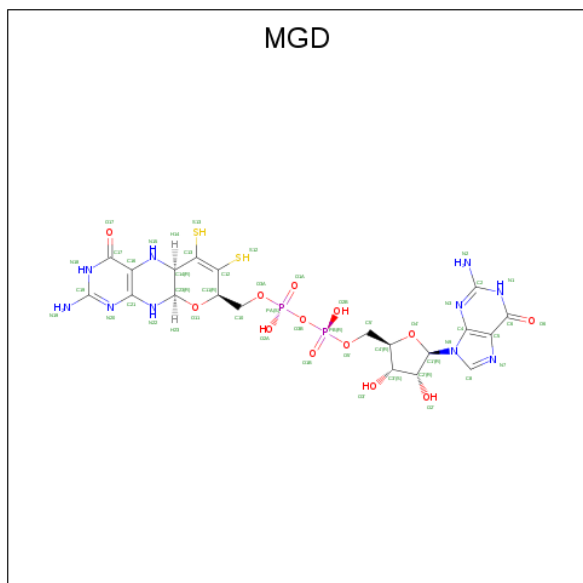


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is MOLYBDENUM(VI) ION (three-letter code: 6MO) (formula: Mo).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mo 1 1	0	0
3	F	1	Total Mo 1 1	0	0

- Molecule 4 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 (three-letter code: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	F	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	F	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

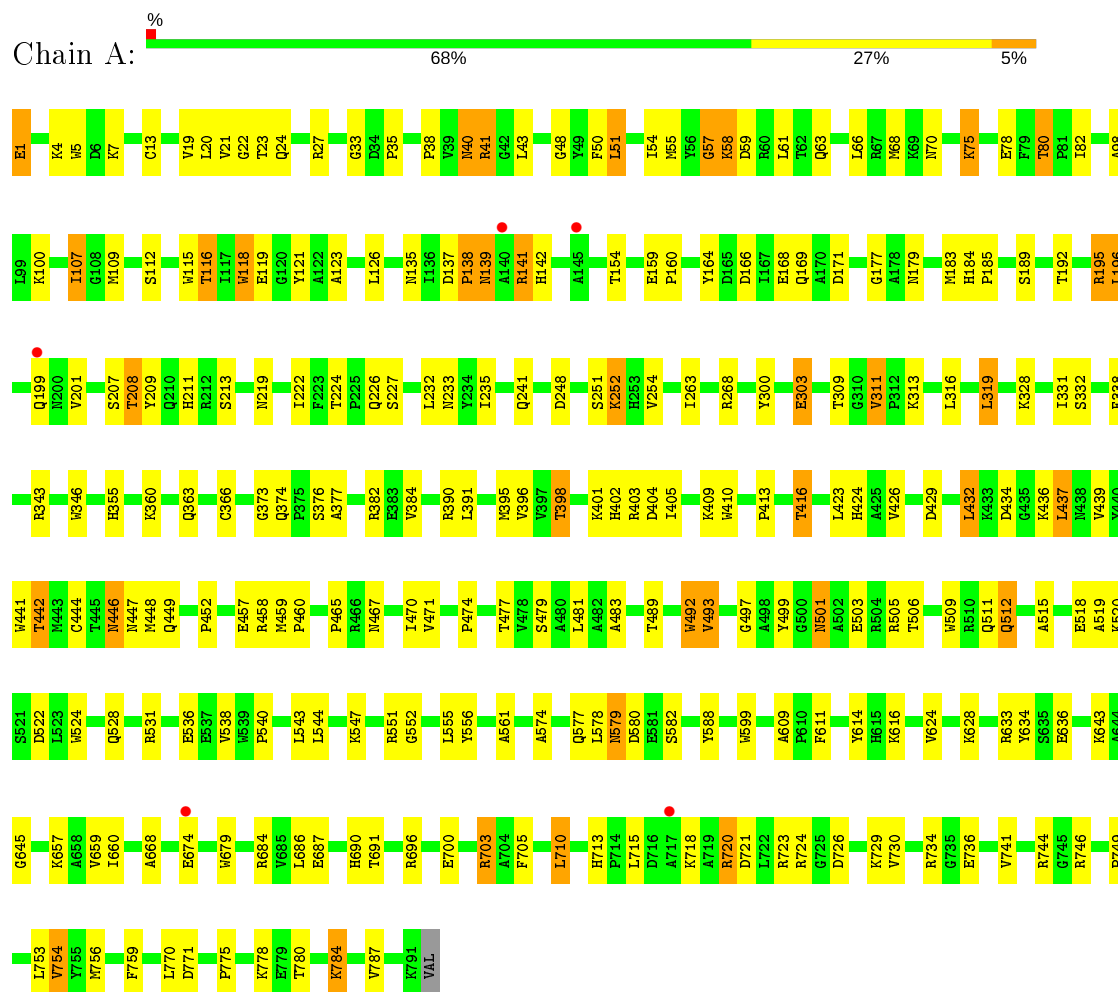
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	489	Total O 489 489	0	0
5	F	436	Total O 436 436	0	0

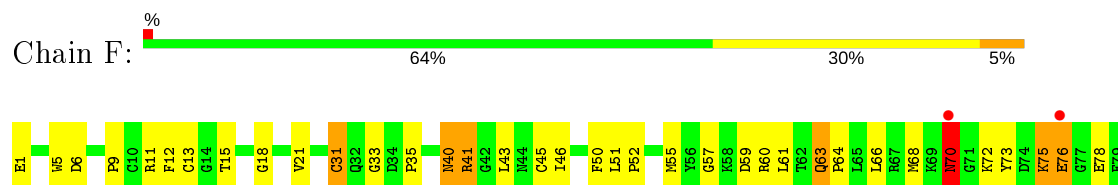
3 Residue-property plots

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

• Molecule 1: Periplasmic nitrate reductase



• Molecule 1: Periplasmic nitrate reductase



T80	L196	Q308	K408	A502	H606	V731
E93	S197	T309	K409	E503	Y614	S732
M109	M198	Q310	P413	R504	R733	R733
T116	Q199	V311	T416	T506	G619	G735
I117	T202	P312	I421	Q507	R621	I740
W118	V203	D314	G422	F508	K628	V741
E119	L206	Q315	L423	R510	Q631	N747
G120	S207	L316	H424	Q511	Q512	R748
Y121	T208	E317	A427	Q512	D639	P749
A122	Y209	Q318	A515	A515		P750
A123	D210	I319	A519	A519	V642	
L126	R211	T331	K432	K520	K643	L753
N135	R212	S332	K433	K520	A644	V754
Y136	F214	S213	D434	Q525	G652	Y755
D137	E215	Q336	L437	Q528	V659	F759
P138	G337	F337	T442	R531	I660	L764
N139	I218	Q338	M443	R532	A668	L768
A140	N219	D340	C444	F533	D673	T769
R141	I222	T342	T445	N446	E674	L770
H142	F223	R343	N447	V538		
C143	T224	Q346	P452	W539	R684	P775
V148	F225	N353	E456	L543	V685	E779
T154	S227	L354	E457	L544	L686	T780
F155	I231	R355	N467	R551	H690	K783
M161	L232	C366	V471	T554	R696	K784
G162	N233	Q373	S472	Y556	R697	V787
D165	I234	Q374	P474	A561	E700	K791
D166	I235	P375	S479	E572	L701	VAL
I167	I240	S376	A483	L573	H702	
E168	Q241	R382	D484	A574	A704	
Q169	I245	V384	L485	Q577	F705	
A172	D248	R390	L486	L578	P706	
L175	S251	L391	L487	D580	V709	
M179	R253	K395	T489	E581	L710	
M180	L256	V396	A490	S582	F711	
M183	R268	V397	N491	F587	I712	
H184	G281	T398	W492	Y588	H713	
P185	E291	K401	E494	L589	A719	
I186	T301	R403	K495	Y597	R720	
L187	L302	D404	E496	L722	D721	
R190	E303	I405	G497	A598	R723	
Y191	R304	C406	Y499	F600	D726	
T192	T305	E407	N501	G601	V730	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.45Å 94.60Å 131.21Å 90.00° 96.34° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 49.69 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (50.00-2.50) 97.1 (49.69-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.181 , 0.243 0.181 , 0.241	Depositor DCC
R_{free} test set	2860 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13733	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.11% 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: 6MO, SF4, MGD

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	0.72	1/6470 (0.0%)	0.80	3/8770 (0.0%)
1	F	0.68	0/6470	0.76	2/8770 (0.0%)
All	All	0.70	1/12940 (0.0%)	0.78	5/17540 (0.0%)

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
1	F	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	TRP	CB-CG	-5.06	1.41	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	GLY	O-C-N	-5.99	113.12	122.70
1	A	720	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	F	578	LEU	CA-CB-CG	5.20	127.25	115.30
1	F	319	LEU	CA-CB-CG	5.20	127.25	115.30
1	A	720	ARG	NE-CZ-NH2	-5.18	117.71	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	PRO	Peptide
1	F	313	LYS	Peptide
1	F	57	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	6301	0	6155	215	0
1	F	6301	0	6155	247	0
2	A	8	0	0	0	0
2	F	8	0	0	0	0
3	A	1	0	0	0	0
3	F	1	0	0	0	0
4	A	94	0	44	15	0
4	F	94	0	44	17	0
5	A	489	0	0	15	0
5	F	436	0	0	29	1
All	All	13733	0	12398	458	1

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 18.

The worst 5 of 458 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:F:783:LYS:HG3	5:F:7033:HOH:O	1.43	1.18
1:F:109:MET:CE	1:F:123:ALA:HB1	1.95	0.96
1:F:684:ARG:NH2	4:F:6001:MGD:H15	1.63	0.95
1:F:193:ASN:HB3	5:F:7024:HOH:O	1.68	0.93
1:F:668:ALA:HA	5:F:7032:HOH:O	1.67	0.93

All (1) 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)
5:F:7379:HOH:O	5:F:7409:HOH:O[2_655]	1.98	0.22

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	789/792 (100%)	736 (93%)	47 (6%)	6 (1%)	19	35
1	F	789/792 (100%)	725 (92%)	55 (7%)	9 (1%)	14	26
All	All	1578/1584 (100%)	1461 (93%)	102 (6%)	15 (1%)	15	28

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	F	70	ASN
1	F	215	GLU
1	F	314	ASP
1	F	241	GLN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	661/663 (100%)	600 (91%)	61 (9%)	9	18
1	F	661/663 (100%)	603 (91%)	58 (9%)	10	19
All	All	1322/1326 (100%)	1203 (91%)	119 (9%)	9	19

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	703	ARG
1	F	45	CYS
1	F	578	LEU
1	A	710	LEU
1	A	787	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	690	HIS
1	F	179	ASN
1	F	525	GLN
1	F	40	ASN
1	F	200	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MGD	F	7001	3	41,52,52	1.54	3 (7%)	43,81,81	2.25	11 (25%)
2	SF4	A	2001	1	0,12,12	0.00	-	-		
2	SF4	F	5001	1	0,12,12	0.00	-	-		
4	MGD	A	3001	3	41,52,52	1.50	6 (14%)	43,81,81	2.57	17 (39%)
4	MGD	A	4001	3	41,52,52	1.40	4 (9%)	43,81,81	2.36	14 (32%)
4	MGD	F	6001	3	41,52,52	1.55	6 (14%)	43,81,81	2.58	18 (41%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MGD	F	7001	3	-	6/18/66/66	0/6/6/6
2	SF4	A	2001	1	-	-	0/6/5/5
2	SF4	F	5001	1	-	-	0/6/5/5
4	MGD	A	3001	3	-	6/18/66/66	0/6/6/6
4	MGD	A	4001	3	-	6/18/66/66	0/6/6/6
4	MGD	F	6001	3	-	4/18/66/66	0/6/6/6

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	7001	MGD	C17-C16	6.24	1.50	1.41
4	A	3001	MGD	C17-C16	5.63	1.49	1.41
4	A	4001	MGD	C17-C16	5.21	1.48	1.41
4	F	6001	MGD	C17-C16	4.91	1.48	1.41
4	A	3001	MGD	C6-C5	4.57	1.49	1.41

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	4001	MGD	C17-C16-N15	6.89	124.91	119.12
4	A	3001	MGD	C17-C16-N15	6.20	124.33	119.12
4	F	7001	MGD	C2-N3-C4	5.76	121.93	115.36
4	F	6001	MGD	O11-C23-C14	-5.40	105.36	108.96
4	F	7001	MGD	C17-C16-N15	5.30	123.57	119.12

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

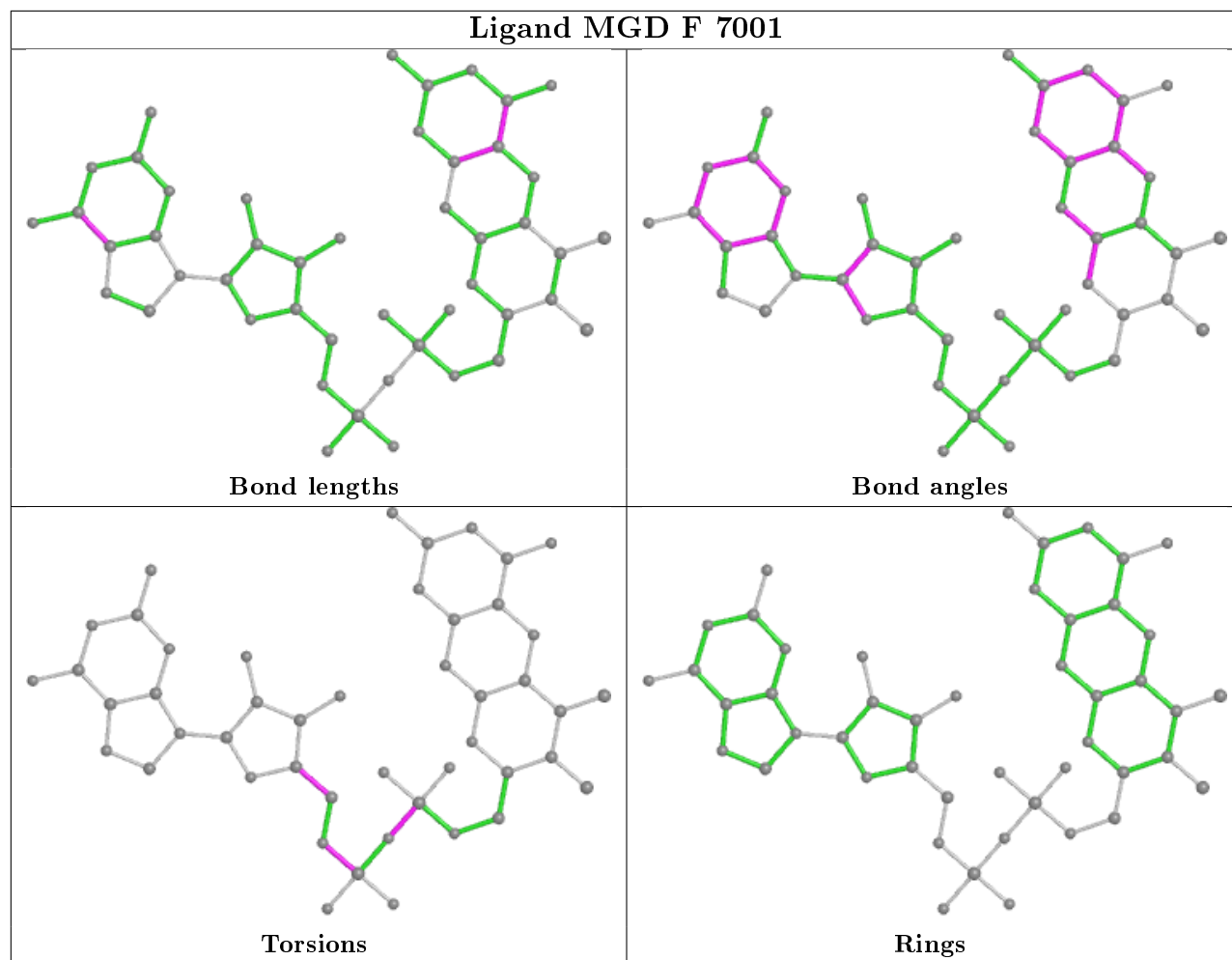
Mol	Chain	Res	Type	Atoms
4	F	7001	MGD	C5'-O5'-PB-O2B
4	A	3001	MGD	PA-O3B-PB-O5'
4	A	3001	MGD	C5'-O5'-PB-O2B
4	A	3001	MGD	C5'-O5'-PB-O3B
4	A	4001	MGD	C5'-O5'-PB-O1B

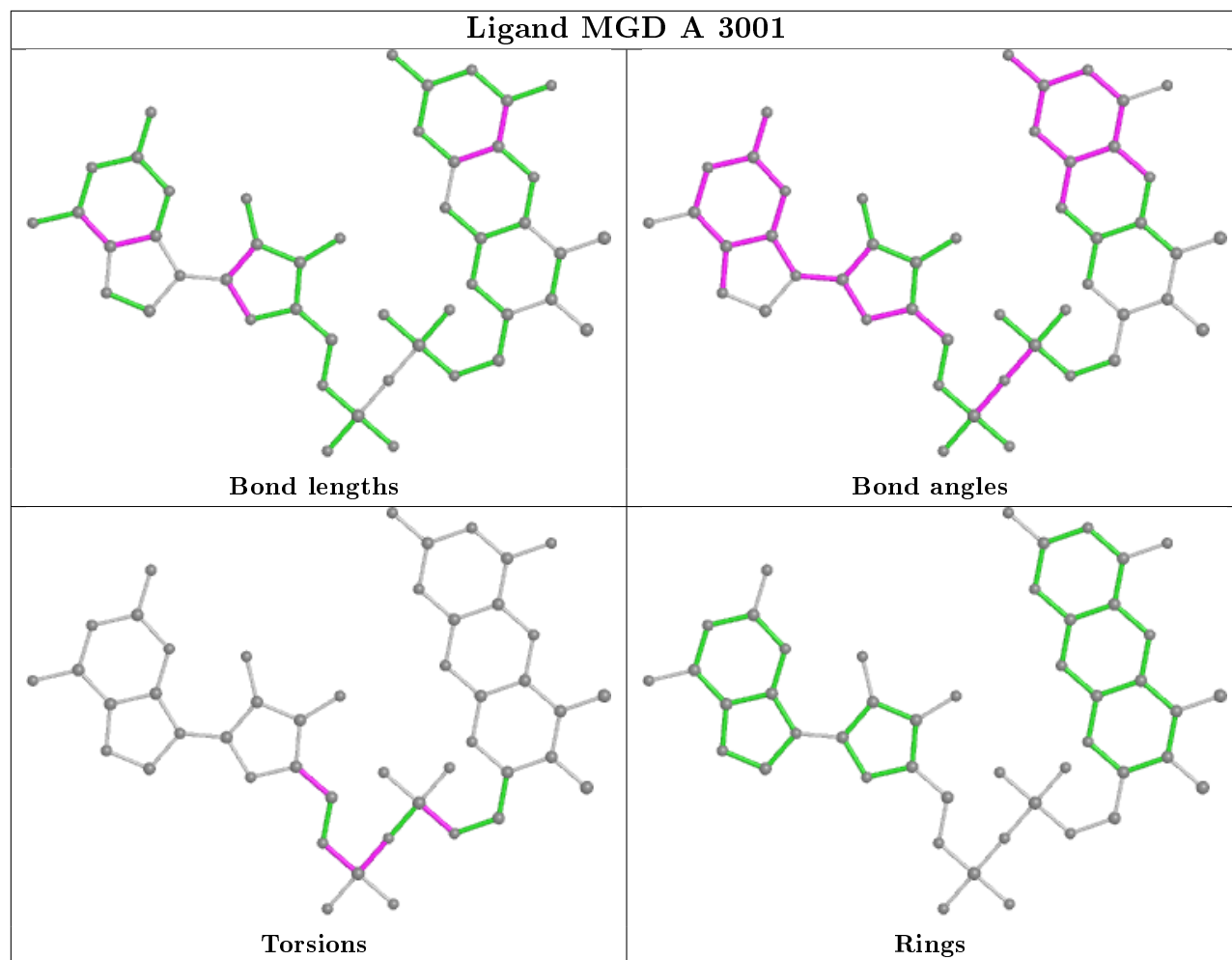
There are no ring outliers.

4 monomers are involved in 32 short contacts:

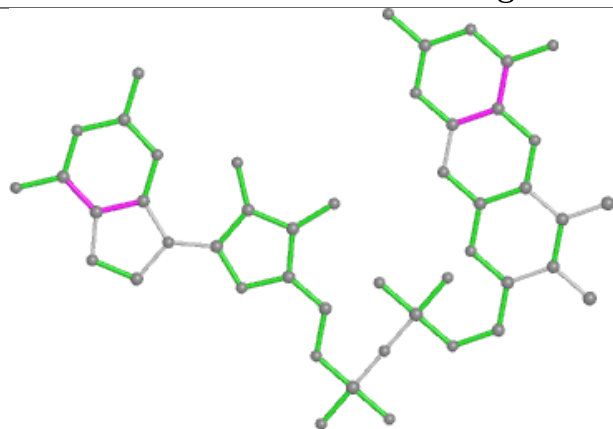
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	7001	MGD	8	0
4	A	3001	MGD	7	0
4	A	4001	MGD	8	0
4	F	6001	MGD	9	0

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.

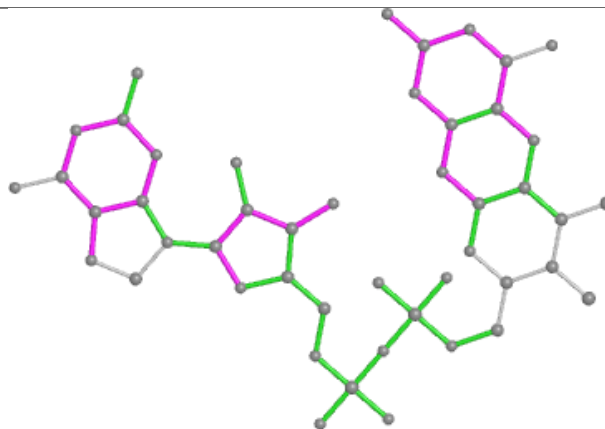




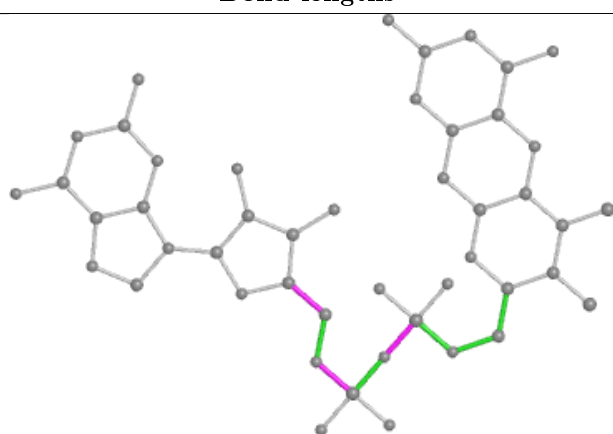
Ligand MGD A 4001



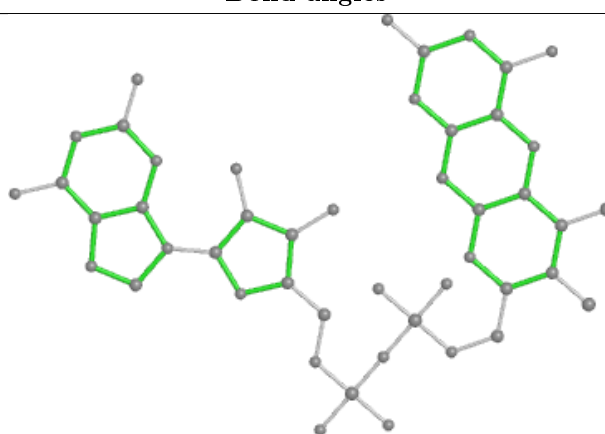
Bond lengths



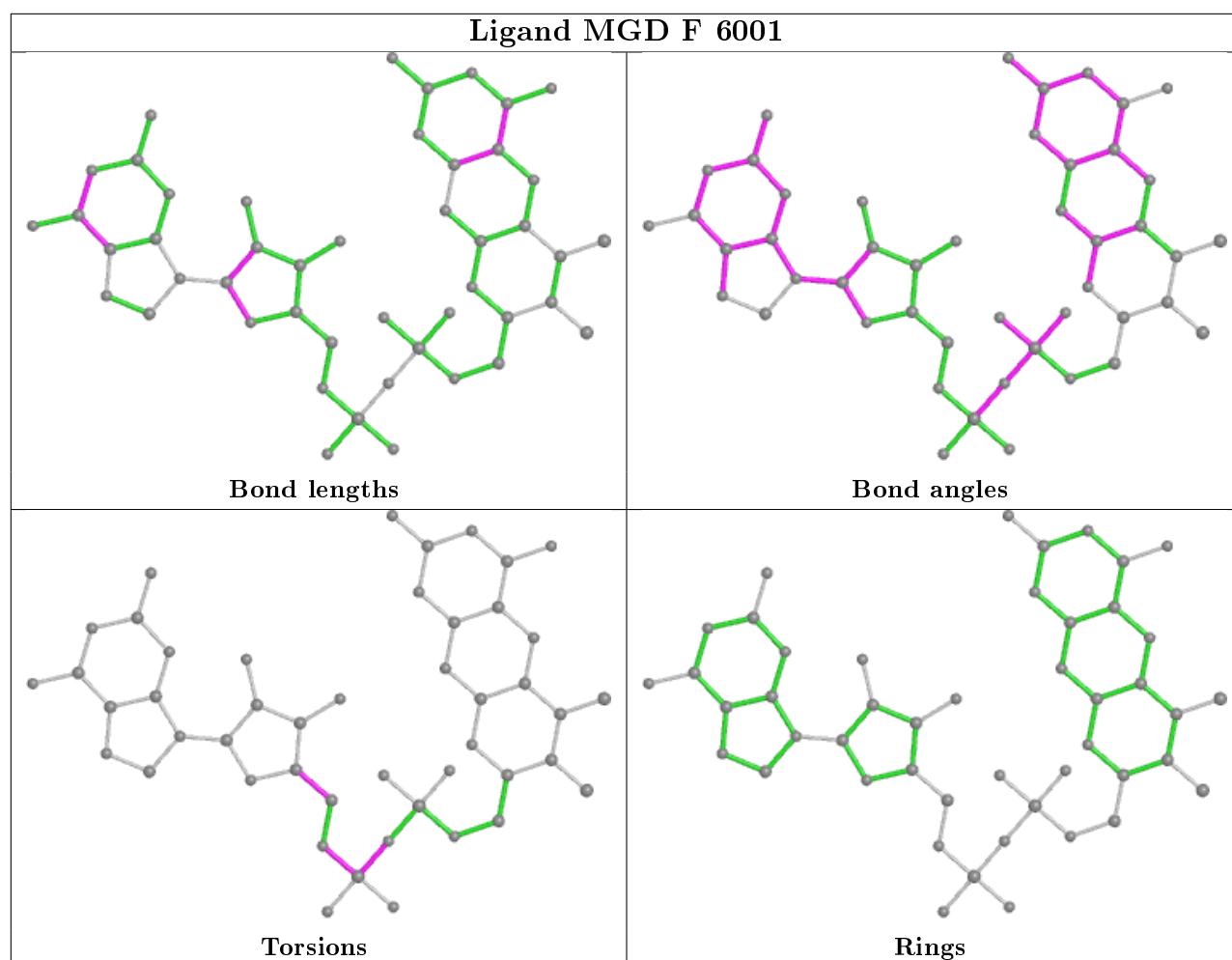
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	791/792 (99%)	-0.19	5 (0%) 89 90	13, 24, 37, 46	0
1	F	791/792 (99%)	0.00	9 (1%) 80 82	17, 30, 45, 55	0
All	All	1582/1584 (99%)	-0.09	14 (0%) 84 86	13, 27, 42, 55	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	723	ARG	3.7
1	F	140	ALA	3.6
1	A	717	ALA	3.1
1	F	76	GLU	2.7
1	F	644	ALA	2.6

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

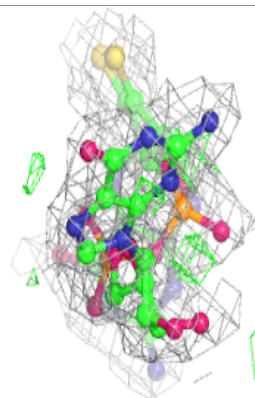
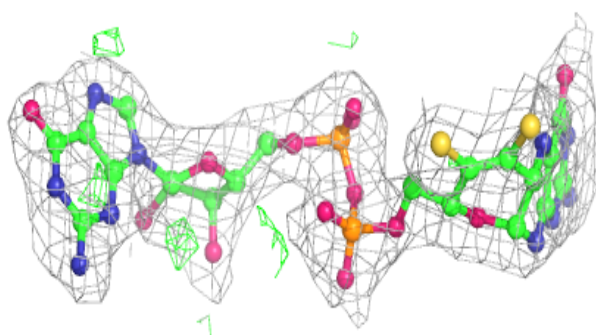
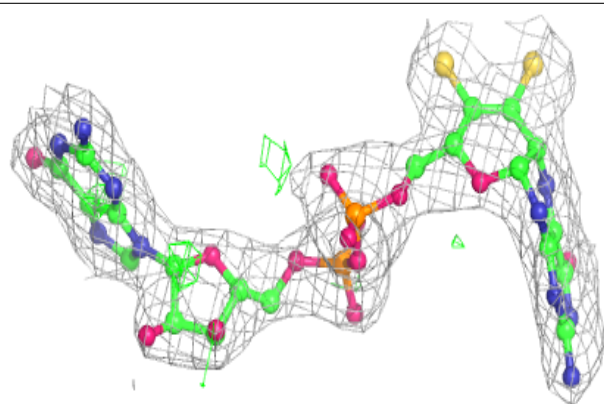
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MGD	F	7001	47/47	0.97	0.15	18,22,27,31	0
2	SF4	F	5001	8/8	0.97	0.06	25,26,29,30	0
4	MGD	A	3001	47/47	0.98	0.15	11,16,17,20	0
4	MGD	A	4001	47/47	0.98	0.17	13,21,26,30	0
4	MGD	F	6001	47/47	0.98	0.15	15,19,21,22	0
2	SF4	A	2001	8/8	0.99	0.06	24,26,28,28	0
3	6MO	F	5002	1/1	1.00	0.10	24,24,24,24	0
3	6MO	A	2002	1/1	1.00	0.12	20,20,20,20	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.

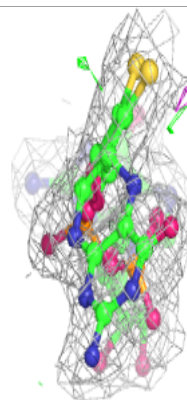
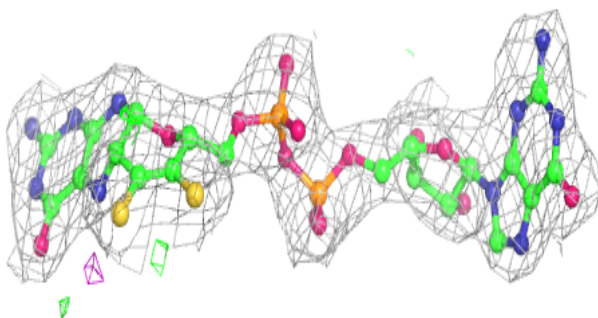
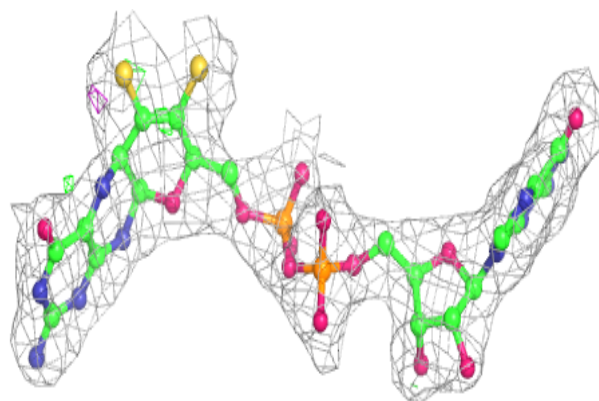
Electron density around MGD F 7001:

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

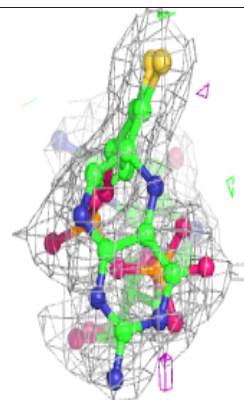
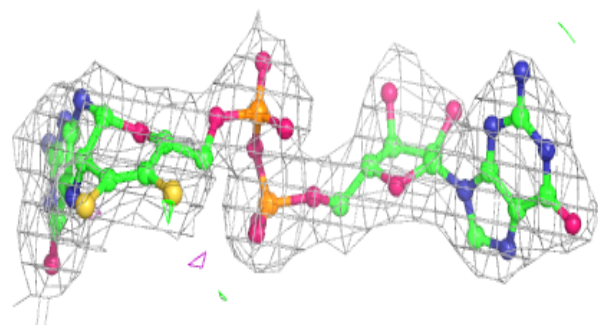
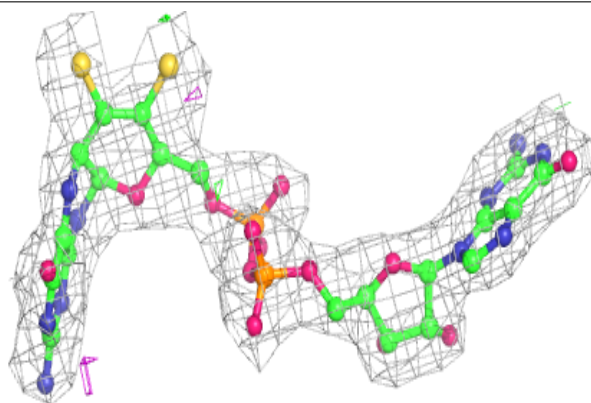


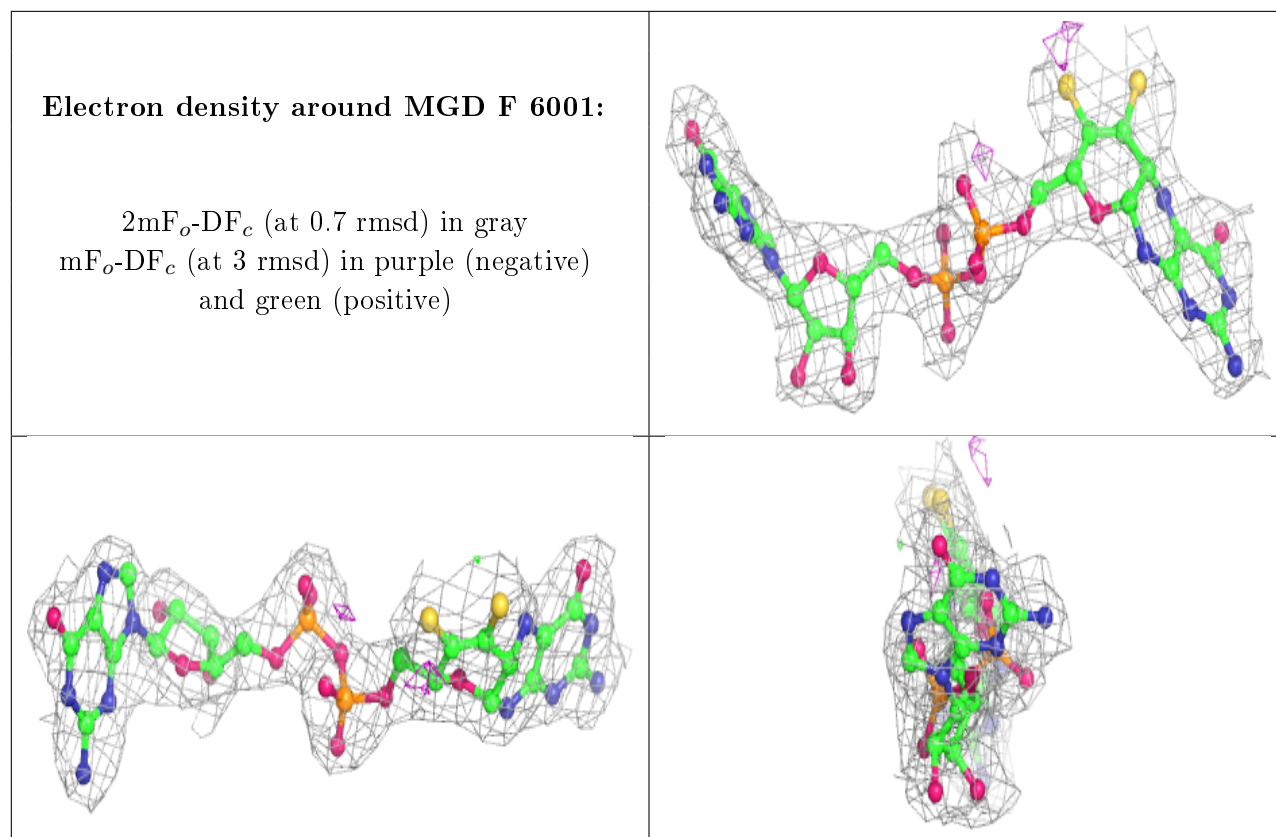
Electron density around MGD A 3001:

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

**Electron density around MGD A 4001:**

$2mF_o-DF_c$ (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.