Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2023 – 07:58 PM EDT

PDB ID	:	4ZU4
Title	:	X-ray structure of the 3,4-ketoisomerase domain of FdtD from Shewanella denitrificans
Authors	:	Thoden, J.B.; Vinogradov, E.; Gilbert, M.; Salinger, A.J.; Holden, H.M.
Deposited on	:	2015-05-15
Resolution	:	1.70 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:

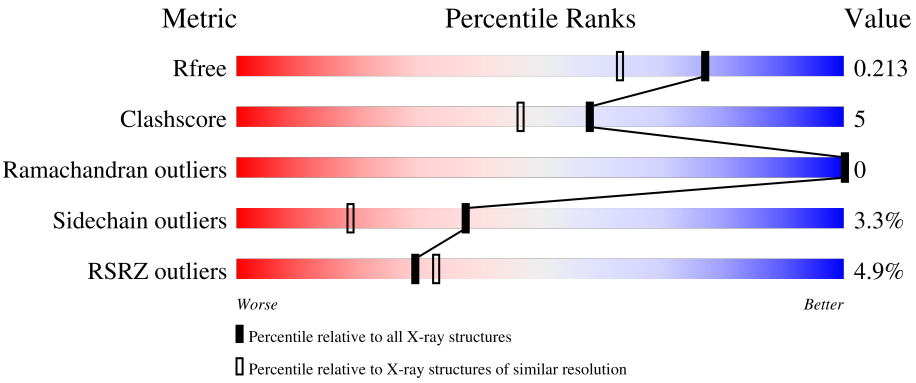
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	148	2% 86% 11%
1	B	148	8% 85% 9%
1	C	148	5% 89% 10%
1	D	148	6% 80% 16%
1	E	148	3% 84% 12%

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Mol	Chain	Length	Quality of chain
1	F	148	

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
2	4TG	B	401	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8024 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 WxcM-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	2	0
			1187	762	198	221	6			
1	B	142	Total	C	N	O	S	0	0	0
			1162	747	194	215	6			
1	C	146	Total	C	N	O	S	0	4	0
			1212	776	203	226	7			
1	D	143	Total	C	N	O	S	0	2	0
			1180	760	196	217	7			
1	E	144	Total	C	N	O	S	0	3	0
			1187	762	197	222	6			
1	F	142	Total	C	N	O	S	0	0	0
			1162	747	194	215	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	157	GLY	-	expression tag	UNP Q12KT8
A	158	HIS	-	expression tag	UNP Q12KT8
A	159	MET	-	expression tag	UNP Q12KT8
B	157	GLY	-	expression tag	UNP Q12KT8
B	158	HIS	-	expression tag	UNP Q12KT8
B	159	MET	-	expression tag	UNP Q12KT8
C	157	GLY	-	expression tag	UNP Q12KT8
C	158	HIS	-	expression tag	UNP Q12KT8
C	159	MET	-	expression tag	UNP Q12KT8
D	157	GLY	-	expression tag	UNP Q12KT8
D	158	HIS	-	expression tag	UNP Q12KT8
D	159	MET	-	expression tag	UNP Q12KT8
E	157	GLY	-	expression tag	UNP Q12KT8
E	158	HIS	-	expression tag	UNP Q12KT8
E	159	MET	-	expression tag	UNP Q12KT8
F	157	GLY	-	expression tag	UNP Q12KT8
F	158	HIS	-	expression tag	UNP Q12KT8

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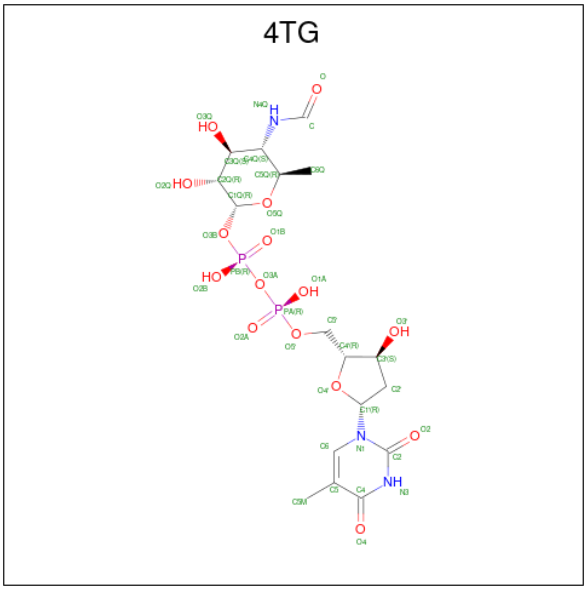
Chain	Residue	Modelled	Actual	Comment	Reference
F	159	MET	-	expression tag	UNP Q12KT8

- Molecule 2 is dTDP-4,6-dideoxy-4-formamido-glucose (three-letter code: 4TG) (formula: $C_{17}H_{27}N_3O_{15}P_2$).

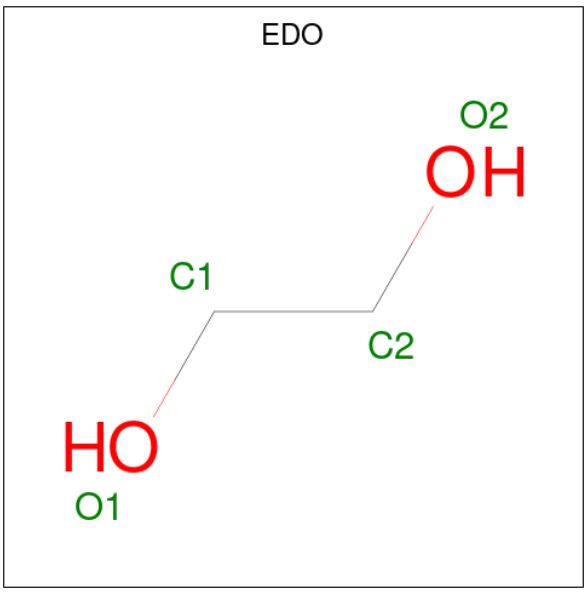


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			74	34	6	30	4		
2	B	1	Total	C	N	O	P	0	0
			37	17	3	15	2		
2	C	1	Total	C	N	O	P	0	0
			37	17	3	15	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	D	2	Total	Cl	0	0
			2	2		
3	E	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

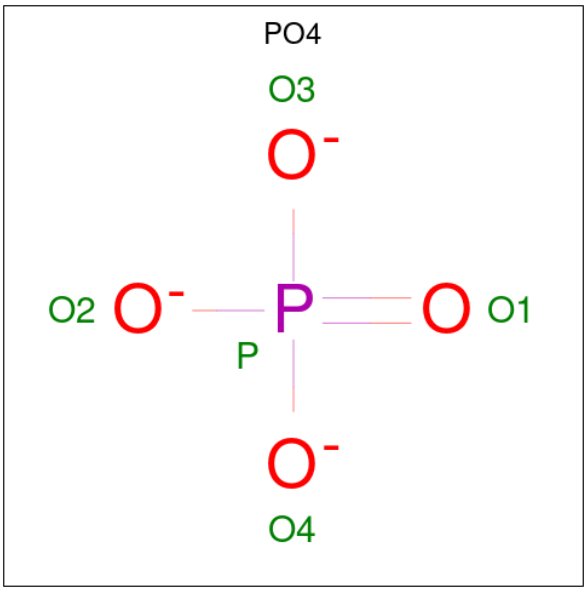


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	C	1	Total Na 1 1	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total O P 5 4 1	0	0

- Molecule 7 is water.

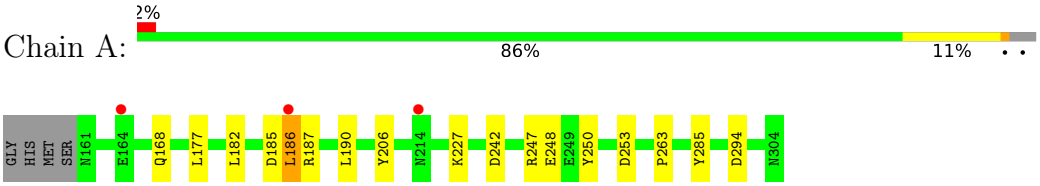
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	143	Total O 143 143	0	0
7	B	77	Total O 77 77	0	0
7	C	128	Total O 128 128	0	0
7	D	107	Total O 107 107	0	0
7	E	140	Total O 140 140	0	0
7	F	154	Total O 154 154	0	0

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.

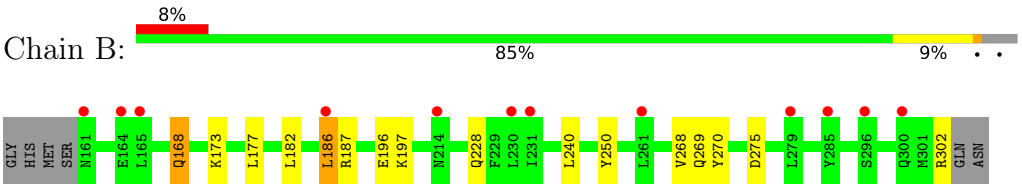
• Molecule 1: WxcM-like protein

Chain A:



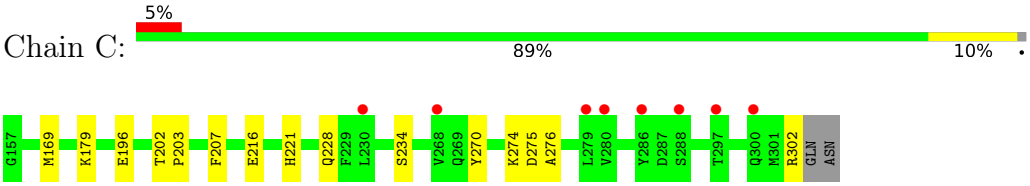
• Molecule 1: WxcM-like protein

Chain B:



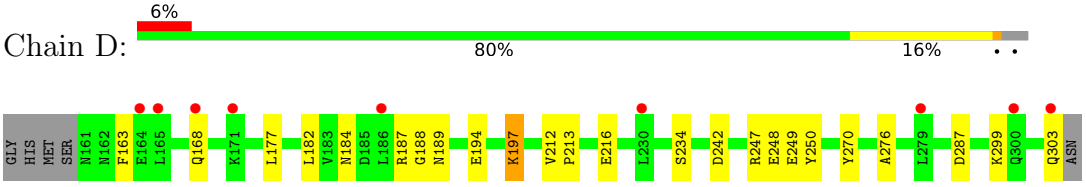
• Molecule 1: WxcM-like protein

Chain C:



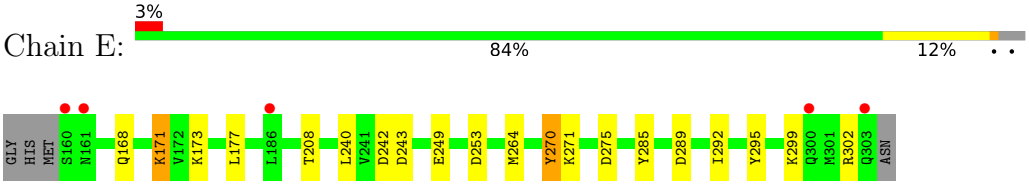
• Molecule 1: WxcM-like protein

Chain D:



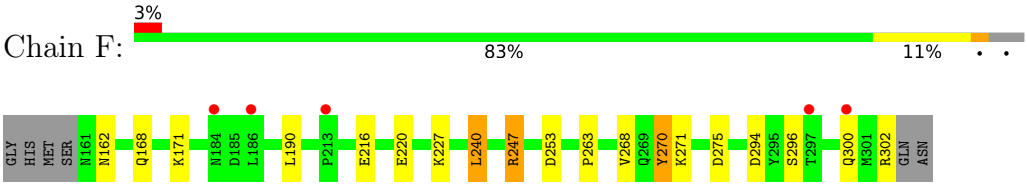
• Molecule 1: WxcM-like protein

Chain E:



• Molecule 1: WxcM-like protein

Chain F:


3%
83%
11%
GLY
HIS
MET
SER
N161
N162
Q168
K171
N184
D185
L186
L190
P213
E216
E220
K227
L240
R247
D253
P263
V268
Q269
Y270
K271
D275
D294
Y295
S296
T297
Q300
M301
R302
GLN
ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.41Å 64.58Å 112.97Å 90.00° 111.39° 90.00°	Depositor
Resolution (Å)	28.28 – 1.70 28.26 – 1.70	Depositor EDS
% Data completeness (in resolution range)	91.7 (28.28-1.70) 91.8 (28.26-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	9.66 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.171 , 0.207 0.178 , 0.213	Depositor DCC
R_{free} test set	5776 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8024	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 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CL, PO4, EDO, 4TG

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	0.67	0/1222	0.99	3/1646 (0.2%)
1	B	0.57	0/1191	0.91	2/1605 (0.1%)
1	C	0.72	0/1254	1.06	6/1689 (0.4%)
1	D	0.68	0/1215	1.01	4/1637 (0.2%)
1	E	0.69	0/1225	1.04	5/1651 (0.3%)
1	F	0.73	0/1191	1.10	4/1605 (0.2%)
All	All	0.68	0/7298	1.02	24/9833 (0.2%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	275[A]	ASP	CB-CG-OD1	10.24	127.51	118.30
1	C	275[B]	ASP	CB-CG-OD1	10.24	127.51	118.30
1	C	302	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	A	242	ASP	CB-CG-OD2	-7.63	111.44	118.30
1	B	302	ARG	NE-CZ-NH2	6.78	123.69	120.30
1	F	275	ASP	CB-CG-OD1	6.72	124.35	118.30
1	E	275	ASP	CB-CG-OD1	6.42	124.07	118.30
1	B	275	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	294	ASP	CB-CG-OD1	-6.18	112.74	118.30
1	D	242	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	E	285	TYR	CB-CG-CD1	5.92	124.56	121.00
1	E	302	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	D	287	ASP	CB-CG-OD1	5.86	123.57	118.30
1	A	253	ASP	CB-CG-OD1	5.57	123.31	118.30
1	F	302	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	E	253	ASP	CB-CG-OD1	5.44	123.19	118.30
1	F	247	ARG	NE-CZ-NH1	-5.39	117.60	120.30
1	D	299	LYS	CD-CE-NZ	-5.39	99.30	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	275[A]	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	C	275[B]	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	E	242	ASP	CB-CG-OD1	5.25	123.02	118.30
1	C	169	MET	CG-SD-CE	5.17	108.47	100.20
1	F	253	ASP	CB-CG-OD1	5.14	122.93	118.30
1	D	247	ARG	NE-CZ-NH1	-5.10	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1187	0	1158	9	0
1	B	1162	0	1131	9	0
1	C	1212	0	1182	10	0
1	D	1180	0	1157	14	0
1	E	1187	0	1155	12	0
1	F	1162	0	1131	9	0
2	A	74	0	52	0	0
2	B	37	0	26	8	0
2	C	37	0	26	8	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	8	0	12	3	0
4	B	4	0	6	0	0
4	E	8	0	12	2	0
4	F	4	0	6	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	E	5	0	0	0	0
7	A	143	0	0	0	0
7	B	77	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	128	0	0	1	0
7	D	107	0	0	1	0
7	E	140	0	0	1	0
7	F	154	0	0	1	0
All	All	8024	0	7054	68	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 5.

All (68) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:GLN:HE22	2:B:401:4TG:H9	1.32	0.95
1:C:179:LYS:HE2	7:C:608:HOH:O	1.72	0.89
1:E:264:MET:SD	1:E:292:ILE:CD1	2.73	0.76
1:D:184:ASN:HA	1:D:189:ASN:HD22	1.51	0.76
1:F:294:ASP:OD2	1:F:296:SER:OG	2.06	0.73
1:A:186:LEU:H	1:A:186:LEU:HD23	1.54	0.73
1:E:295:TYR:CE2	1:E:299:LYS:HD2	2.26	0.71
1:C:228[A]:GLN:HE22	2:C:401:4TG:H9	1.57	0.70
1:C:228[B]:GLN:OE1	2:C:401:4TG:N4Q	2.29	0.65
1:B:177:LEU:HD11	1:B:250:TYR:CE1	2.32	0.64
1:D:177:LEU:HD21	1:D:250:TYR:CD1	2.33	0.63
4:A:404:EDO:O1	2:B:401:4TG:C5'	2.47	0.62
1:D:184:ASN:HA	1:D:189:ASN:ND2	2.14	0.62
1:D:194:GLU:OE1	1:D:197:LYS:HE2	2.00	0.61
1:D:213:PRO:HD2	1:D:216:GLU:HG3	1.83	0.60
1:D:248:GLU:HG2	1:D:250:TYR:CZ	2.37	0.59
1:A:186:LEU:HG	1:A:187:ARG:HG3	1.85	0.59
1:E:171:LYS:H	4:E:402:EDO:HO1	1.52	0.58
1:D:177:LEU:HD21	1:D:250:TYR:CE1	2.38	0.58
4:A:404:EDO:O1	2:B:401:4TG:H18	2.04	0.57
1:E:264:MET:SD	1:E:292:ILE:HD12	2.44	0.57
1:C:221:HIS:NE2	2:C:401:4TG:H12	2.21	0.56
1:B:228:GLN:NE2	2:B:401:4TG:H9	2.14	0.53
4:E:403:EDO:O2	7:E:501:HOH:O	2.19	0.53
1:F:270:TYR:CZ	1:F:271:LYS:HE3	2.43	0.53
1:B:186:LEU:HD23	1:B:187:ARG:HG3	1.91	0.52
1:D:234:SER:O	1:D:276:ALA:HA	2.08	0.52
1:E:240:LEU:HD23	1:E:249[A]:GLU:HB2	1.92	0.52
1:C:216:GLU:OE1	1:D:187:ARG:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:GLU:HG3	1:C:202:THR:OG1	2.09	0.51
1:D:249:GLU:OE1	1:D:270:TYR:OH	2.19	0.51
1:B:269:GLN:HE22	2:B:401:4TG:C	2.23	0.51
2:C:401:4TG:C	2:C:401:4TG:H6	2.42	0.50
1:D:249:GLU:OE2	1:F:296:SER:HB3	2.12	0.49
1:E:264:MET:SD	1:E:292:ILE:HD11	2.53	0.49
4:A:404:EDO:O1	2:B:401:4TG:H17	2.12	0.49
1:E:240:LEU:CD2	1:E:249[A]:GLU:HB2	2.42	0.49
2:B:401:4TG:O1A	2:B:401:4TG:O2Q	2.22	0.49
1:D:188:GLY:C	7:D:501:HOH:O	2.51	0.48
1:D:163:PHE:CZ	1:D:177:LEU:HD23	2.49	0.47
1:B:177:LEU:HD11	1:B:250:TYR:CD1	2.49	0.47
1:C:234:SER:O	1:C:276:ALA:HA	2.15	0.47
1:F:162:ASN:HA	7:F:501:HOH:O	2.14	0.47
1:F:220:GLU:HG2	1:F:268:VAL:HG22	1.97	0.47
1:E:270:TYR:CZ	1:E:271:LYS:HD2	2.50	0.46
1:C:228[A]:GLN:HE22	2:C:401:4TG:C4Q	2.27	0.46
1:A:186:LEU:H	1:A:186:LEU:CD2	2.26	0.44
2:C:401:4TG:O2Q	2:C:401:4TG:H25	2.17	0.44
2:B:401:4TG:H11	2:B:401:4TG:H5	1.48	0.44
1:A:247:ARG:C	1:A:248:GLU:HG2	2.39	0.43
1:C:202:THR:HG23	1:C:203:PRO:HD2	2.00	0.43
1:A:177:LEU:HD11	1:A:250:TYR:CE1	2.54	0.43
1:B:240:LEU:HB2	1:B:268:VAL:HB	2.01	0.42
1:F:227:LYS:HG2	1:F:263:PRO:HD3	2.01	0.42
1:E:177:LEU:HD22	1:E:177:LEU:N	2.35	0.42
1:A:227:LYS:HG2	1:A:263:PRO:HD3	2.01	0.42
1:E:208:THR:O	1:F:190:LEU:HA	2.20	0.41
1:F:240:LEU:HD21	1:F:247:ARG:CZ	2.50	0.41
1:A:206:TYR:CD2	1:A:206:TYR:C	2.92	0.41
1:A:185:ASP:HB2	1:A:186:LEU:HD23	2.03	0.41
1:B:168:GLN:HG2	1:B:177:LEU:HB2	2.02	0.41
1:D:212:VAL:HA	1:D:213:PRO:HD3	1.94	0.41
1:E:173:LYS:HE3	1:E:243:ASP:OD2	2.21	0.41
1:F:240:LEU:HD21	1:F:247:ARG:NE	2.36	0.41
1:A:285:TYR:CE1	1:B:197:LYS:HE3	2.56	0.40
2:C:401:4TG:C	2:C:401:4TG:C6Q	2.99	0.40
1:E:295:TYR:HE2	1:E:299:LYS:HD2	1.80	0.40
1:C:207:PHE:CZ	2:C:401:4TG:H14	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	144/148 (97%)	142 (99%)	2 (1%)	0	100	100
1	B	140/148 (95%)	138 (99%)	2 (1%)	0	100	100
1	C	148/148 (100%)	142 (96%)	6 (4%)	0	100	100
1	D	143/148 (97%)	140 (98%)	3 (2%)	0	100	100
1	E	145/148 (98%)	143 (99%)	2 (1%)	0	100	100
1	F	140/148 (95%)	136 (97%)	4 (3%)	0	100	100
All	All	860/888 (97%)	841 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	133/135 (98%)	129 (97%)	4 (3%)	41	22
1	B	129/135 (96%)	123 (95%)	6 (5%)	26	10
1	C	137/135 (102%)	135 (98%)	2 (2%)	65	51
1	D	132/135 (98%)	128 (97%)	4 (3%)	41	22
1	E	133/135 (98%)	129 (97%)	4 (3%)	41	22
1	F	129/135 (96%)	123 (95%)	6 (5%)	26	10
All	All	793/810 (98%)	767 (97%)	26 (3%)	38	19

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	GLN
1	A	182	LEU
1	A	186	LEU
1	A	190	LEU
1	B	168	GLN
1	B	173	LYS
1	B	182	LEU
1	B	186	LEU
1	B	196	GLU
1	B	270	TYR
1	C	270	TYR
1	C	274	LYS
1	D	168	GLN
1	D	182	LEU
1	D	197	LYS
1	D	303	GLN
1	E	168	GLN
1	E	171	LYS
1	E	270	TYR
1	E	289	ASP
1	F	168	GLN
1	F	171	LYS
1	F	216	GLU
1	F	240	LEU
1	F	270	TYR
1	F	300	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	221	HIS
1	B	228	GLN
1	C	236	ASN
1	D	162	ASN
1	D	189	ASN
1	D	246	ASN
1	E	184	ASN
1	E	189	ASN
1	E	300	GLN
1	F	162	ASN
1	F	184	ASN

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Mol	Chain	Res	Type
1	F	189	ASN
1	F	228	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
2	4TG	B	401	-	35,39,39	1.85	5 (14%)	50,59,59	2.41	14 (28%)
4	EDO	F	402	-	3,3,3	0.44	0	2,2,2	0.29	0
4	EDO	A	404	-	3,3,3	0.47	0	2,2,2	0.51	0
6	PO4	E	404	-	4,4,4	0.88	0	6,6,6	0.88	0
4	EDO	B	403	-	3,3,3	0.49	0	2,2,2	0.25	0
2	4TG	A	401[A]	-	35,39,39	1.90	6 (17%)	50,59,59	2.11	10 (20%)
4	EDO	E	403	-	3,3,3	0.42	0	2,2,2	0.43	0
2	4TG	A	401[B]	-	35,39,39	1.95	7 (20%)	50,59,59	2.17	11 (22%)
2	4TG	C	401	-	35,39,39	1.94	5 (14%)	50,59,59	2.26	13 (26%)
4	EDO	E	402	-	3,3,3	0.20	0	2,2,2	0.12	0
4	EDO	A	403	-	3,3,3	0.67	0	2,2,2	0.32	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
2	4TG	B	401	-	-	4/24/56/56	0/3/3/3
4	EDO	F	402	-	-	0/1/1/1	-
4	EDO	A	404	-	-	0/1/1/1	-
4	EDO	B	403	-	-	1/1/1/1	-
2	4TG	A	401[A]	-	-	2/24/56/56	0/3/3/3
4	EDO	E	403	-	-	0/1/1/1	-
2	4TG	A	401[B]	-	-	3/24/56/56	0/3/3/3
2	4TG	C	401	-	-	3/24/56/56	0/3/3/3
4	EDO	E	402	-	-	0/1/1/1	-
4	EDO	A	403	-	-	0/1/1/1	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	4TG	O2-C2	7.12	1.36	1.23
2	A	401[A]	4TG	O2-C2	7.12	1.36	1.23
2	A	401[B]	4TG	O2-C2	7.12	1.36	1.23
2	B	401	4TG	O2-C2	7.11	1.36	1.23
2	C	401	4TG	O4-C4	6.10	1.35	1.23
2	A	401[A]	4TG	O4-C4	6.06	1.35	1.23
2	A	401[B]	4TG	O4-C4	6.06	1.35	1.23
2	B	401	4TG	O4-C4	6.00	1.35	1.23
2	A	401[A]	4TG	C4-C5	-3.50	1.39	1.44
2	A	401[B]	4TG	C4-C5	-3.50	1.39	1.44
2	C	401	4TG	C4-C5	-3.28	1.39	1.44
2	B	401	4TG	C4-C5	-2.83	1.40	1.44
2	C	401	4TG	C6-C5	2.81	1.39	1.34
2	C	401	4TG	C2-N1	-2.79	1.34	1.38
2	B	401	4TG	C6-N1	-2.62	1.33	1.38
2	A	401[B]	4TG	C4Q-N4Q	2.53	1.50	1.45
2	A	401[A]	4TG	C6-C5	2.43	1.38	1.34
2	A	401[B]	4TG	C6-C5	2.43	1.38	1.34
2	B	401	4TG	C2-N1	-2.37	1.34	1.38
2	A	401[A]	4TG	C6-N1	-2.12	1.34	1.38
2	A	401[B]	4TG	C6-N1	-2.12	1.34	1.38
2	A	401[A]	4TG	C2-N1	-2.10	1.35	1.38
2	A	401[B]	4TG	C2-N1	-2.10	1.35	1.38

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	4TG	C5-C4-N3	7.21	121.47	115.31
2	B	401	4TG	C5-C4-N3	7.02	121.30	115.31
2	B	401	4TG	C4-N3-C2	-6.96	118.34	127.35
2	A	401[A]	4TG	C4-N3-C2	-6.87	118.46	127.35
2	A	401[B]	4TG	C4-N3-C2	-6.87	118.46	127.35
2	A	401[A]	4TG	C5-C4-N3	6.75	121.08	115.31
2	A	401[B]	4TG	C5-C4-N3	6.75	121.08	115.31
2	C	401	4TG	C4-N3-C2	-6.06	119.50	127.35
2	B	401	4TG	C5M-C5-C4	5.53	124.85	118.77
2	C	401	4TG	C5M-C5-C4	5.19	124.48	118.77
2	A	401[A]	4TG	C5-C6-N1	-4.85	118.35	123.34
2	A	401[B]	4TG	C5-C6-N1	-4.85	118.35	123.34
2	A	401[A]	4TG	N3-C2-N1	4.76	121.20	114.89
2	A	401[B]	4TG	N3-C2-N1	4.76	121.20	114.89
2	B	401	4TG	O4-C4-C5	-4.65	119.52	124.90
2	C	401	4TG	C5-C6-N1	-4.51	118.69	123.34
2	A	401[A]	4TG	O4-C4-C5	-4.43	119.76	124.90
2	A	401[B]	4TG	O4-C4-C5	-4.43	119.76	124.90
2	B	401	4TG	N3-C2-N1	4.37	120.69	114.89
2	C	401	4TG	O3A-PB-O3B	3.99	110.53	102.48
2	B	401	4TG	C5M-C5-C6	-3.92	117.61	122.85
2	C	401	4TG	N3-C2-N1	3.78	119.91	114.89
2	C	401	4TG	O5Q-C1Q-O3B	-3.78	106.43	111.36
2	B	401	4TG	O5Q-C5Q-C4Q	3.66	117.17	110.10
2	B	401	4TG	O2B-PB-O1B	3.56	129.85	112.24
2	C	401	4TG	C5M-C5-C6	-3.55	118.10	122.85
2	A	401[B]	4TG	C3Q-C4Q-N4Q	3.09	116.37	110.62
2	B	401	4TG	C5-C6-N1	-3.07	120.18	123.34
2	B	401	4TG	C1'-N1-C6	-3.02	115.57	120.77
2	B	401	4TG	O2-C2-N1	-2.84	119.01	122.79
2	C	401	4TG	C2'-C1'-N1	-2.82	107.27	113.77
2	A	401[B]	4TG	O3Q-C3Q-C2Q	-2.71	104.09	110.35
2	C	401	4TG	O4-C4-N3	-2.50	115.33	120.12
2	C	401	4TG	PB-O3B-C1Q	-2.47	110.18	119.74
2	B	401	4TG	C1'-N1-C2	2.45	122.47	117.64
2	A	401[B]	4TG	C2Q-C3Q-C4Q	2.41	113.86	110.34
2	A	401[A]	4TG	C5M-C5-C4	2.31	121.31	118.77
2	A	401[B]	4TG	C5M-C5-C4	2.31	121.31	118.77
2	A	401[A]	4TG	C5M-C5-C6	-2.31	119.77	122.85
2	A	401[B]	4TG	C5M-C5-C6	-2.31	119.77	122.85
2	A	401[A]	4TG	C1'-N1-C6	-2.21	116.96	120.77
2	A	401[B]	4TG	C1'-N1-C6	-2.21	116.96	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401[A]	4TG	O3Q-C3Q-C2Q	-2.16	105.35	110.35
2	A	401[A]	4TG	C3Q-C4Q-N4Q	2.14	114.60	110.62
2	B	401	4TG	PB-O3B-C1Q	-2.11	111.58	119.74
2	B	401	4TG	C2'-C3'-C4'	2.03	107.00	102.76
2	C	401	4TG	PA-O3A-PB	-2.03	125.87	132.83
2	C	401	4TG	C2Q-C3Q-C4Q	2.01	113.29	110.34

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401[A]	4TG	C5Q-C4Q-N4Q-C
2	A	401[A]	4TG	C3Q-C4Q-N4Q-C
2	A	401[B]	4TG	C5Q-C4Q-N4Q-C
2	A	401[B]	4TG	C3Q-C4Q-N4Q-C
2	A	401[B]	4TG	O-C-N4Q-C4Q
2	B	401	4TG	C5Q-C4Q-N4Q-C
2	B	401	4TG	O-C-N4Q-C4Q
2	C	401	4TG	PA-O3A-PB-O3B
2	C	401	4TG	C5Q-C4Q-N4Q-C
2	C	401	4TG	O-C-N4Q-C4Q
2	B	401	4TG	O4'-C4'-C5'-O5'
2	B	401	4TG	C3'-C4'-C5'-O5'
4	B	403	EDO	O1-C1-C2-O2

There are no ring outliers.

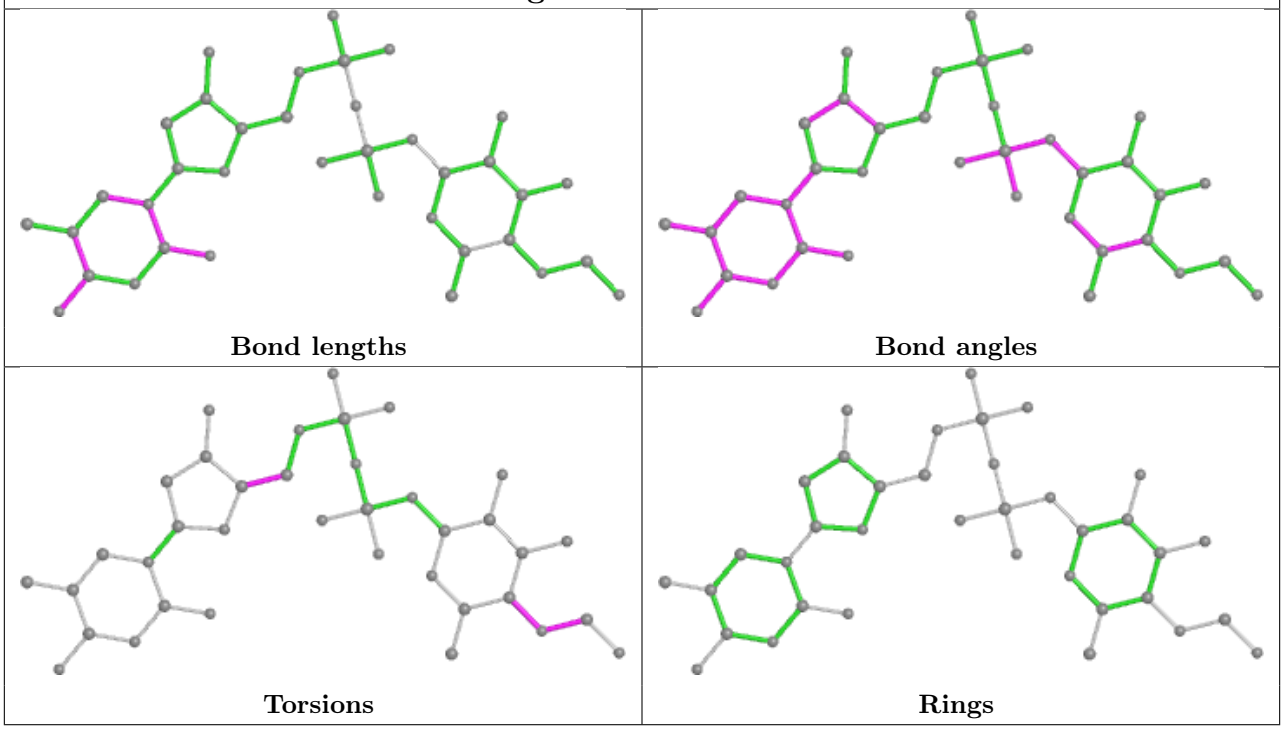
5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	4TG	8	0
4	A	404	EDO	3	0
4	E	403	EDO	1	0
2	C	401	4TG	8	0
4	E	402	EDO	1	0

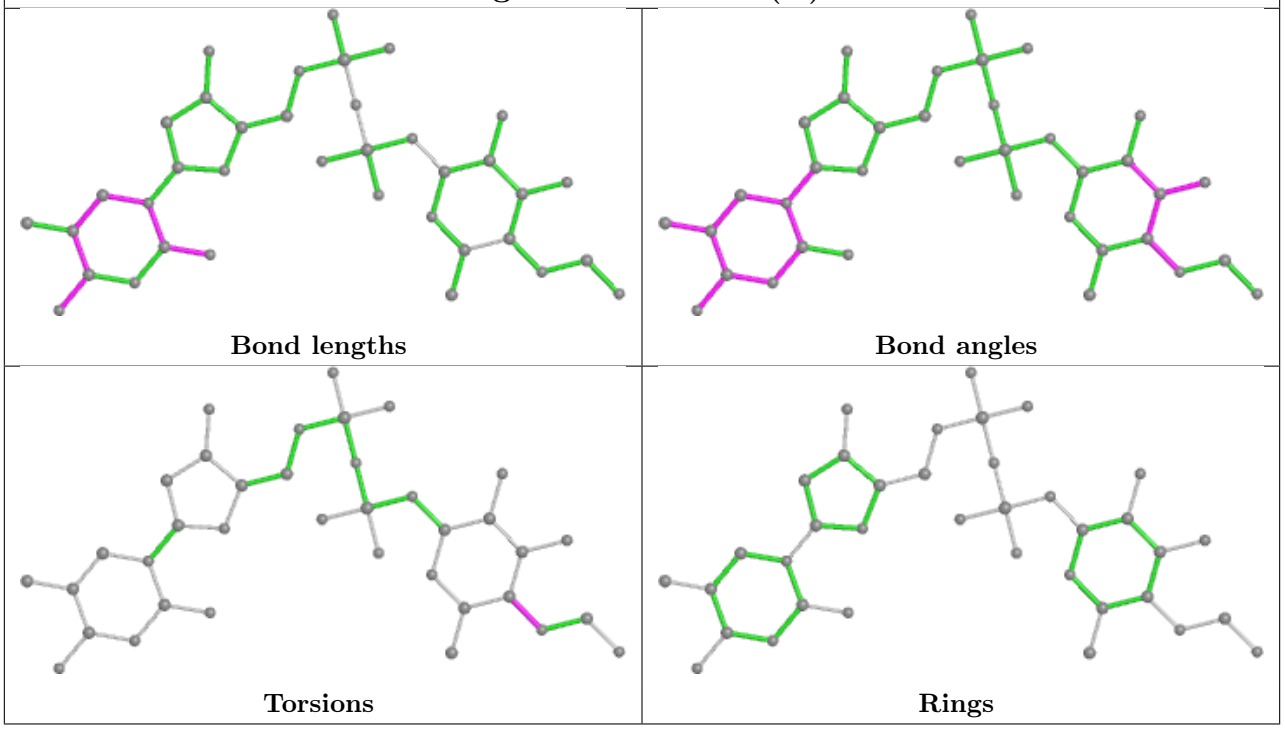
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

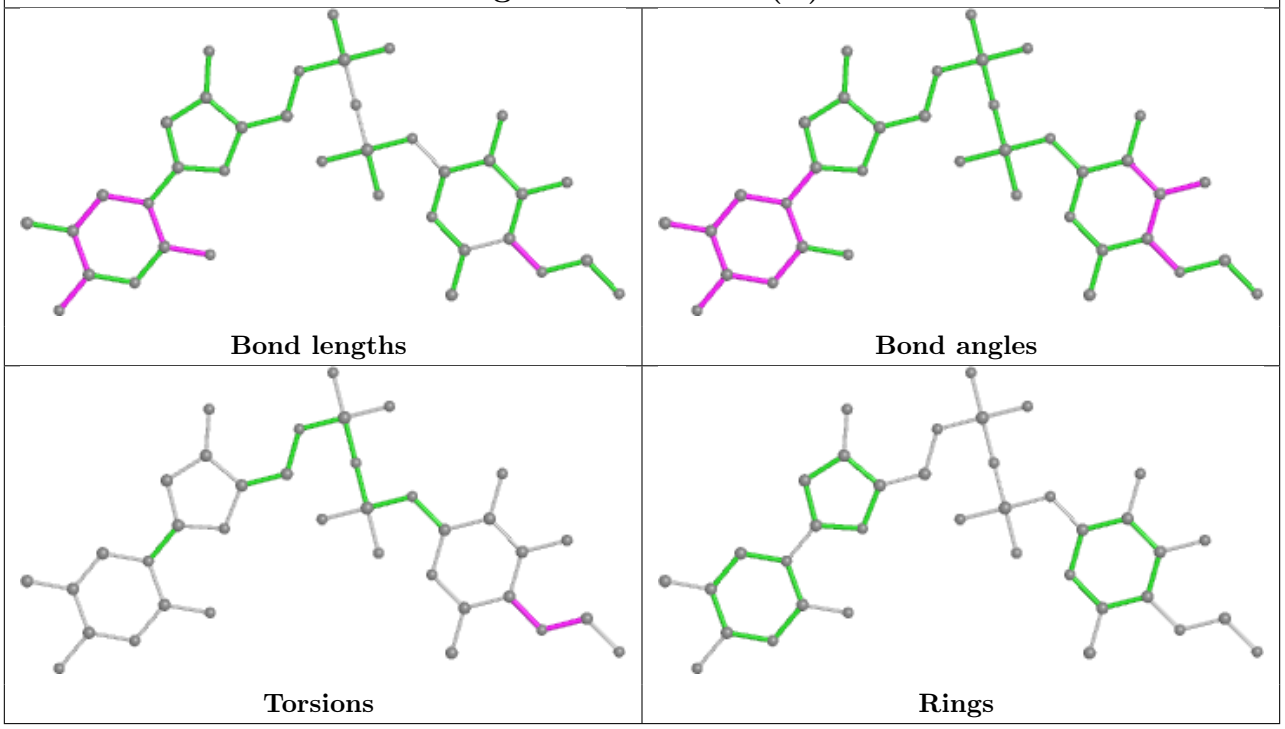
Ligand 4TG B 401



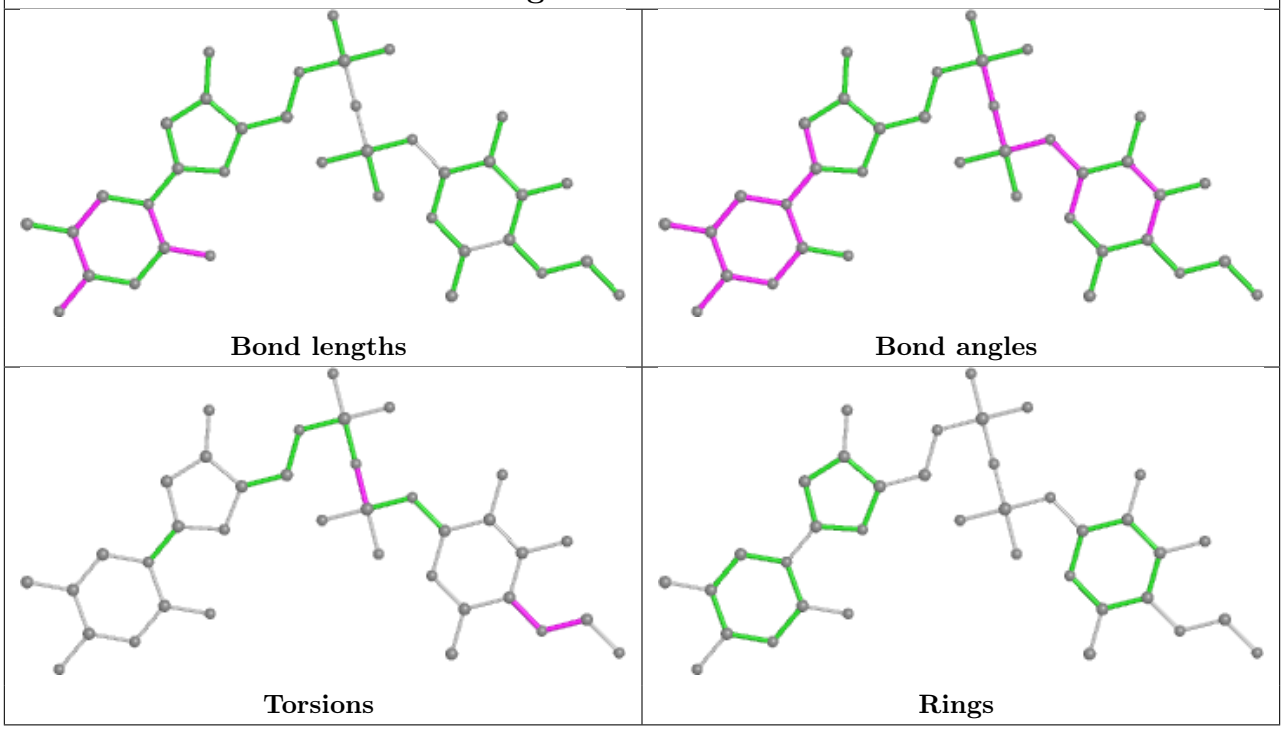
Ligand 4TG A 401 (A)



Ligand 4TG A 401 (B)



Ligand 4TG C 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	144/148 (97%)	0.03	3 (2%)	63	67	16, 24, 42, 58	0
1	B	142/148 (95%)	0.30	12 (8%)	10	12	22, 30, 50, 68	0
1	C	146/148 (98%)	0.09	8 (5%)	25	27	14, 23, 45, 68	0
1	D	143/148 (96%)	0.16	9 (6%)	20	22	16, 26, 47, 74	0
1	E	144/148 (97%)	0.06	5 (3%)	44	49	15, 22, 43, 64	0
1	F	142/148 (95%)	-0.02	5 (3%)	44	49	13, 21, 43, 67	0
All	All	861/888 (96%)	0.10	42 (4%)	29	33	13, 25, 46, 74	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	303	GLN	5.2
1	A	186	LEU	5.1
1	C	300	GLN	4.8
1	D	186	LEU	4.3
1	F	186	LEU	4.0
1	E	186	LEU	3.9
1	E	160	SER	3.6
1	F	300	GLN	3.3
1	B	300	GLN	3.3
1	B	164	GLU	3.3
1	E	161	ASN	3.0
1	D	300	GLN	3.0
1	C	288	SER	3.0
1	C	297	THR	2.8
1	B	285	TYR	2.8
1	D	164	GLU	2.8
1	C	286	TYR	2.8
1	B	165	LEU	2.8
1	D	230	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	279	LEU	2.6
1	B	279	LEU	2.6
1	E	300	GLN	2.6
1	F	184	ASN	2.5
1	C	230	LEU	2.5
1	F	297	THR	2.4
1	B	231	ILE	2.3
1	D	165	LEU	2.3
1	D	168	GLN	2.2
1	C	280	VAL	2.2
1	D	171	LYS	2.2
1	C	268	VAL	2.2
1	B	296	SER	2.1
1	B	214	ASN	2.1
1	A	164	GLU	2.1
1	B	261	LEU	2.1
1	F	213	PRO	2.1
1	E	303	GLN	2.1
1	B	186	LEU	2.1
1	B	230	LEU	2.1
1	D	279	LEU	2.1
1	A	214	ASN	2.0
1	B	161	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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.

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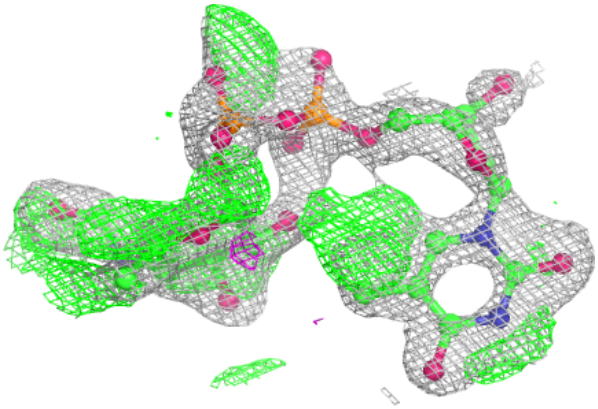
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

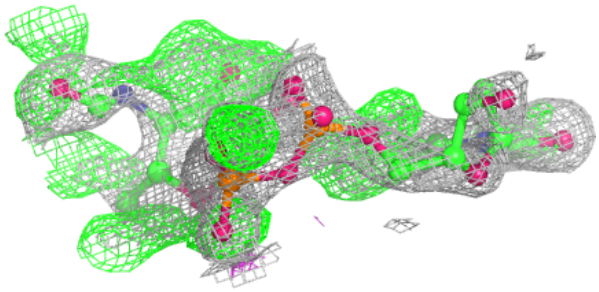
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	4TG	B	401	37/37	0.55	0.51	22,31,34,37	37
2	4TG	C	401	37/37	0.73	0.39	14,26,33,39	37
4	EDO	A	403	4/4	0.90	0.11	29,31,33,38	0
4	EDO	E	403	4/4	0.90	0.09	34,34,37,38	0
3	CL	D	402	1/1	0.93	0.07	46,46,46,46	0
2	4TG	A	401[B]	37/37	0.94	0.10	22,24,30,34	37
4	EDO	A	404	4/4	0.94	0.17	39,41,42,42	0
4	EDO	B	403	4/4	0.94	0.15	46,49,49,51	0
4	EDO	E	402	4/4	0.94	0.15	33,35,38,39	0
2	4TG	A	401[A]	37/37	0.94	0.10	16,24,30,34	37
3	CL	D	401	1/1	0.95	0.05	34,34,34,34	0
6	PO4	E	404	5/5	0.95	0.12	34,36,38,42	5
4	EDO	F	402	4/4	0.97	0.05	30,33,33,34	0
3	CL	B	402	1/1	0.98	0.07	38,38,38,38	0
3	CL	E	401	1/1	0.99	0.04	27,27,27,27	0
5	NA	A	405	1/1	0.99	0.07	23,23,23,23	0
5	NA	C	402	1/1	0.99	0.09	27,27,27,27	0
3	CL	A	402	1/1	0.99	0.05	29,29,29,29	0
3	CL	F	401	1/1	1.00	0.04	22,22,22,22	0

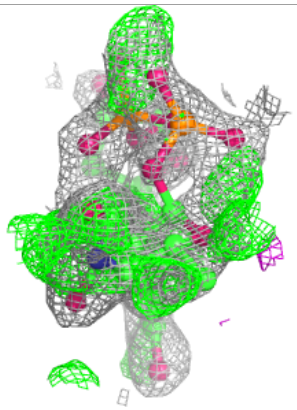
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 4TG B 401:

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

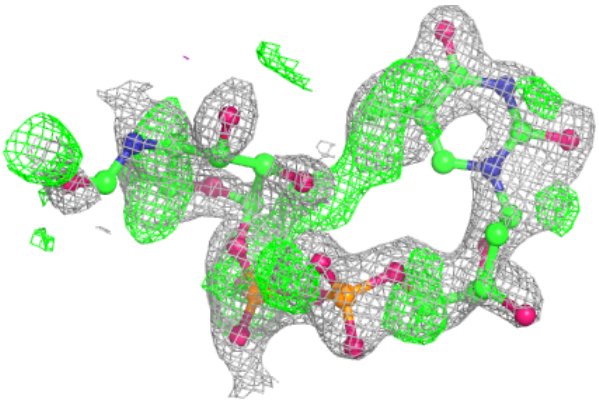


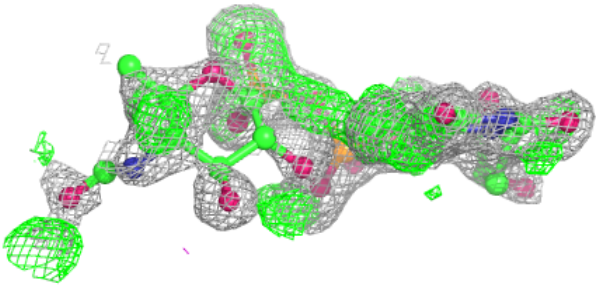


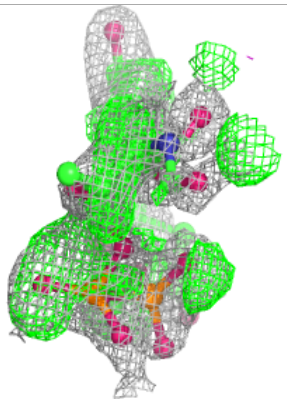


Electron density around 4TG C 401:

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

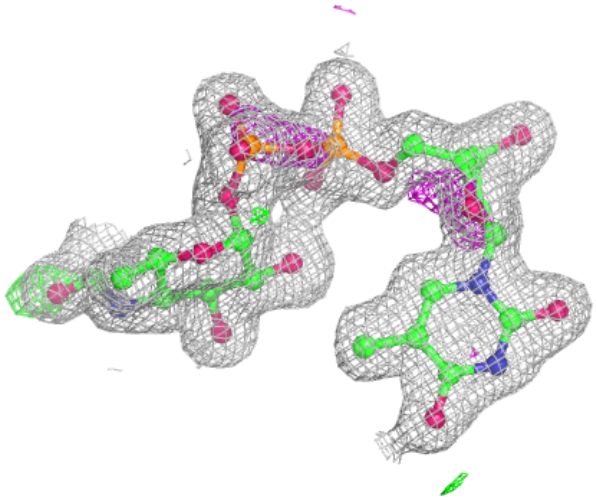


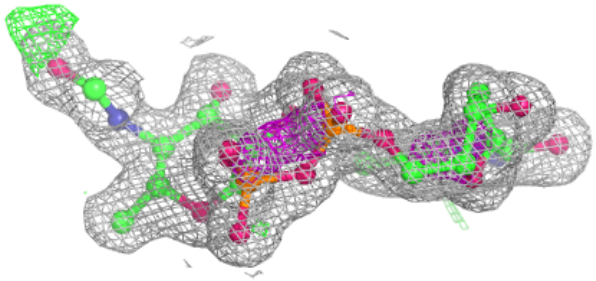




Electron density around 4TG A 401 (B):

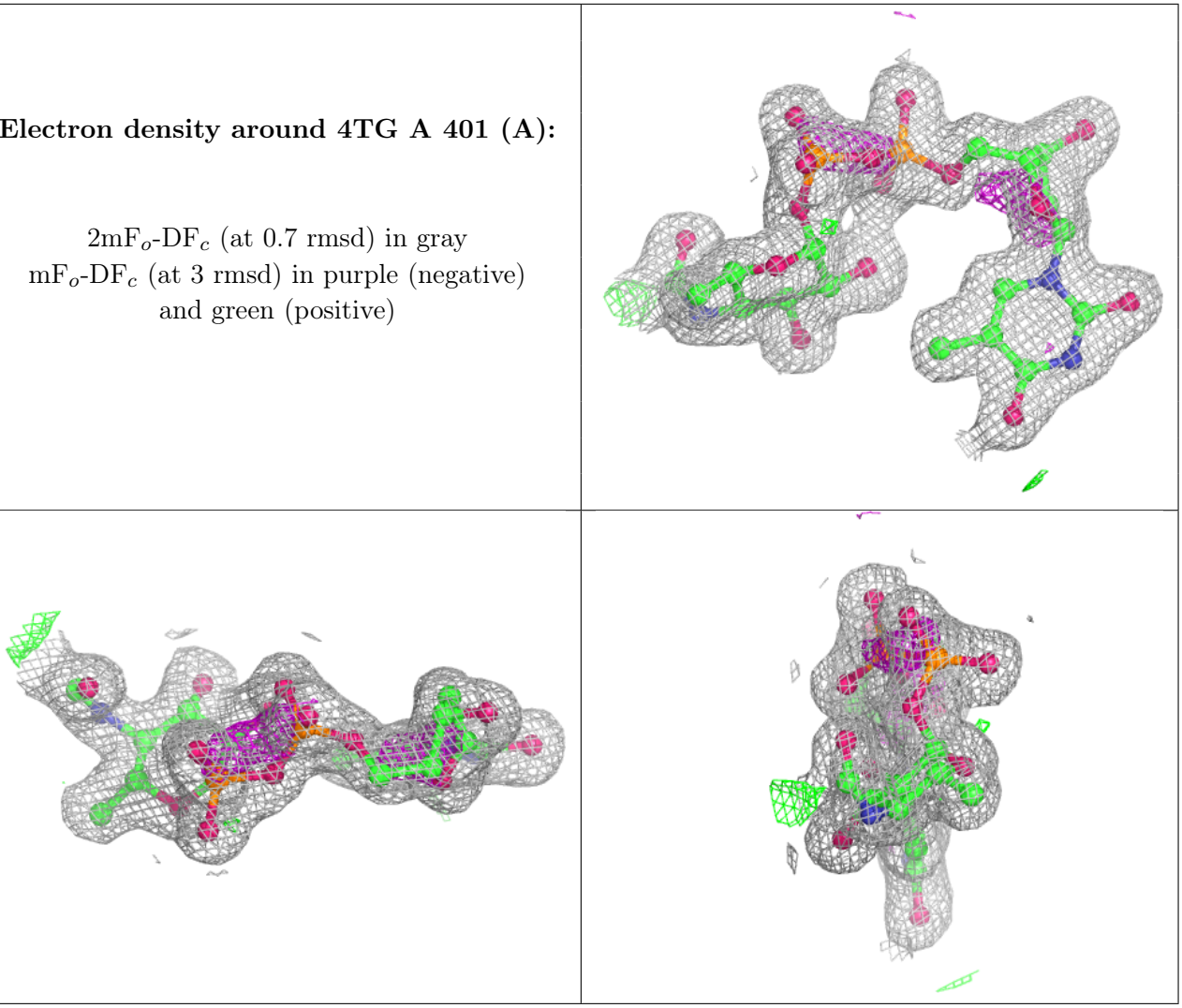
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around 4TG A 401 (A):

$2mF_o$-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

There are no such residues in this entry.