



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:06 AM UTC

PDB ID : 4ZU4 / pdb_00004zu4
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:

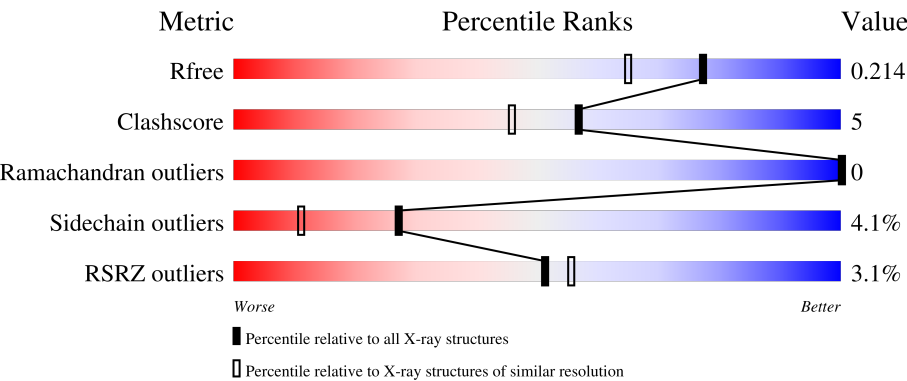
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 $\leq 5\%$. 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	148	2% 87% 9% ..
1	B	148	2% 86% 9% ..
1	C	148	5% 88% 10% ..
1	D	148	5% 80% 16% ..
1	E	148	2% 86% 9% ..

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Mol	Chain	Length	Quality of chain
1	F	148	2% 83% 11%

2 Entry composition

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:

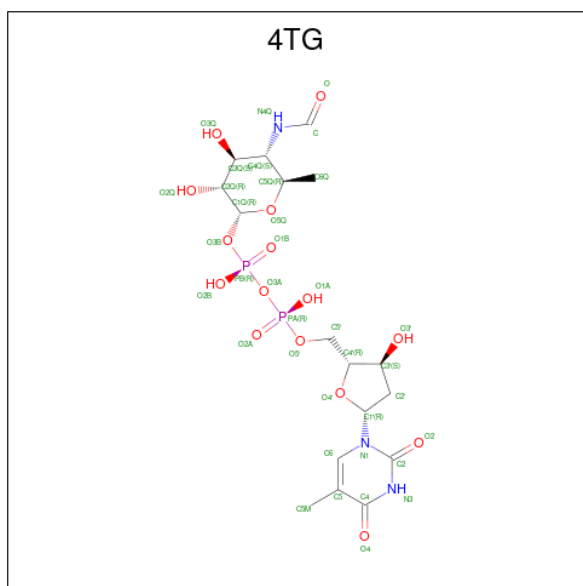
Chain	Residue	Modelled	Actual	Comment	Reference
A	157	GLY	-	expression tag	UNP Q12KT8
A	158	HIS	-	expression tag	UNP Q12KT8
A	159	MET	-	expression tag	UNP Q12KT8
B	157	GLY	-	expression tag	UNP Q12KT8
B	158	HIS	-	expression tag	UNP Q12KT8
B	159	MET	-	expression tag	UNP Q12KT8
C	157	GLY	-	expression tag	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 (CCD ID: 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 (CCD ID: 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 (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

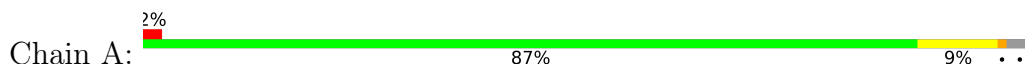
- Molecule 7 is water.

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

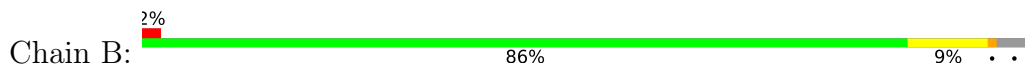
3 Residue-property plots [i](#)

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

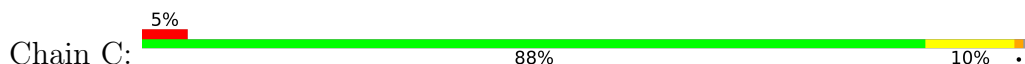
- Molecule 1: WxcM-like protein



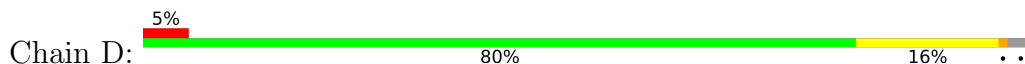
- Molecule 1: WxcM-like protein



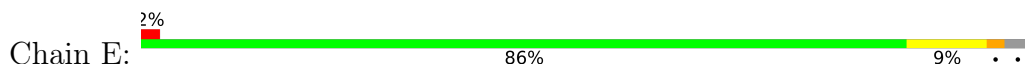
- Molecule 1: WxcM-like protein



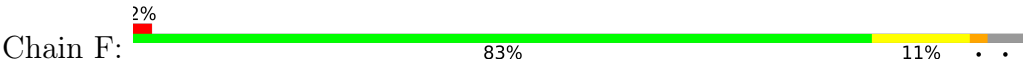
- Molecule 1: WxcM-like protein



- Molecule 1: WxcM-like protein



- Molecule 1: WxcM-like protein



4 Data and refinement statistics

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 28.28 – 1.70	Depositor EDS
% Data completeness (in resolution range)	91.7 (28.28-1.70) 91.8 (28.28-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.66 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.171 , 0.207 0.178 , 0.214	Depositor DCC
R_{free} test set	5776 reflections (4.59%)	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 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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: CL, EDO, PO4, NA, 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	0.86	1/1222 (0.1%)	1.07	2/1646 (0.1%)
1	B	0.74	0/1191	1.02	0/1605
1	C	0.93	3/1254 (0.2%)	1.08	0/1689
1	D	0.87	0/1215	1.09	1/1637 (0.1%)
1	E	0.87	0/1225	1.10	0/1651
1	F	0.95	1/1191 (0.1%)	1.22	5/1605 (0.3%)
All	All	0.87	5/7298 (0.1%)	1.10	8/9833 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	201	PHE	N-CA	-5.29	1.39	1.46
1	C	193	GLY	N-CA	5.21	1.51	1.45
1	C	242	ASP	N-CA	5.12	1.52	1.46
1	A	261	LEU	C-O	-5.12	1.19	1.24
1	C	172	VAL	N-CA	-5.09	1.40	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	162	ASN	N-CA-C	8.30	122.66	112.54
1	A	261	LEU	CA-C-N	-6.63	113.55	120.38
1	A	261	LEU	C-N-CA	-6.63	113.55	120.38
1	F	162	ASN	N-CA-C	-6.23	101.71	110.50
1	F	212	VAL	CA-C-N	-6.04	113.51	120.04
1	F	212	VAL	C-N-CA	-6.04	113.51	120.04
1	F	202	THR	CA-C-N	-5.65	114.15	120.14
1	F	202	THR	C-N-CA	-5.65	114.15	120.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1187	0	1158	9	0
1	B	1162	0	1131	9	0
1	C	1212	0	1182	9	0
1	D	1180	0	1157	17	0
1	E	1187	0	1155	13	0
1	F	1162	0	1131	10	0
2	A	74	0	52	0	0
2	B	37	0	26	6	0
2	C	37	0	26	2	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
7	C	128	0	0	2	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	66	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 (66) 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: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:E:171:LYS:H	4:E:402:EDO:HO1	1.49	0.59
1:A:186:LEU:HG	1:A:187:ARG:HG3	1.85	0.59
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:C:169:MET:HE3	7:C:544:HOH:O	2.06	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:188:GLY:C	7:D:501:HOH:O	2.51	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
1:C:196:GLU:HG3	1:C:202:THR:OG1	2.09	0.51
1:B:269:GLN:HE22	2:B:401:4TG:C	2.23	0.51
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
1:A:247:ARG:C	1:A:248:GLU:HG2	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:LYS:NZ	1:F:294:ASP:OD1	2.41	0.46
1:A:206:TYR:CD2	1:A:206:TYR:C	2.92	0.46
1:A:186:LEU:H	1:A:186:LEU:CD2	2.26	0.44
1:D:249:GLU:OE1	1:D:270:TYR:OH	2.19	0.44
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:184:ASN:ND2	1:E:184:ASN:C	2.78	0.41
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:C:297:THR:CG2	1:C:301:MET:HE3	2.50	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:D:243:ASP:OD1	1:D:243:ASP:C	2.63	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
1:D:185:ASP:OD1	1:D:185:ASP:C	2.65	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	128 (96%)	5 (4%)	29	13
1	B	129/135 (96%)	122 (95%)	7 (5%)	20	6
1	C	137/135 (102%)	135 (98%)	2 (2%)	57	43
1	D	132/135 (98%)	126 (96%)	6 (4%)	24	9
1	E	133/135 (98%)	127 (96%)	6 (4%)	24	9
1	F	129/135 (96%)	123 (95%)	6 (5%)	23	9
All	All	793/810 (98%)	761 (96%)	32 (4%)	27	12

All (32) 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	A	261	LEU
1	B	168	GLN
1	B	173	LYS
1	B	182	LEU

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Mol	Chain	Res	Type
1	B	186	LEU
1	B	196	GLU
1	B	246	ASN
1	B	270	TYR
1	C	179	LYS
1	C	274	LYS
1	D	168	GLN
1	D	182	LEU
1	D	187	ARG
1	D	196	GLU
1	D	197	LYS
1	D	303	GLN
1	E	168	GLN
1	E	171	LYS
1	E	179	LYS
1	E	184	ASN
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 (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	HIS
1	A	303	GLN
1	B	184	ASN
1	B	189	ASN
1	B	221	HIS
1	B	228	GLN
1	B	269	GLN
1	C	214	ASN
1	D	162	ASN
1	D	181	HIS
1	D	189	ASN
1	E	162	ASN
1	E	184	ASN
1	E	189	ASN

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Mol	Chain	Res	Type
1	F	162	ASN
1	F	184	ASN
1	F	189	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	C	401	-	38,39,39	2.07	8 (21%)	54,59,59	2.13	11 (20%)
4	EDO	E	403	-	3,3,3	0.38	0	2,2,2	0.36	0
2	4TG	B	401	-	38,39,39	1.86	5 (13%)	54,59,59	2.41	17 (31%)
2	4TG	A	401[A]	-	38,39,39	1.93	7 (18%)	54,59,59	2.06	11 (20%)
4	EDO	F	402	-	3,3,3	0.42	0	2,2,2	0.34	0
4	EDO	A	404	-	3,3,3	0.44	0	2,2,2	0.53	0
6	PO4	E	404	-	4,4,4	0.94	0	6,6,6	0.92	0
4	EDO	B	403	-	3,3,3	0.46	0	2,2,2	0.30	0
2	4TG	A	401[B]	-	38,39,39	1.97	8 (21%)	54,59,59	2.11	12 (22%)
4	EDO	A	403	-	3,3,3	0.63	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	E	402	-	3,3,3	0.18	0	2,2,2	0.18	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	C	401	-	-	3/24/56/56	0/3/3/3
4	EDO	E	403	-	-	0/1/1/1	-
2	4TG	B	401	-	-	4/24/56/56	0/3/3/3
2	4TG	A	401[A]	-	-	2/24/56/56	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[B]	-	-	3/24/56/56	0/3/3/3
4	EDO	A	403	-	-	0/1/1/1	-
4	EDO	E	402	-	-	0/1/1/1	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	4TG	O2-C2	7.34	1.36	1.23
2	A	401[A]	4TG	O2-C2	7.34	1.36	1.23
2	A	401[B]	4TG	O2-C2	7.34	1.36	1.23
2	B	401	4TG	O2-C2	7.33	1.36	1.23
2	C	401	4TG	O4-C4	6.13	1.35	1.23
2	A	401[A]	4TG	O4-C4	6.09	1.35	1.23
2	A	401[B]	4TG	O4-C4	6.09	1.35	1.23
2	B	401	4TG	O4-C4	6.03	1.35	1.23
2	C	401	4TG	PB-O3A	3.95	1.63	1.59
2	A	401[A]	4TG	C4-C5	-3.60	1.39	1.44
2	A	401[B]	4TG	C4-C5	-3.60	1.39	1.44
2	C	401	4TG	C4-C5	-3.37	1.39	1.44
2	C	401	4TG	PA-O3A	3.30	1.63	1.59
2	A	401[A]	4TG	PA-O3A	2.93	1.62	1.59
2	B	401	4TG	C4-C5	-2.92	1.40	1.44
2	A	401[B]	4TG	PA-O3A	2.88	1.62	1.59
2	C	401	4TG	C2-N1	-2.87	1.34	1.38
2	C	401	4TG	C6-C5	2.82	1.39	1.34
2	B	401	4TG	C6-N1	-2.60	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401[B]	4TG	C4Q-N4Q	2.60	1.50	1.45
2	B	401	4TG	C2-N1	-2.44	1.34	1.38
2	A	401[A]	4TG	C6-C5	2.44	1.38	1.34
2	A	401[B]	4TG	C6-C5	2.44	1.38	1.34
2	A	401[A]	4TG	C2-N1	-2.16	1.35	1.38
2	A	401[B]	4TG	C2-N1	-2.16	1.35	1.38
2	A	401[A]	4TG	C6-N1	-2.10	1.34	1.38
2	A	401[B]	4TG	C6-N1	-2.10	1.34	1.38
2	C	401	4TG	C2-N3	-2.01	1.34	1.38

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	4TG	C5-C4-N3	7.07	121.47	115.32
2	B	401	4TG	C5-C4-N3	6.88	121.30	115.32
2	B	401	4TG	C4-N3-C2	-6.86	118.34	127.34
2	A	401[A]	4TG	C4-N3-C2	-6.77	118.46	127.34
2	A	401[B]	4TG	C4-N3-C2	-6.77	118.46	127.34
2	A	401[A]	4TG	C5-C4-N3	6.62	121.08	115.32
2	A	401[B]	4TG	C5-C4-N3	6.62	121.08	115.32
2	C	401	4TG	C4-N3-C2	-5.98	119.50	127.34
2	B	401	4TG	C5M-C5-C4	5.69	124.85	118.78
2	C	401	4TG	C5M-C5-C4	5.34	124.48	118.78
2	A	401[A]	4TG	N3-C2-N1	4.85	121.20	114.89
2	A	401[B]	4TG	N3-C2-N1	4.85	121.20	114.89
2	B	401	4TG	O4-C4-C5	-4.72	119.52	124.92
2	A	401[A]	4TG	C5-C6-N1	-4.57	118.35	123.31
2	A	401[B]	4TG	C5-C6-N1	-4.57	118.35	123.31
2	A	401[A]	4TG	O4-C4-C5	-4.51	119.76	124.92
2	A	401[B]	4TG	O4-C4-C5	-4.51	119.76	124.92
2	B	401	4TG	N3-C2-N1	4.45	120.69	114.89
2	C	401	4TG	C5-C6-N1	-4.25	118.69	123.31
2	B	401	4TG	C5M-C5-C6	-3.87	117.61	122.85
2	C	401	4TG	N3-C2-N1	3.85	119.91	114.89
2	C	401	4TG	O5Q-C1Q-O3B	-3.78	106.43	111.36
2	B	401	4TG	O2B-PB-O1B	3.74	129.85	112.44
2	B	401	4TG	C6Q-C5Q-C4Q	-3.56	107.04	113.57
2	C	401	4TG	C5M-C5-C6	-3.51	118.10	122.85
2	A	401[B]	4TG	C3Q-C4Q-N4Q	3.19	116.37	110.62
2	B	401	4TG	C1'-N1-C6	-3.08	115.57	120.74
2	B	401	4TG	O3A-PB-O1B	-3.01	101.65	110.70
2	A	401[A]	4TG	C6Q-C5Q-C4Q	-2.98	108.10	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401[B]	4TG	C6Q-C5Q-C4Q	-2.97	108.13	113.57
2	B	401	4TG	O5Q-C5Q-C4Q	2.95	117.17	110.52
2	B	401	4TG	O2-C2-N1	-2.91	119.01	122.80
2	B	401	4TG	C5-C6-N1	-2.89	120.18	123.31
2	C	401	4TG	PB-O3B-C1Q	-2.71	110.18	121.21
2	A	401[B]	4TG	O3Q-C3Q-C2Q	-2.67	104.09	110.38
2	B	401	4TG	C5Q-C4Q-N4Q	-2.63	105.67	111.23
2	C	401	4TG	C2'-C1'-N1	-2.62	107.27	113.81
2	C	401	4TG	O4-C4-N3	-2.54	115.33	120.11
2	B	401	4TG	C1'-N1-C2	2.46	122.47	117.66
2	A	401[B]	4TG	C2Q-C3Q-C4Q	2.38	113.86	110.40
2	B	401	4TG	PB-O3B-C1Q	-2.37	111.58	121.21
2	A	401[A]	4TG	C5M-C5-C4	2.36	121.31	118.78
2	A	401[B]	4TG	C5M-C5-C4	2.36	121.31	118.78
2	A	401[A]	4TG	C5M-C5-C6	-2.28	119.77	122.85
2	A	401[B]	4TG	C5M-C5-C6	-2.28	119.77	122.85
2	C	401	4TG	O3A-PB-O1B	-2.25	103.94	110.70
2	A	401[A]	4TG	C1'-N1-C6	-2.25	116.96	120.74
2	A	401[B]	4TG	C1'-N1-C6	-2.25	116.96	120.74
2	A	401[A]	4TG	C3Q-C4Q-N4Q	2.21	114.60	110.62
2	A	401[A]	4TG	O3Q-C3Q-C2Q	-2.13	105.35	110.38
2	B	401	4TG	C2'-C3'-C4'	2.07	107.00	102.80

There are no chirality outliers.

All (13) torsion outliers are listed below:

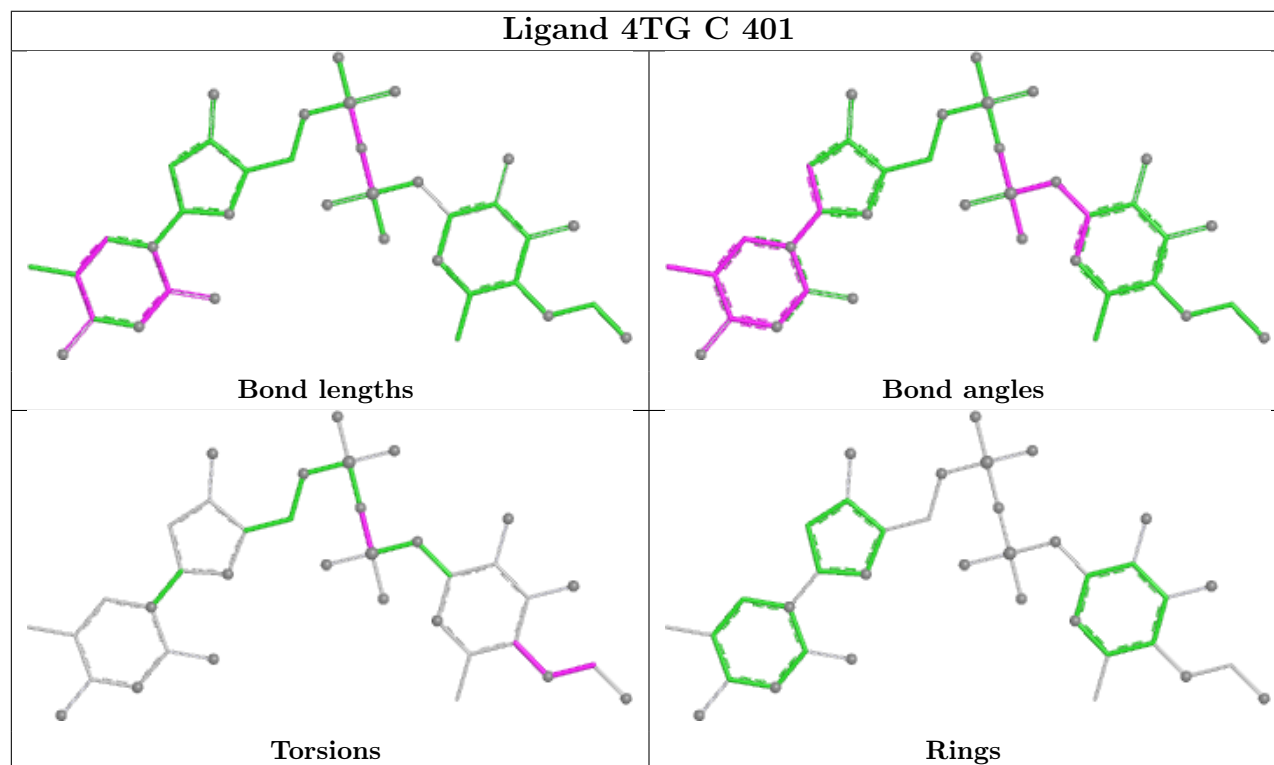
Mol	Chain	Res	Type	Atoms
2	A	401[A]	4TG	C5Q-C4Q-N4Q-C
2	A	401[A]	4TG	C3Q-C4Q-N4Q-C
2	A	401[B]	4TG	C5Q-C4Q-N4Q-C
2	A	401[B]	4TG	C3Q-C4Q-N4Q-C
2	A	401[B]	4TG	O-C-N4Q-C4Q
2	B	401	4TG	C5Q-C4Q-N4Q-C
2	B	401	4TG	O-C-N4Q-C4Q
2	C	401	4TG	PA-O3A-PB-O3B
2	C	401	4TG	C5Q-C4Q-N4Q-C
2	C	401	4TG	O-C-N4Q-C4Q
2	B	401	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.

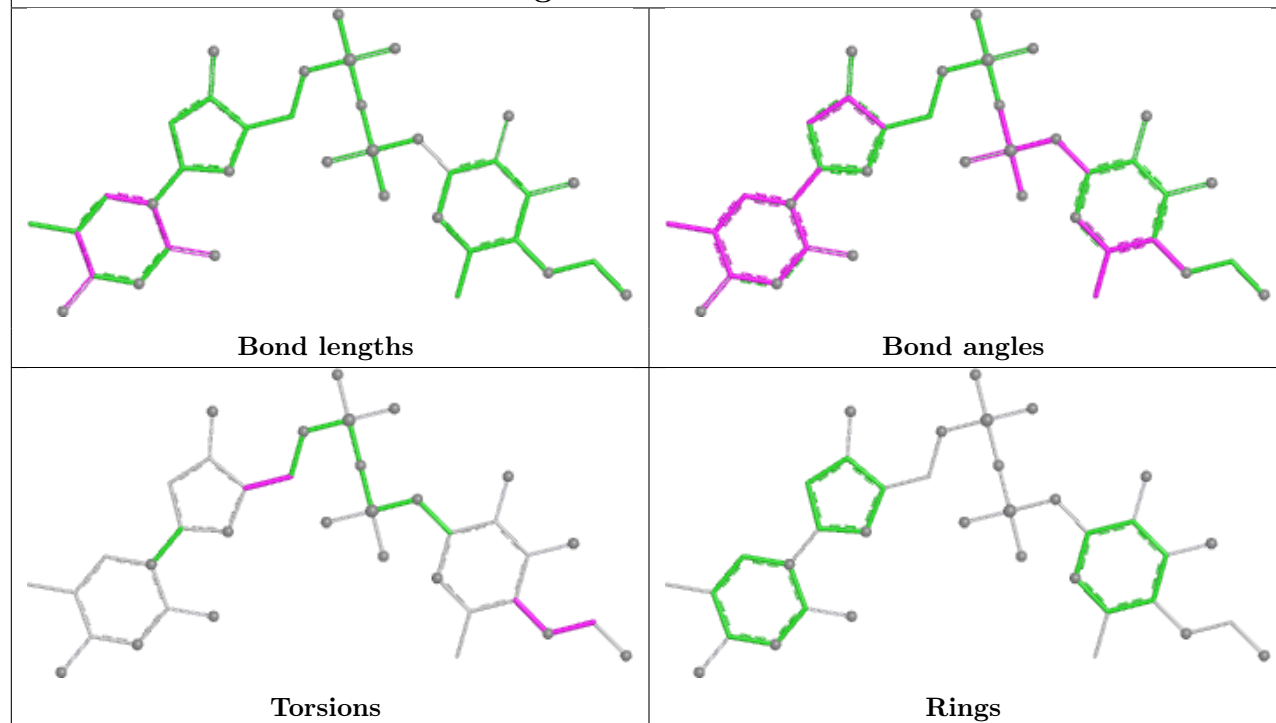
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	4TG	2	0
4	E	403	EDO	1	0
2	B	401	4TG	6	0
4	A	404	EDO	3	0
4	E	402	EDO	1	0

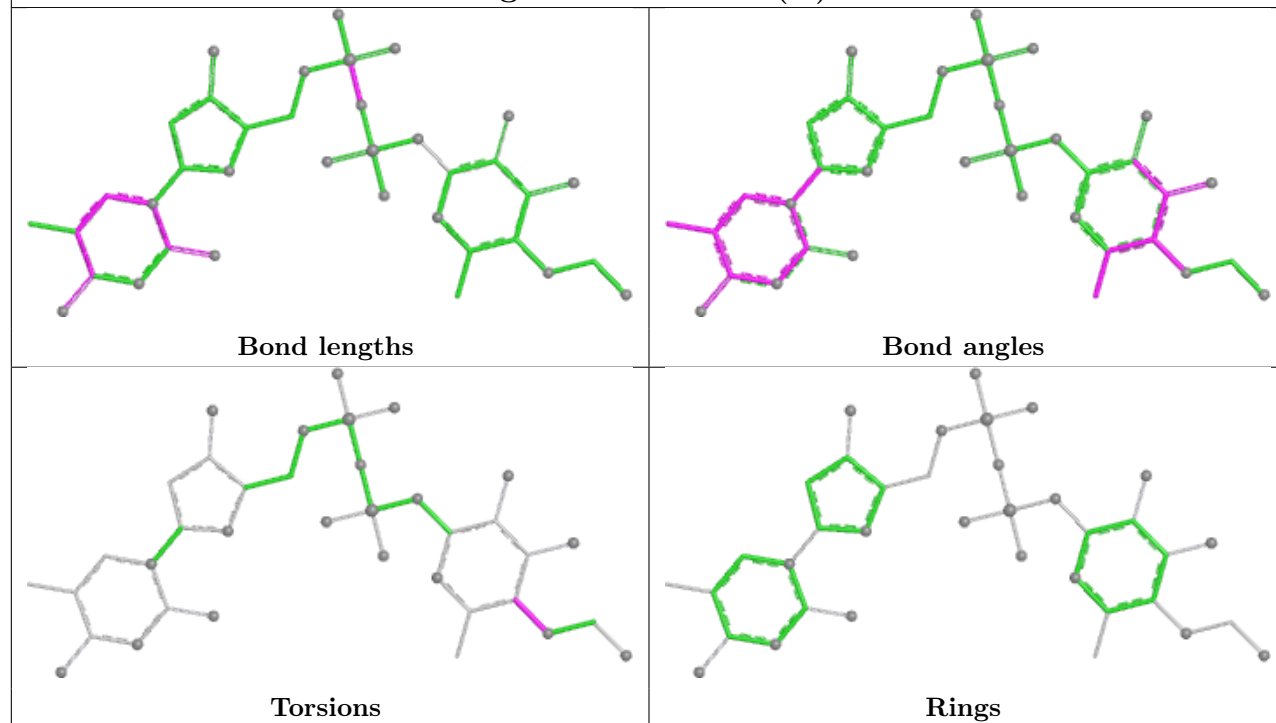
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

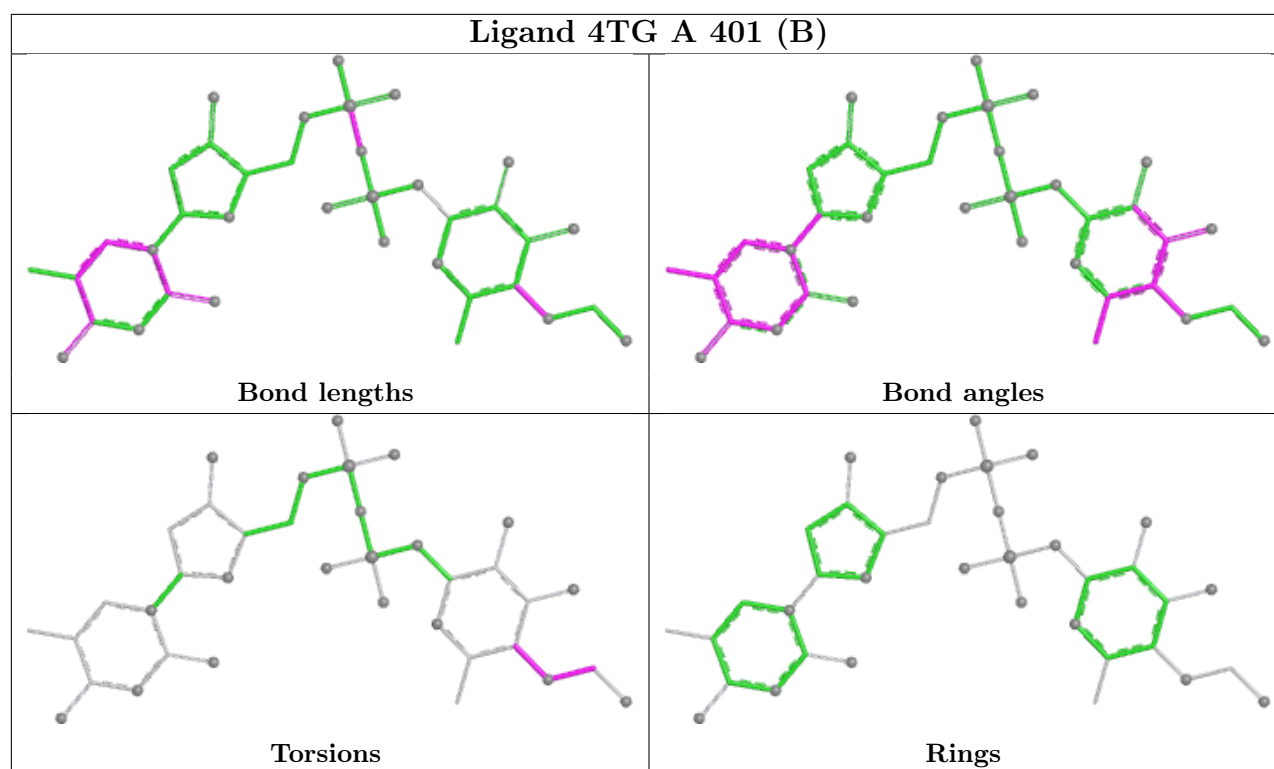


Ligand 4TG B 401



Ligand 4TG A 401 (A)





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	144/148 (97%)	0.05	3 (2%) 63 68	13, 24, 42, 58	2 (1%)
1	B	142/148 (95%)	0.37	3 (2%) 63 68	22, 30, 50, 68	0
1	C	146/148 (98%)	0.08	8 (5%) 30 34	13, 23, 45, 68	4 (2%)
1	D	143/148 (96%)	0.28	7 (4%) 35 38	14, 25, 47, 74	2 (1%)
1	E	144/148 (97%)	-0.04	3 (2%) 63 68	13, 22, 43, 64	3 (2%)
1	F	142/148 (95%)	0.10	3 (2%) 63 68	13, 21, 43, 67	0
All	All	861/888 (96%)	0.14	27 (3%) 51 55	13, 25, 46, 74	11 (1%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	186	LEU	5.2
1	E	160	SER	4.5
1	E	303	GLN	3.8
1	D	168	GLN	3.6
1	A	161	ASN	3.2
1	C	286	TYR	3.2
1	D	186	LEU	3.1
1	D	161	ASN	3.0
1	F	186	LEU	3.0
1	F	161	ASN	2.9
1	C	300	GLN	2.7
1	F	181	HIS	2.6
1	C	288	SER	2.6
1	D	215	LYS	2.6
1	D	303	GLN	2.4
1	E	161	ASN	2.4
1	B	186	LEU	2.4
1	C	285	TYR	2.4
1	C	301	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	161	ASN	2.3
1	D	219	GLY	2.2
1	B	214	ASN	2.2
1	A	275	ASP	2.1
1	C	302	ARG	2.1
1	C	297	THR	2.1
1	D	171	LYS	2.1
1	C	291	TYR	2.1

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
2	4TG	B	401	37/37	0.69	0.25	22,31,34,37	37
2	4TG	C	401	37/37	0.80	0.22	14,26,33,39	37
4	EDO	A	403	4/4	0.90	0.14	29,31,33,38	0
4	EDO	B	403	4/4	0.90	0.11	46,49,49,51	0
4	EDO	A	404	4/4	0.91	0.11	39,41,42,42	0
4	EDO	E	403	4/4	0.91	0.10	34,34,37,38	0
4	EDO	E	402	4/4	0.92	0.12	33,35,38,39	0
3	CL	D	402	1/1	0.92	0.12	46,46,46,46	0
6	PO4	E	404	5/5	0.92	0.11	34,36,38,42	5
3	CL	D	401	1/1	0.95	0.09	34,34,34,34	0
2	4TG	A	401[A]	37/37	0.96	0.07	16,24,30,34	37
4	EDO	F	402	4/4	0.96	0.07	30,33,33,34	0
5	NA	A	405	1/1	0.96	0.09	23,23,23,23	0
2	4TG	A	401[B]	37/37	0.96	0.07	22,24,30,34	37
3	CL	E	401	1/1	0.98	0.04	27,27,27,27	0

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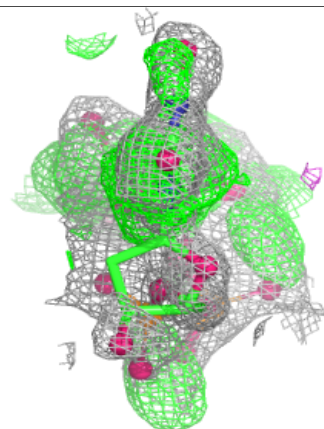
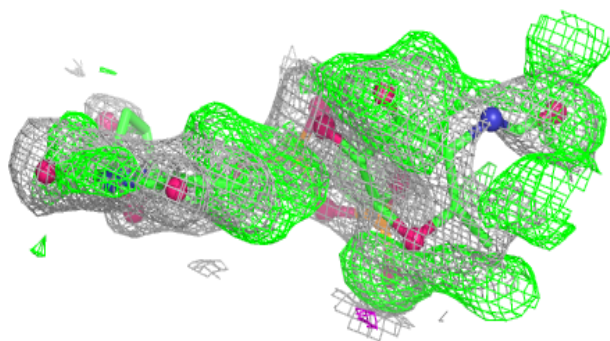
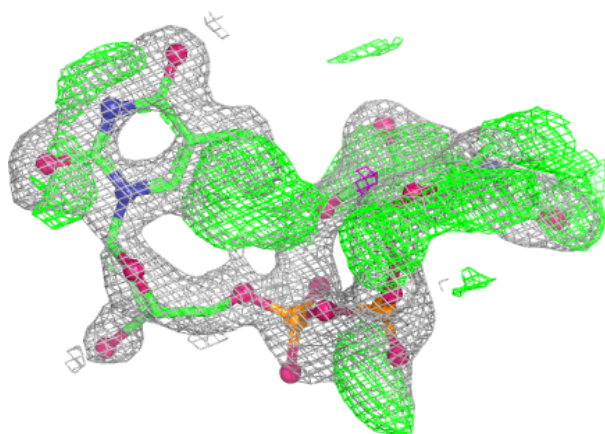
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	A	402	1/1	0.98	0.07	29,29,29,29	0
3	CL	B	402	1/1	0.98	0.09	38,38,38,38	0
5	NA	C	402	1/1	0.99	0.06	27,27,27,27	0
3	CL	F	401	1/1	0.99	0.03	22,22,22,22	0

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.

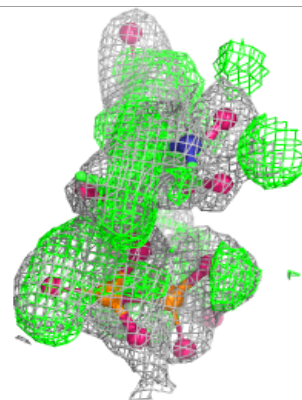
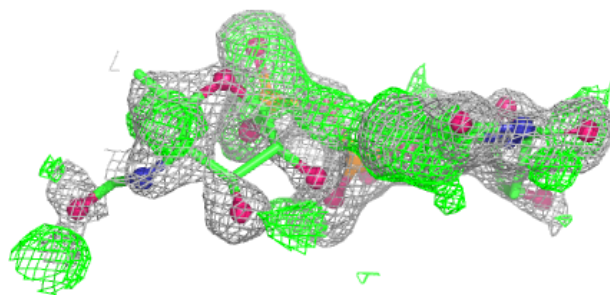
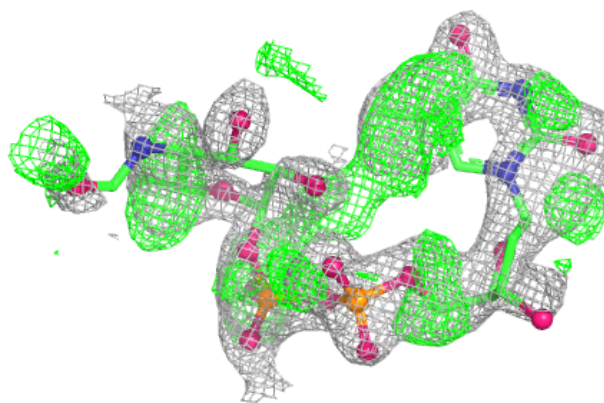
Electron density around 4TG B 401:

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



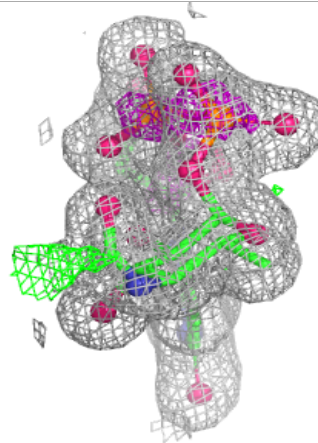
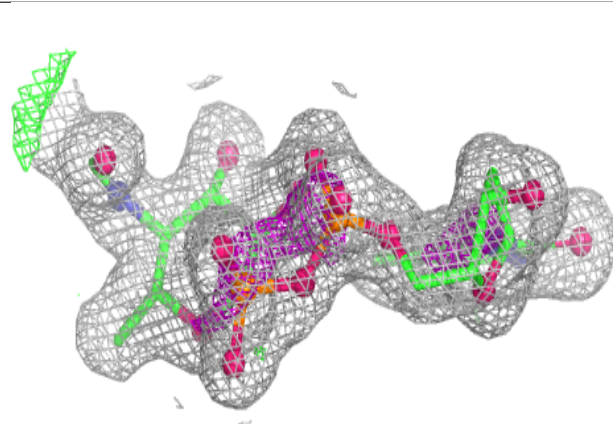
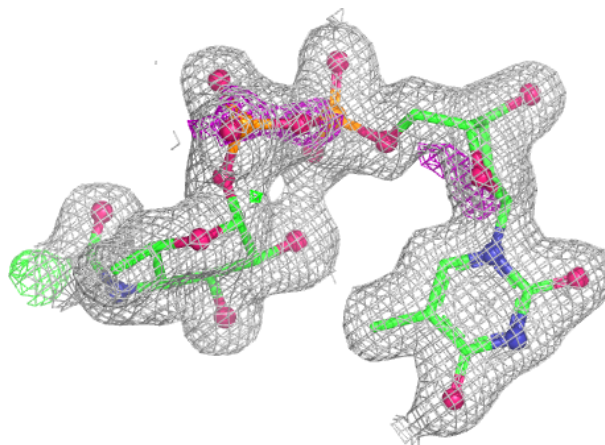
Electron density around 4TG C 401:

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



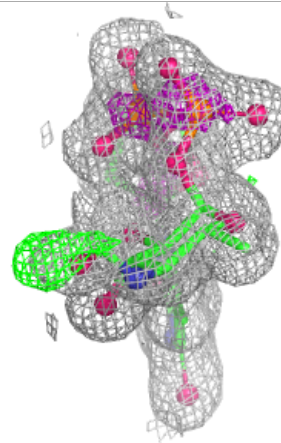
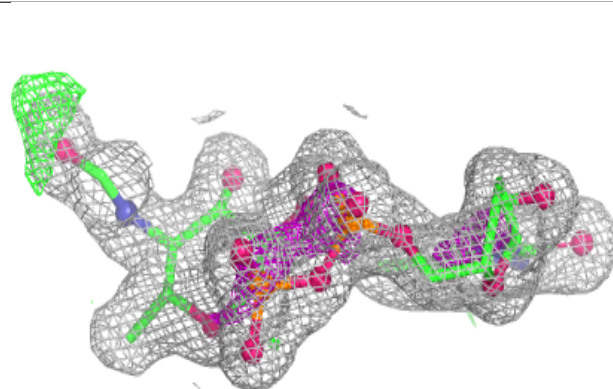
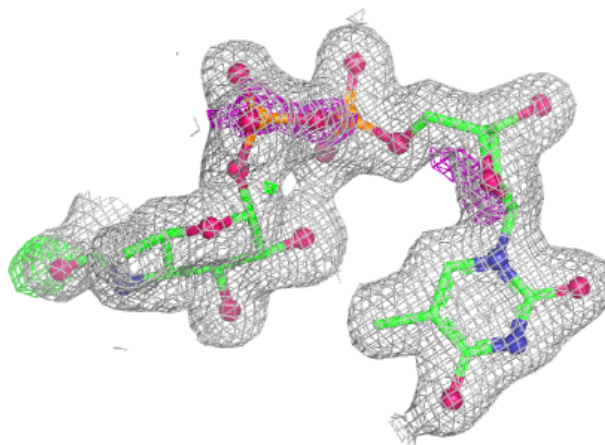
Electron density around 4TG A 401 (A):

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.