



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:21 PM UTC

PDB ID : 3FKB / pdb_00003fkb
Title : Structure of NDPK H122G and tenofovir-diphosphate
Authors : Morera, S.; Chen, Y.X.
Deposited on : 2008-12-16
Resolution : 1.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

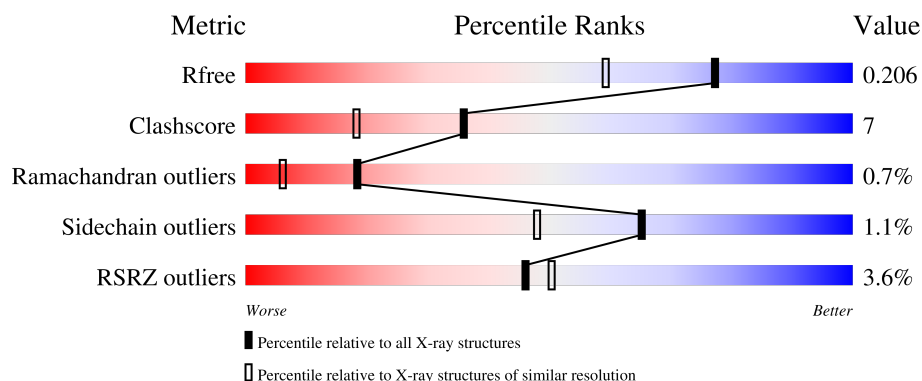
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	155	5% 81% 14% ..
1	B	155	3% 78% 17% ..
1	C	155	5% 84% 11% ..
1	D	155	3% 79% 13% ..
1	E	155	2% 85% 11% ..

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Mol	Chain	Length	Quality of chain
1	F	155	

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
5	GOL	C	157	-	X	-	-
5	GOL	D	157	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8284 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.

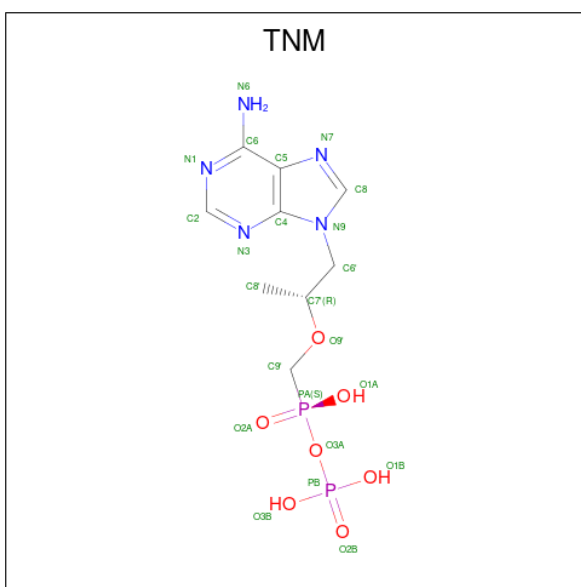
- Molecule 1 is a protein called Nucleoside diphosphate kinase, cytosolic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1140	732	196	210	2			
1	B	150	Total	C	N	O	S	0	0	0
			1140	732	196	210	2			
1	C	150	Total	C	N	O	S	0	0	0
			1140	732	196	210	2			
1	D	149	Total	C	N	O	S	0	0	0
			1133	727	195	209	2			
1	E	149	Total	C	N	O	S	0	0	0
			1133	727	195	209	2			
1	F	150	Total	C	N	O	S	0	0	0
			1140	732	196	210	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	122	GLY	HIS	engineered mutation	UNP P22887
B	122	GLY	HIS	engineered mutation	UNP P22887
C	122	GLY	HIS	engineered mutation	UNP P22887
D	122	GLY	HIS	engineered mutation	UNP P22887
E	122	GLY	HIS	engineered mutation	UNP P22887
F	122	GLY	HIS	engineered mutation	UNP P22887

- Molecule 2 is [(2R)-1-(6-aminopurin-9-yl)propan-2-yl]oxymethyl-phosphonooxy-phosphinic acid (CCD ID: TNM) (formula: C₉H₁₅N₅O₇P₂).

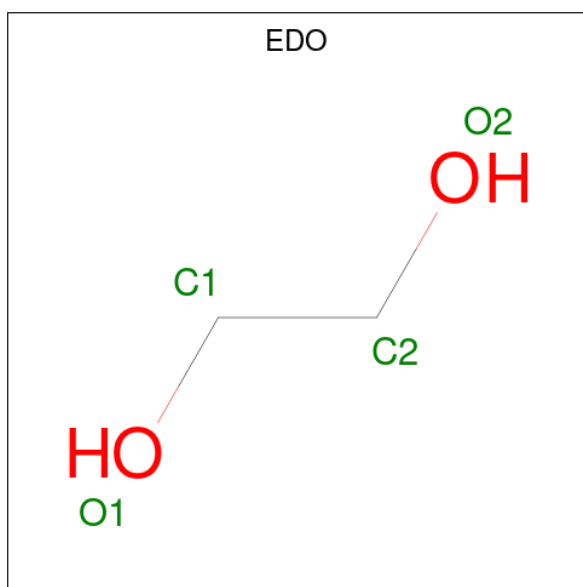


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	9	5	7	2		
2	B	1	Total	C	N	O	P	0	0
			23	9	5	7	2		
2	C	1	Total	C	N	O	P	0	0
			23	9	5	7	2		
2	E	1	Total	C	N	O	P	0	0
			23	9	5	7	2		
2	F	1	Total	C	N	O	P	0	0
			23	9	5	7	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

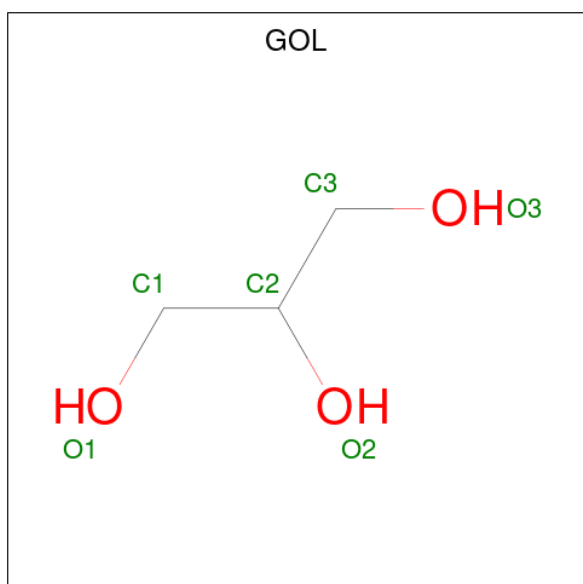
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



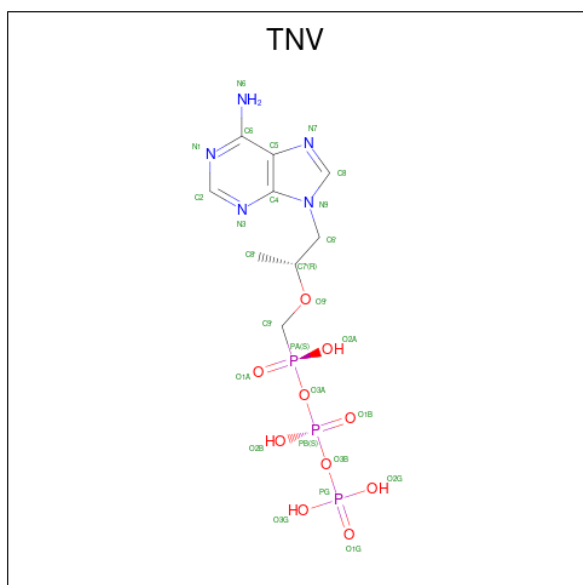
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is [2-(6-AMINO-9H-PURIN-9-YL)-1-METHYLETHOXY]METHYL-TRIPHOSPHATE (CCD ID: TNV) (formula: $C_9H_{16}N_5O_{10}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	0	0
			27	9	5	10	3		

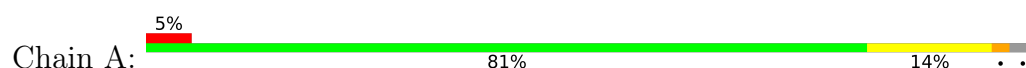
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	203	Total	O	0	0
			203	203		
7	B	200	Total	O	0	0
			200	200		
7	C	212	Total	O	0	0
			212	212		
7	D	210	Total	O	0	0
			210	210		
7	E	239	Total	O	0	0
			239	239		
7	F	214	Total	O	0	0
			214	214		

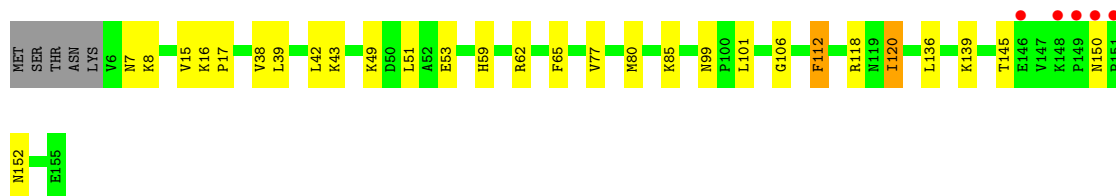
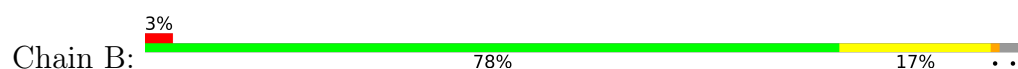
3 Residue-property plots [i](#)

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.

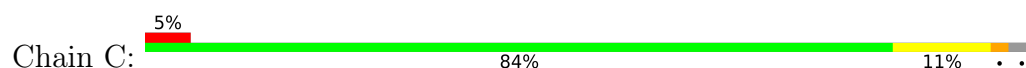
- Molecule 1: Nucleoside diphosphate kinase, cytosolic



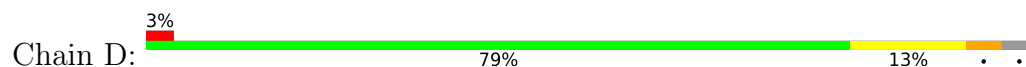
- Molecule 1: Nucleoside diphosphate kinase, cytosolic



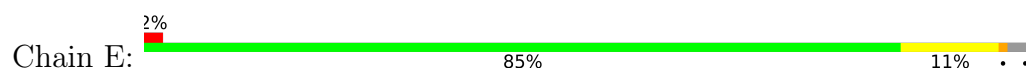
- Molecule 1: Nucleoside diphosphate kinase, cytosolic



- Molecule 1: Nucleoside diphosphate kinase, cytosolic

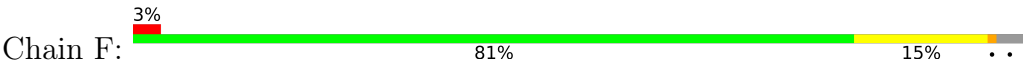


- Molecule 1: Nucleoside diphosphate kinase, cytosolic





● Molecule 1: Nucleoside diphosphate kinase, cytosolic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.42Å 104.57Å 69.21Å 90.00° 117.96° 90.00°	Depositor
Resolution (Å)	20.00 – 1.65 20.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-1.65) 99.8 (20.00-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.45 (at 1.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.181 , 0.205 0.181 , 0.206	Depositor DCC
R_{free} test set	5276 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	12.0	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.004 for l,k,-h-l 0.004 for -h-l,k,h 0.018 for -h-l,-k,l 0.019 for h,-k,-h-l 0.021 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8284	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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: EDO, GOL, TNV, TNM, MG

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	0.32	0/1163	0.88	4/1573 (0.3%)
1	B	0.32	0/1163	0.85	6/1573 (0.4%)
1	C	0.31	0/1163	0.86	4/1573 (0.3%)
1	D	0.33	0/1156	0.87	4/1563 (0.3%)
1	E	0.34	0/1156	0.89	4/1563 (0.3%)
1	F	0.32	0/1163	0.87	3/1573 (0.2%)
All	All	0.32	0/6964	0.87	25/9418 (0.3%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	120	ILE	N-CA-C	6.55	122.97	109.34
1	F	120	ILE	N-CA-C	6.48	122.82	109.34
1	A	120	ILE	N-CA-C	5.88	121.58	109.34
1	C	151	PRO	N-CA-C	-5.74	106.52	114.27
1	A	15	VAL	N-CA-C	-5.56	99.59	107.98
1	E	15	VAL	N-CA-C	-5.53	99.63	107.98
1	E	145	THR	N-CA-C	-5.50	107.11	113.88
1	D	106	GLY	N-CA-C	-5.42	107.45	113.79
1	B	112	PHE	N-CA-C	5.39	121.62	114.12
1	C	120	ILE	N-CA-C	5.33	120.42	109.34
1	B	120	ILE	N-CA-C	5.32	120.39	109.34
1	D	120	ILE	N-CA-C	5.30	120.36	109.34
1	B	139	LYS	N-CA-C	-5.26	103.04	110.29
1	D	112	PHE	N-CA-C	5.24	121.41	114.12
1	C	15	VAL	N-CA-C	-5.23	100.09	107.98
1	E	112	PHE	N-CA-C	5.21	121.36	114.12
1	F	15	VAL	N-CA-C	-5.18	99.65	107.73
1	D	139	LYS	N-CA-C	-5.16	103.17	110.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106	GLY	N-CA-C	-5.15	107.76	113.79
1	B	145	THR	N-CA-C	-5.13	107.40	113.97
1	F	112	PHE	N-CA-C	5.08	121.18	114.12
1	B	15	VAL	N-CA-C	-5.05	100.35	107.98
1	A	112	PHE	N-CA-C	5.05	121.14	114.12
1	C	106	GLY	N-CA-C	-5.03	107.91	113.79
1	A	106	GLY	N-CA-C	-5.01	107.93	113.79

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	1140	0	1163	16	0
1	B	1140	0	1163	19	0
1	C	1140	0	1163	19	0
1	D	1133	0	1154	22	0
1	E	1133	0	1154	13	0
1	F	1140	0	1163	17	0
2	A	23	0	12	0	0
2	B	23	0	12	0	0
2	C	23	0	12	0	0
2	E	23	0	12	0	0
2	F	23	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	4	0	6	1	0
4	B	4	0	6	1	0
4	D	4	0	6	0	0
4	F	8	0	12	0	0
5	C	6	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	6	0	3	0	0
6	D	27	0	12	0	0
7	A	203	0	0	3	0
7	B	200	0	0	2	0
7	C	212	0	0	3	0
7	D	210	0	0	1	0
7	E	239	0	0	1	0
7	F	214	0	0	2	0
All	All	8284	0	7068	103	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 7.

All (103) 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:D:146:GLU:HG3	1:D:147:VAL:H	1.35	0.92
1:F:6:VAL:HG13	1:F:8:LYS:H	1.41	0.86
1:A:151:PRO:HD2	7:A:2265:HOH:O	1.84	0.78
1:D:56:TYR:CD2	1:D:68:LEU:HD21	2.20	0.76
1:E:148:LYS:HD2	1:E:149:PRO:HD2	1.70	0.73
1:A:6:VAL:HG13	1:A:8:LYS:H	1.53	0.72
1:D:68:LEU:C	1:D:68:LEU:HD23	2.17	0.70
1:B:150:ASN:HD21	1:B:152:ASN:HD22	1.41	0.69
1:B:62:ARG:HA	1:B:62:ARG:HE	1.59	0.68
1:C:149:PRO:C	1:C:150:ASN:HD22	2.04	0.64
1:C:150:ASN:HB2	1:C:153:LEU:HD23	1.81	0.63
1:D:8:LYS:HD3	1:D:83:GLU:OE2	2.00	0.62
1:C:16:LYS:HE3	7:C:1855:HOH:O	1.99	0.61
1:E:150:ASN:HD22	1:E:150:ASN:C	2.11	0.59
1:C:149:PRO:HG3	1:C:154:TYR:HE2	1.69	0.58
1:D:150:ASN:C	1:D:150:ASN:HD22	2.12	0.58
1:A:49:LYS:O	1:A:53:GLU:HG3	2.04	0.57
1:A:141:GLU:H	1:A:141:GLU:CD	2.12	0.57
1:D:146:GLU:HG3	1:D:147:VAL:N	2.13	0.57
1:F:6:VAL:HG22	1:F:7:ASN:H	1.70	0.57
1:A:6:VAL:HG22	1:A:7:ASN:N	2.20	0.56
1:A:6:VAL:HG22	1:A:7:ASN:H	1.70	0.56
1:C:151:PRO:HD2	7:C:1910:HOH:O	2.06	0.56
1:B:38:VAL:HG13	4:B:157:EDO:H21	1.89	0.55
1:E:147:VAL:O	1:E:148:LYS:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LEU:HD21	1:A:114:VAL:HG13	1.89	0.54
1:E:150:ASN:ND2	1:E:152:ASN:H	2.04	0.54
1:F:141:GLU:H	1:F:141:GLU:CD	2.16	0.54
1:B:150:ASN:ND2	1:B:152:ASN:HB2	2.24	0.53
1:D:146:GLU:O	1:D:147:VAL:HB	2.10	0.52
1:D:150:ASN:ND2	1:D:152:ASN:H	2.08	0.51
1:C:17:PRO:HD3	1:C:77:VAL:HG22	1.92	0.51
1:B:8:LYS:HE2	7:B:2156:HOH:O	2.10	0.51
1:E:150:ASN:HD22	1:E:151:PRO:N	2.09	0.50
1:A:54:SER:HB3	1:A:136:LEU:HD11	1.93	0.50
1:D:49:LYS:O	1:D:53:GLU:HG3	2.11	0.50
1:F:80:MET:HE3	1:F:82:PHE:HE1	1.76	0.50
1:B:51:LEU:CD1	1:B:136:LEU:HG	2.43	0.49
1:E:8:LYS:O	1:E:8:LYS:HD3	2.10	0.49
1:F:6:VAL:HG22	1:F:7:ASN:N	2.27	0.49
1:F:39:LEU:HD21	1:F:42:LEU:HD22	1.93	0.49
1:A:39:LEU:HD21	1:A:42:LEU:HD22	1.93	0.49
1:D:7:ASN:N	7:D:1879:HOH:O	2.45	0.49
1:F:51:LEU:CD1	1:F:136:LEU:HG	2.42	0.49
1:B:59:HIS:O	1:B:65:PHE:HB2	2.13	0.48
1:C:149:PRO:C	1:C:150:ASN:ND2	2.71	0.48
1:D:51:LEU:CD1	1:D:136:LEU:HD22	2.44	0.48
1:E:49:LYS:O	1:E:53:GLU:HG3	2.14	0.47
7:A:1068:HOH:O	1:D:34:LYS:HE3	2.15	0.46
1:A:112:PHE:HB2	1:A:120:ILE:HD13	1.98	0.46
1:C:149:PRO:HG3	1:C:154:TYR:CE2	2.48	0.46
1:D:150:ASN:HD22	1:D:151:PRO:N	2.13	0.46
1:B:39:LEU:HD21	1:B:42:LEU:HD22	1.98	0.46
1:B:8:LYS:HD2	7:B:2229:HOH:O	2.16	0.46
1:B:17:PRO:HD3	1:B:77:VAL:HG22	1.97	0.46
1:E:39:LEU:HD21	1:E:42:LEU:HD22	1.98	0.46
1:F:58:GLU:HG2	7:F:1899:HOH:O	2.15	0.45
1:B:62:ARG:HA	1:B:62:ARG:NE	2.27	0.45
1:D:112:PHE:HB2	1:D:120:ILE:HD13	1.98	0.45
1:A:51:LEU:HD12	1:A:136:LEU:HD22	1.99	0.45
1:F:59:HIS:O	1:F:65:PHE:HB2	2.18	0.44
1:F:80:MET:HE3	1:F:82:PHE:CE1	2.52	0.44
1:D:16:LYS:HE2	1:D:56:TYR:OH	2.17	0.44
1:B:118:ARG:NH1	1:C:155:GLU:OE2	2.50	0.44
1:C:39:LEU:HD21	1:C:42:LEU:HD22	1.99	0.44
1:C:43:LYS:HA	1:F:42:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:LYS:HZ3	1:D:147:VAL:HG21	1.82	0.43
1:A:150:ASN:OD1	1:A:152:ASN:HB2	2.18	0.43
1:A:51:LEU:CD1	1:A:136:LEU:HD22	2.48	0.43
1:D:68:LEU:C	1:D:68:LEU:CD2	2.88	0.43
1:C:112:PHE:HB2	1:C:120:ILE:HD13	2.00	0.43
1:F:130:ALA:O	1:F:134:ILE:HG13	2.19	0.43
1:B:49:LYS:O	1:B:53:GLU:HG3	2.19	0.42
1:D:60:LYS:HA	1:D:65:PHE:CD1	2.54	0.42
1:D:147:VAL:O	1:D:148:LYS:HB2	2.19	0.42
1:C:128:GLU:H	1:C:128:GLU:CD	2.27	0.42
1:A:60:LYS:HA	1:A:65:PHE:CD1	2.55	0.42
1:A:60:LYS:HE2	7:A:1275:HOH:O	2.18	0.42
1:C:16:LYS:HB3	1:C:17:PRO:HD2	2.02	0.42
1:D:60:LYS:HA	1:D:65:PHE:CG	2.54	0.42
1:C:6:VAL:N	7:C:2046:HOH:O	2.53	0.41
1:E:150:ASN:HD22	1:E:151:PRO:CD	2.33	0.41
1:A:150:ASN:OD1	1:A:152:ASN:ND2	2.52	0.41
1:B:7:ASN:OD1	1:B:85:LYS:HE3	2.20	0.41
1:B:43:LYS:HA	1:E:42:LEU:O	2.20	0.41
1:F:49:LYS:O	1:F:53:GLU:HG3	2.20	0.41
1:C:16:LYS:CE	1:C:119:ASN:OD1	2.69	0.41
1:F:13:LEU:HB2	1:F:80:MET:HG3	2.02	0.41
1:C:150:ASN:ND2	1:C:150:ASN:N	2.68	0.41
1:E:34:LYS:HE2	7:E:1697:HOH:O	2.19	0.41
1:E:150:ASN:HD22	1:E:152:ASN:H	1.68	0.41
1:B:99:ASN:C	1:B:99:ASN:HD22	2.28	0.41
1:B:112:PHE:HB2	1:B:120:ILE:HD13	2.03	0.41
1:B:16:LYS:HB3	1:B:17:PRO:HD2	2.03	0.40
2:F:160:TNM:H8	7:F:1038:HOH:O	2.21	0.40
1:F:6:VAL:HG13	1:F:8:LYS:N	2.22	0.40
1:C:8:LYS:N	1:C:8:LYS:HD2	2.36	0.40
1:D:62:ARG:HA	1:D:63:PRO:HD3	1.95	0.40
1:F:99:ASN:C	1:F:99:ASN:HD22	2.29	0.40
4:A:157:EDO:H11	1:D:75:GLY:HA3	2.02	0.40
1:B:99:ASN:ND2	1:B:101:LEU:H	2.19	0.40
1:C:42:LEU:O	1:F:43:LYS:HA	2.20	0.40
1:E:17:PRO:HD3	1:E:77:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	148/155 (96%)	141 (95%)	6 (4%)	1 (1%)	18	6
1	B	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
1	C	148/155 (96%)	141 (95%)	6 (4%)	1 (1%)	18	6
1	D	147/155 (95%)	141 (96%)	4 (3%)	2 (1%)	9	1
1	E	147/155 (95%)	142 (97%)	4 (3%)	1 (1%)	18	6
1	F	148/155 (96%)	143 (97%)	4 (3%)	1 (1%)	18	6
All	All	886/930 (95%)	852 (96%)	28 (3%)	6 (1%)	18	6

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	149	PRO
1	A	149	PRO
1	D	148	LYS
1	E	148	LYS
1	F	148	LYS
1	D	147	VAL

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	121/126 (96%)	119 (98%)	2 (2%)	53	32
1	B	121/126 (96%)	120 (99%)	1 (1%)	73	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	121/126 (96%)	121 (100%)	0	100	100
1	D	120/126 (95%)	118 (98%)	2 (2%)	53	32
1	E	120/126 (95%)	120 (100%)	0	100	100
1	F	121/126 (96%)	118 (98%)	3 (2%)	42	18
All	All	724/756 (96%)	716 (99%)	8 (1%)	65	48

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	ASP
1	A	136	LEU
1	B	80	MET
1	D	68	LEU
1	D	136	LEU
1	F	80	MET
1	F	146	GLU
1	F	148	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	99	ASN
1	B	59	HIS
1	B	99	ASN
1	B	150	ASN
1	C	150	ASN
1	C	152	ASN
1	D	7	ASN
1	D	150	ASN
1	E	150	ASN
1	F	7	ASN
1	F	99	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 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	TNM	C	160	3	22,24,24	1.74	7 (31%)	31,36,36	1.24	3 (9%)
4	EDO	F	157	-	3,3,3	0.54	0	2,2,2	0.08	0
4	EDO	F	158	-	3,3,3	0.53	0	2,2,2	0.09	0
4	EDO	D	158	-	3,3,3	0.52	0	2,2,2	0.09	0
5	GOL	C	157	-	5,5,5	4.53	5 (100%)	5,5,5	2.20	2 (40%)
4	EDO	A	157	-	3,3,3	0.56	0	2,2,2	0.03	0
2	TNM	B	160	3	22,24,24	1.75	7 (31%)	31,36,36	1.24	5 (16%)
4	EDO	B	157	-	3,3,3	0.52	0	2,2,2	0.09	0
2	TNM	A	160	3	22,24,24	1.67	7 (31%)	31,36,36	1.21	4 (12%)
6	TNV	D	160	3	26,28,28	2.49	7 (26%)	36,43,43	1.43	4 (11%)
2	TNM	F	160	3	22,24,24	1.71	7 (31%)	31,36,36	1.21	4 (12%)
2	TNM	E	160	3	22,24,24	1.68	6 (27%)	31,36,36	1.19	4 (12%)
5	GOL	D	157	-	5,5,5	4.50	5 (100%)	5,5,5	2.24	2 (40%)

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	TNM	C	160	3	-	4/13/16/16	0/2/2/2
4	EDO	F	157	-	-	1/1/1/1	-
4	EDO	F	158	-	-	1/1/1/1	-
4	EDO	D	158	-	-	1/1/1/1	-
5	GOL	C	157	-	-	4/4/4/4	-
4	EDO	A	157	-	-	0/1/1/1	-
2	TNM	B	160	3	-	3/13/16/16	0/2/2/2
4	EDO	B	157	-	-	1/1/1/1	-
2	TNM	A	160	3	-	1/13/16/16	0/2/2/2
6	TNV	D	160	3	-	4/19/22/22	0/2/2/2
2	TNM	F	160	3	-	1/13/16/16	0/2/2/2
2	TNM	E	160	3	-	1/13/16/16	0/2/2/2
5	GOL	D	157	-	-	4/4/4/4	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	160	TNV	PB-O3B	-9.59	1.49	1.59
5	C	157	GOL	C3-C2	-5.60	1.30	1.51
5	D	157	GOL	C3-C2	-5.60	1.30	1.51
5	C	157	GOL	C1-C2	-5.60	1.30	1.51
5	D	157	GOL	C1-C2	-5.53	1.30	1.51
5	D	157	GOL	O1-C1	3.96	1.59	1.42
5	C	157	GOL	O3-C3	3.96	1.59	1.42
5	C	157	GOL	O1-C1	3.94	1.59	1.42
5	D	157	GOL	O3-C3	3.92	1.58	1.42
2	F	160	TNM	C2-N1	3.13	1.39	1.33
6	D	160	TNV	PA-O2A	-3.11	1.48	1.56
2	B	160	TNM	PA-O1A	-3.06	1.48	1.56
2	E	160	TNM	C2-N1	3.05	1.39	1.33
2	C	160	TNM	C6'-C7'	3.02	1.62	1.51
2	C	160	TNM	C2-N1	2.99	1.39	1.33
6	D	160	TNV	C2-N1	2.99	1.39	1.33
2	B	160	TNM	C6'-C7'	2.99	1.62	1.51
6	D	160	TNV	C6'-C7'	2.99	1.62	1.51
2	A	160	TNM	C2-N1	2.99	1.39	1.33
2	B	160	TNM	C2-N1	2.96	1.39	1.33
2	F	160	TNM	PA-O1A	-2.95	1.49	1.56
2	C	160	TNM	PA-O1A	-2.95	1.49	1.56
5	C	157	GOL	O2-C2	-2.94	1.34	1.43
5	D	157	GOL	O2-C2	-2.90	1.34	1.43
2	A	160	TNM	PA-O1A	-2.89	1.49	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	160	TNM	C6'-C7'	2.82	1.61	1.51
2	E	160	TNM	PA-O1A	-2.81	1.49	1.56
2	F	160	TNM	C6'-C7'	2.81	1.61	1.51
2	E	160	TNM	C6'-C7'	2.72	1.61	1.51
2	E	160	TNM	C4-N3	2.61	1.39	1.34
6	D	160	TNV	C4-N3	2.61	1.39	1.34
2	F	160	TNM	C4-N3	2.54	1.39	1.34
2	C	160	TNM	C4-N3	2.52	1.39	1.34
2	B	160	TNM	C4-N3	2.50	1.39	1.34
2	A	160	TNM	C4-N3	2.49	1.39	1.34
2	B	160	TNM	C2-N3	2.27	1.38	1.33
2	B	160	TNM	C5-C6	2.27	1.47	1.41
2	E	160	TNM	C5-C6	2.24	1.47	1.41
6	D	160	TNV	C5-C6	2.22	1.47	1.41
2	C	160	TNM	C5-C6	2.19	1.47	1.41
2	F	160	TNM	C5-C6	2.18	1.47	1.41
2	B	160	TNM	C5-C4	2.16	1.42	1.39
2	C	160	TNM	C5-C4	2.14	1.42	1.39
2	F	160	TNM	C5-C4	2.12	1.42	1.39
2	F	160	TNM	C2-N3	2.12	1.37	1.33
2	E	160	TNM	C2-N3	2.11	1.37	1.33
2	A	160	TNM	C5-C6	2.09	1.46	1.41
2	C	160	TNM	C2-N3	2.08	1.37	1.33
6	D	160	TNV	C2-N3	2.05	1.37	1.33
2	A	160	TNM	C2-N3	2.04	1.37	1.33
2	A	160	TNM	C5-C4	2.02	1.42	1.39

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	157	GOL	O1-C1-C2	3.50	126.13	110.38
6	D	160	TNV	O3A-PB-O1B	-3.49	100.20	110.70
5	C	157	GOL	O1-C1-C2	3.43	125.82	110.38
5	D	157	GOL	O3-C3-C2	3.42	125.79	110.38
5	C	157	GOL	O3-C3-C2	3.40	125.70	110.38
6	D	160	TNV	O2B-PB-O3B	3.16	115.80	107.27
6	D	160	TNV	PA-O3A-PB	-3.11	122.24	132.37
2	A	160	TNM	PA-O3A-PB	-2.97	121.80	132.45
2	C	160	TNM	PA-O3A-PB	-2.90	122.05	132.45
2	B	160	TNM	PA-O3A-PB	-2.89	122.08	132.45
2	F	160	TNM	PA-O3A-PB	-2.85	122.23	132.45
2	E	160	TNM	PA-O3A-PB	-2.71	122.75	132.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	160	TNM	C6'-N9-C4	2.20	128.96	126.41
2	A	160	TNM	O1A-PA-O2A	2.11	116.81	109.95
2	A	160	TNM	C6'-N9-C4	2.10	128.84	126.41
2	F	160	TNM	C6'-N9-C4	2.09	128.83	126.41
2	B	160	TNM	O3B-PB-O1B	2.09	115.62	107.80
2	A	160	TNM	O3B-PB-O1B	2.08	115.60	107.80
2	C	160	TNM	O1A-PA-O2A	2.07	116.69	109.95
2	F	160	TNM	O3B-PB-O1B	2.07	115.56	107.80
2	B	160	TNM	C7'-C6'-N9	2.05	115.92	112.68
2	B	160	TNM	O1A-PA-O2A	2.05	116.62	109.95
2	F	160	TNM	O1A-PA-O2A	2.05	116.62	109.95
2	C	160	TNM	O3B-PB-O1B	2.05	115.48	107.80
6	D	160	TNV	O2A-PA-O1A	2.04	116.58	109.95
2	E	160	TNM	O3B-PB-O1B	2.04	115.43	107.80
2	E	160	TNM	O1A-PA-O2A	2.03	116.56	109.95
2	B	160	TNM	C6'-N9-C4	2.02	128.75	126.41

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	160	TNM	N9-C6'-C7'-O9'
2	C	160	TNM	N9-C6'-C7'-O9'
5	C	157	GOL	O1-C1-C2-C3
5	C	157	GOL	C1-C2-C3-O3
5	D	157	GOL	O1-C1-C2-C3
5	D	157	GOL	C1-C2-C3-O3
6	D	160	TNV	N9-C6'-C7'-O9'
6	D	160	TNV	N9-C6'-C7'-C8'
5	C	157	GOL	O2-C2-C3-O3
4	B	157	EDO	O1-C1-C2-O2
4	D	158	EDO	O1-C1-C2-O2
2	B	160	TNM	N9-C6'-C7'-C8'
2	C	160	TNM	N9-C6'-C7'-C8'
5	D	157	GOL	O1-C1-C2-O2
4	F	158	EDO	O1-C1-C2-O2
4	F	157	EDO	O1-C1-C2-O2
5	C	157	GOL	O1-C1-C2-O2
5	D	157	GOL	O2-C2-C3-O3
2	C	160	TNM	O9'-C9'-PA-O1A
2	A	160	TNM	PA-C9'-O9'-C7'
2	B	160	TNM	PA-C9'-O9'-C7'

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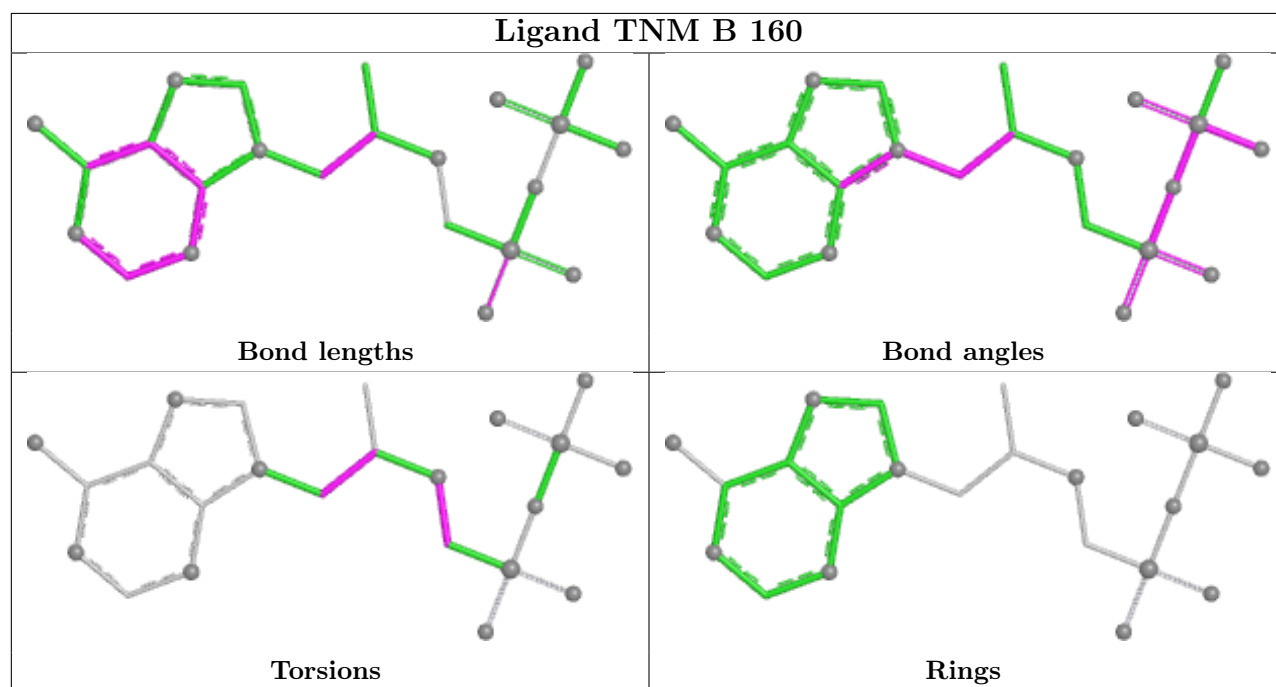
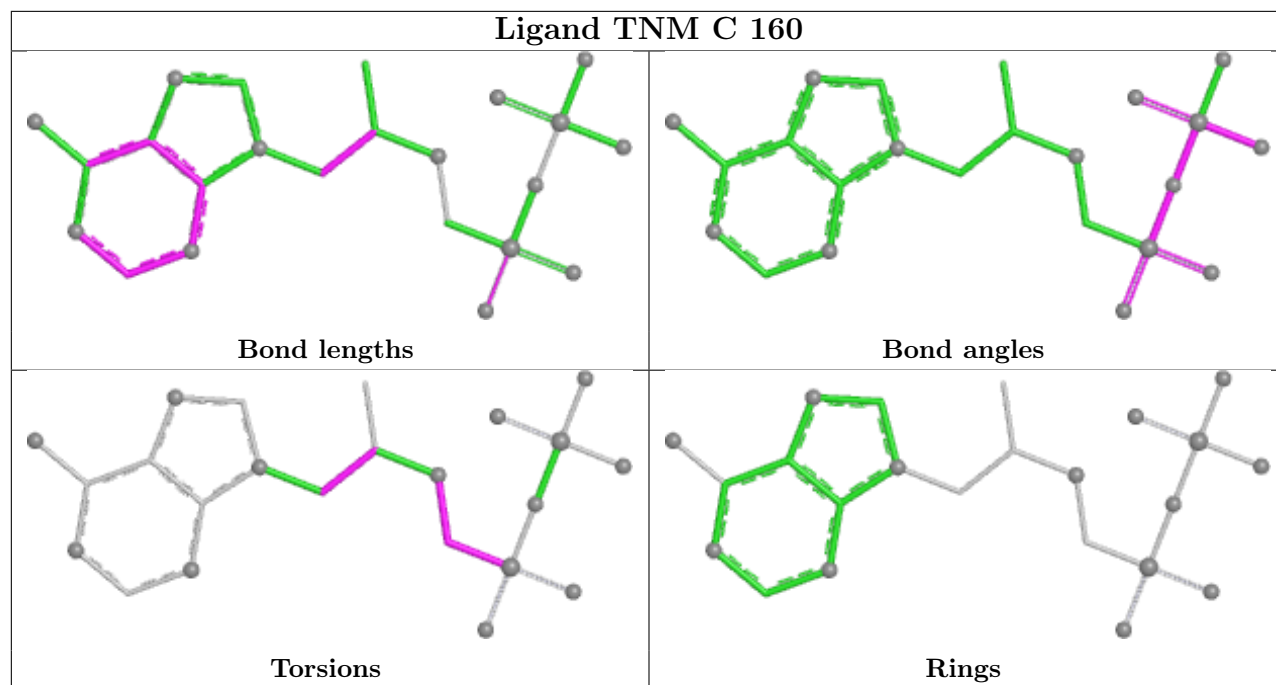
Mol	Chain	Res	Type	Atoms
2	C	160	TNM	PA-C9'-O9'-C7'
2	E	160	TNM	PA-C9'-O9'-C7'
2	F	160	TNM	PA-C9'-O9'-C7'
6	D	160	TNV	PG-O3B-PB-O2B
6	D	160	TNV	PG-O3B-PB-O1B

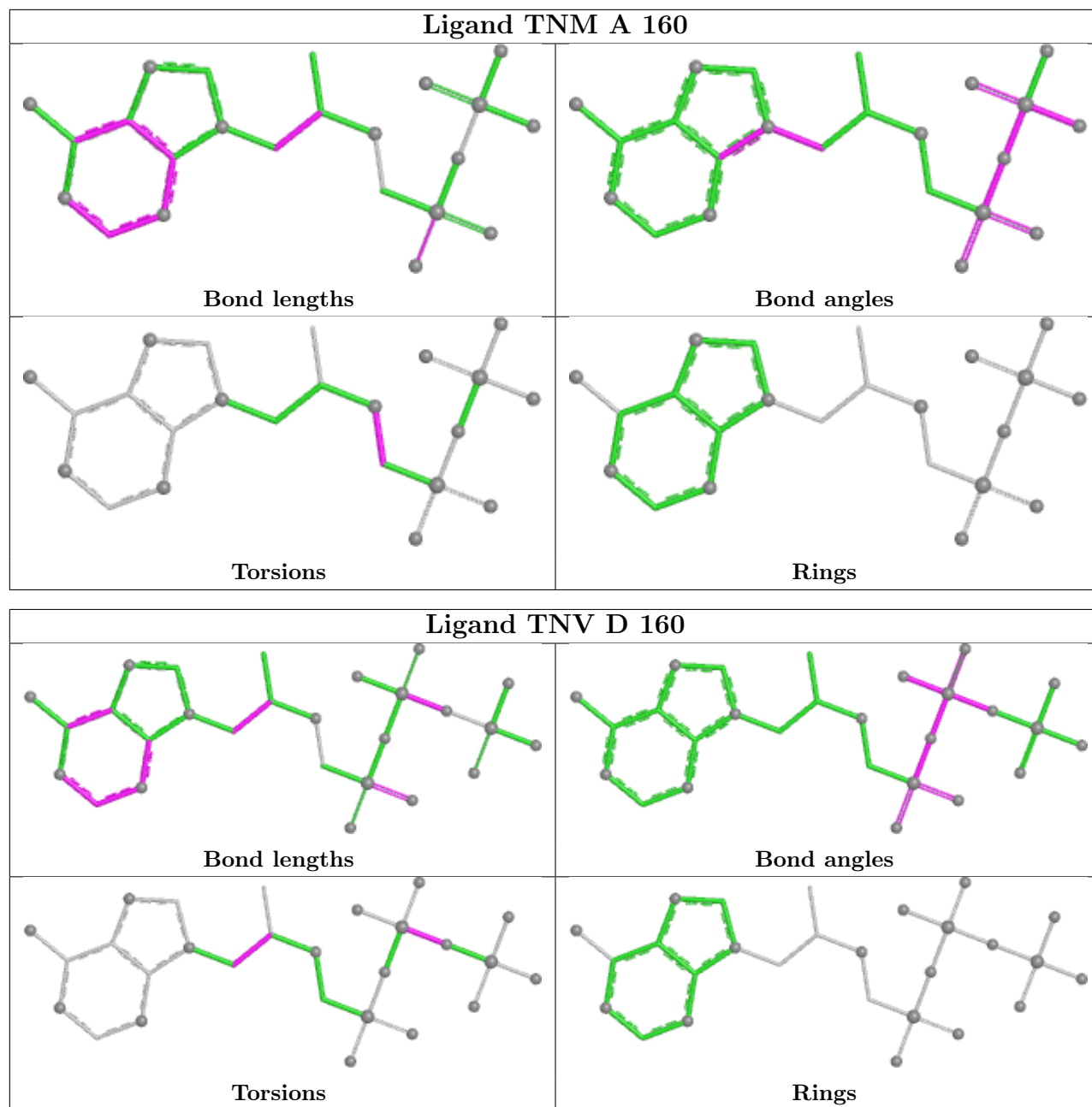
There are no ring outliers.

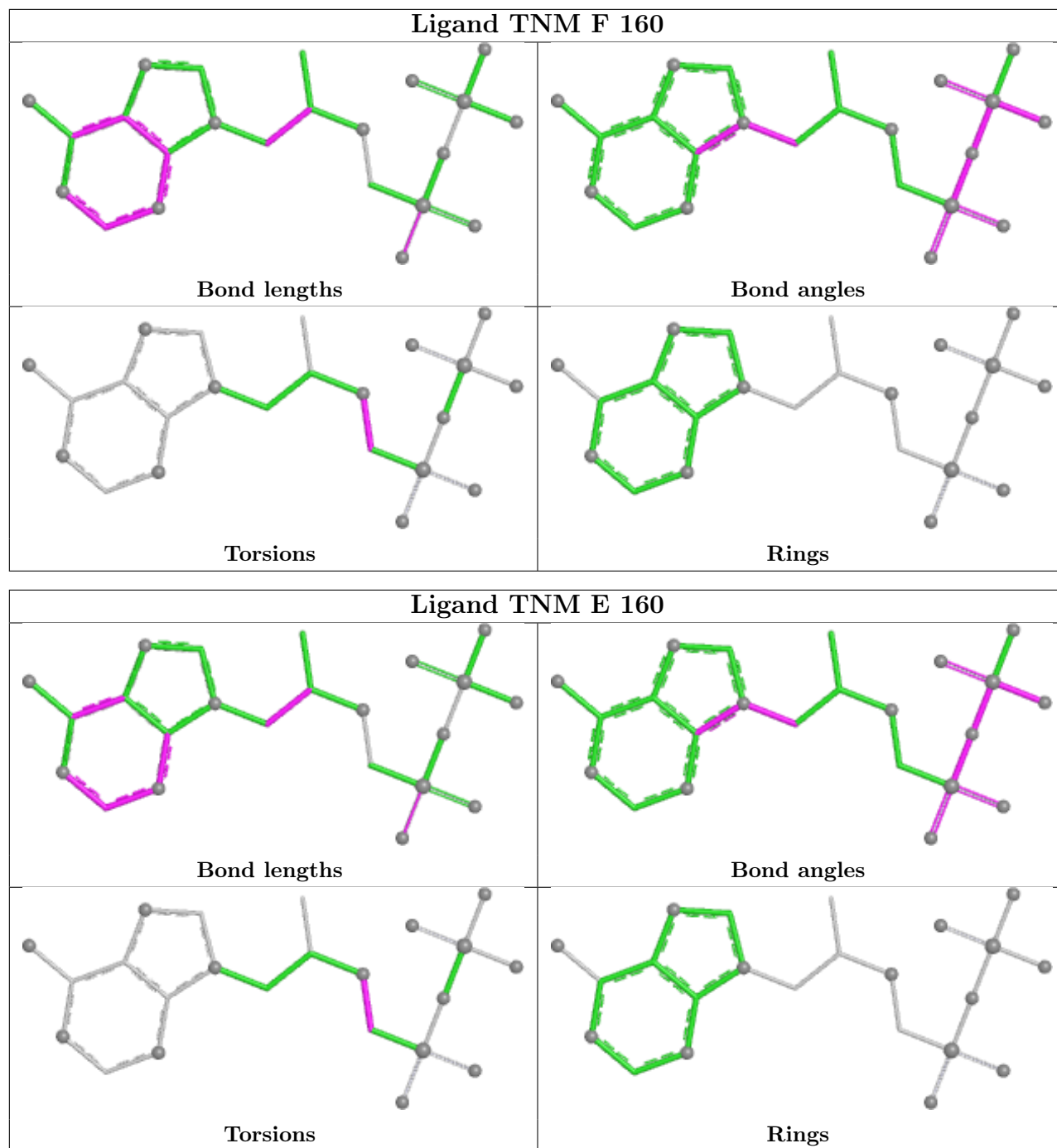
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	157	EDO	1	0
4	B	157	EDO	1	0
2	F	160	TNM	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	150/155 (96%)	-0.16	7 (4%) 36 40	6, 11, 28, 44	0
1	B	150/155 (96%)	-0.09	5 (3%) 49 53	6, 12, 28, 43	0
1	C	150/155 (96%)	0.02	7 (4%) 36 40	6, 13, 37, 45	0
1	D	149/155 (96%)	-0.17	5 (3%) 48 52	7, 12, 24, 41	0
1	E	149/155 (96%)	-0.34	3 (2%) 65 70	6, 10, 24, 39	0
1	F	150/155 (96%)	-0.25	5 (3%) 49 53	7, 11, 27, 42	0
All	All	898/930 (96%)	-0.17	32 (3%) 46 50	6, 11, 28, 45	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	151	PRO	6.5
1	D	147	VAL	6.2
1	C	149	PRO	5.8
1	A	149	PRO	5.3
1	A	6	VAL	4.8
1	A	150	ASN	4.5
1	C	148	LYS	4.5
1	F	146	GLU	4.4
1	B	149	PRO	4.3
1	F	147	VAL	4.2
1	E	147	VAL	4.2
1	F	6	VAL	4.2
1	D	146	GLU	4.0
1	C	150	ASN	4.0
1	D	149	PRO	3.6
1	E	146	GLU	3.6
1	C	147	VAL	3.1
1	D	148	LYS	3.1
1	E	149	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	149	PRO	3.0
1	B	151	PRO	2.9
1	D	56	TYR	2.8
1	F	148	LYS	2.8
1	A	148	LYS	2.7
1	C	50	ASP	2.7
1	A	147	VAL	2.6
1	C	64	PHE	2.5
1	A	153	LEU	2.4
1	B	150	ASN	2.4
1	B	146	GLU	2.1
1	B	148	LYS	2.1
1	C	155	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

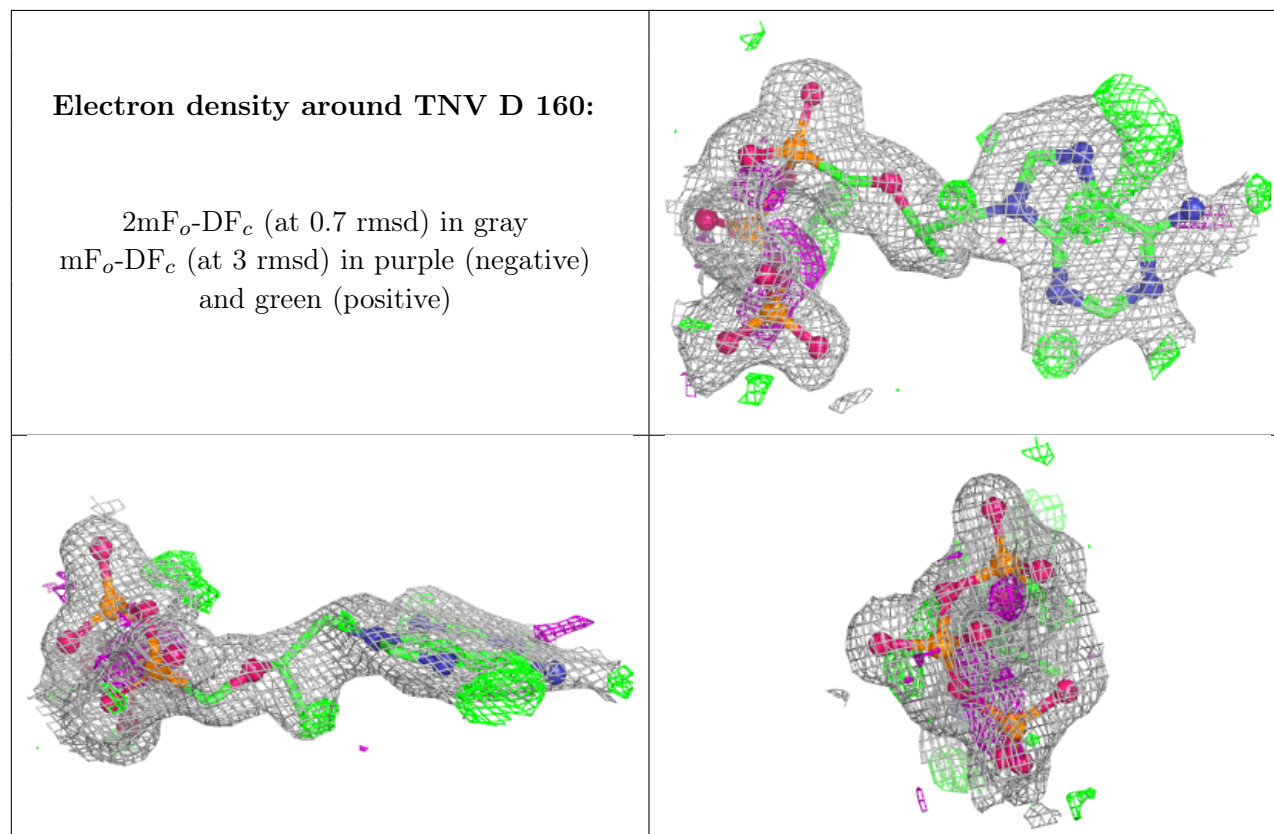
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	F	158	4/4	0.47	0.19	51,51,51,52	0
4	EDO	B	157	4/4	0.67	0.24	40,41,41,43	0
4	EDO	A	157	4/4	0.73	0.17	42,43,43,44	0
5	GOL	C	157	6/6	0.74	0.20	60,60,61,61	0
5	GOL	D	157	6/6	0.75	0.28	76,77,77,77	0
4	EDO	D	158	4/4	0.78	0.16	35,37,37,38	0
4	EDO	F	157	4/4	0.84	0.19	31,32,33,34	0
6	TNV	D	160	27/27	0.88	0.13	24,28,34,36	0
2	TNM	C	160	23/23	0.91	0.12	22,33,40,41	0
2	TNM	B	160	23/23	0.94	0.11	18,27,40,40	0

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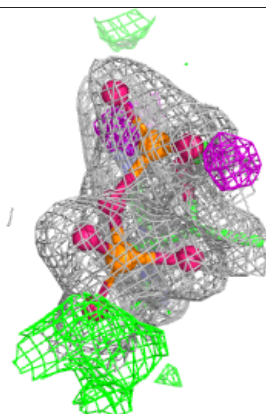
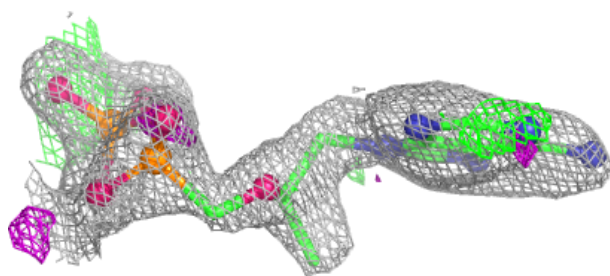
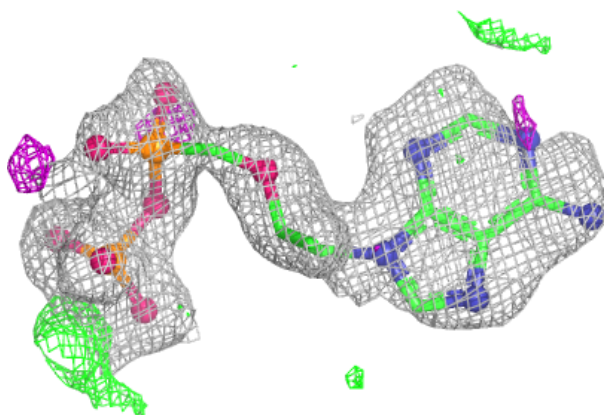
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	D	156	1/1	0.94	0.06	27,27,27,27	0
2	TNM	A	160	23/23	0.95	0.07	15,18,21,22	0
3	MG	C	156	1/1	0.96	0.12	20,20,20,20	0
2	TNM	E	160	23/23	0.96	0.07	11,14,20,23	0
2	TNM	F	160	23/23	0.97	0.06	15,18,25,25	0
3	MG	B	156	1/1	0.97	0.06	15,15,15,15	0
3	MG	E	156	1/1	0.98	0.04	11,11,11,11	0
3	MG	A	156	1/1	0.99	0.06	12,12,12,12	0
3	MG	F	156	1/1	0.99	0.10	11,11,11,11	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.

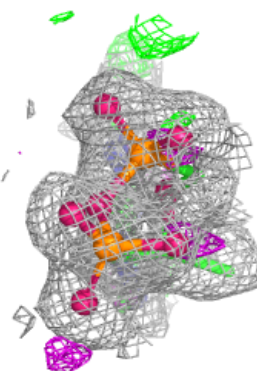
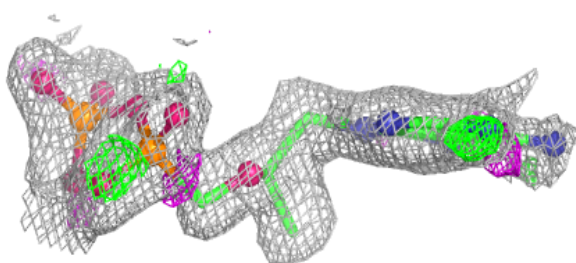
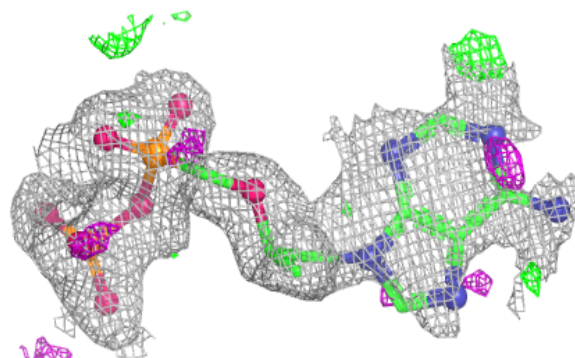


Electron density around TNM C 160:

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

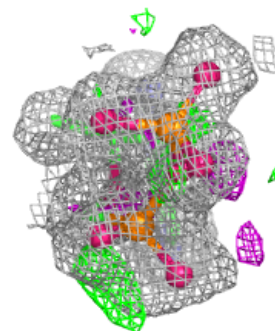
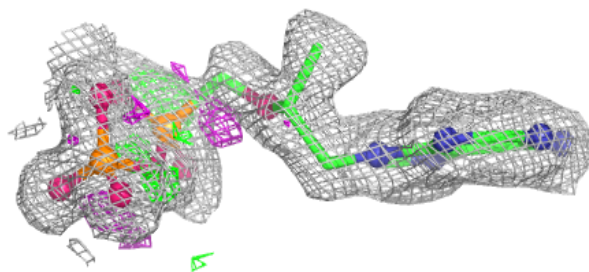
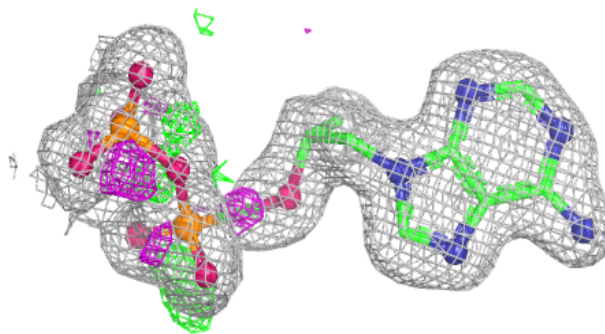
**Electron density around TNM B 160:**

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

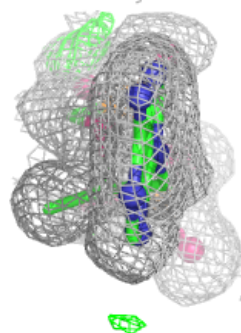
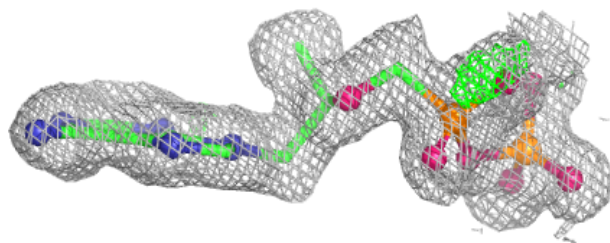
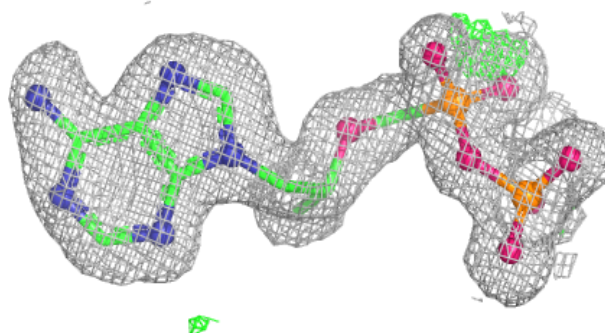


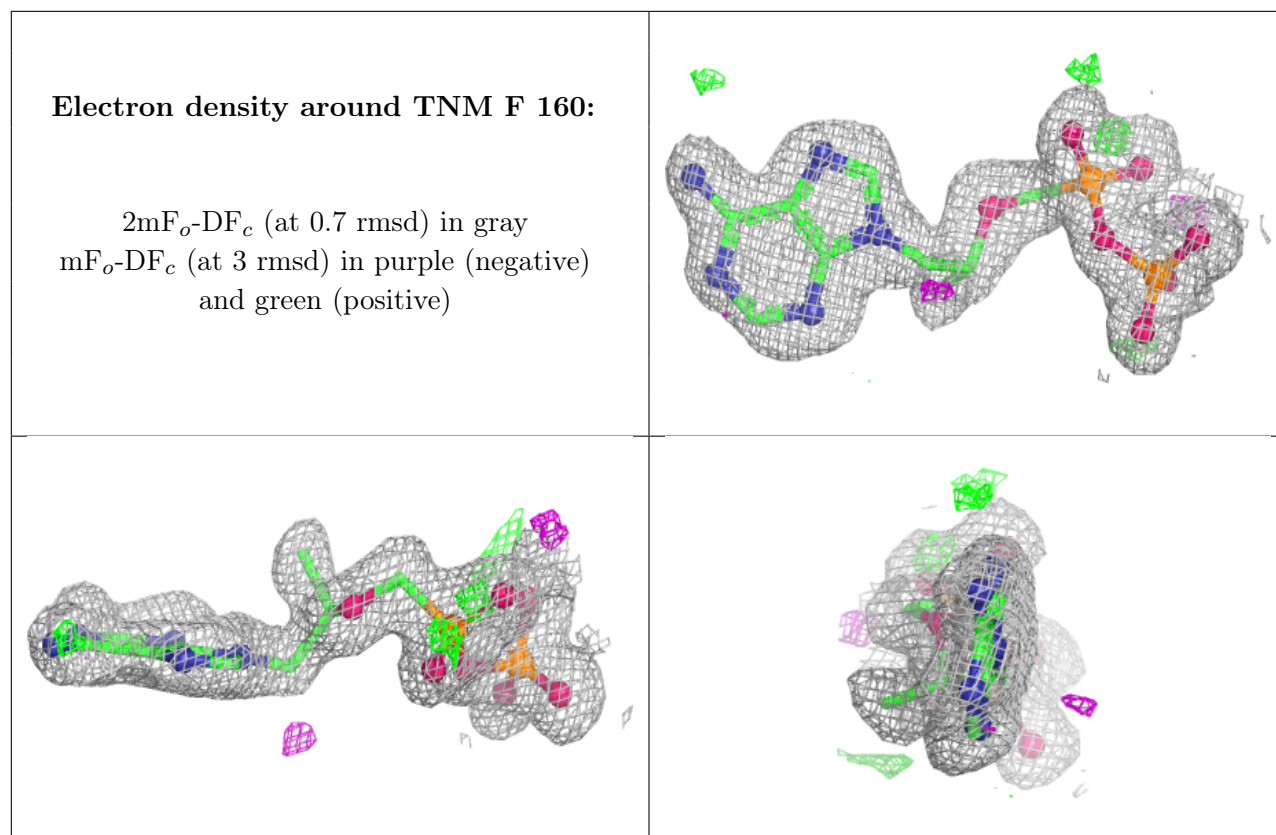
Electron density around TNM A 160:

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

**Electron density around TNM E 160:**

$2mF_o-DF_c$ (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.