WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Aug 23, 2023 – 09:21 AM EDT

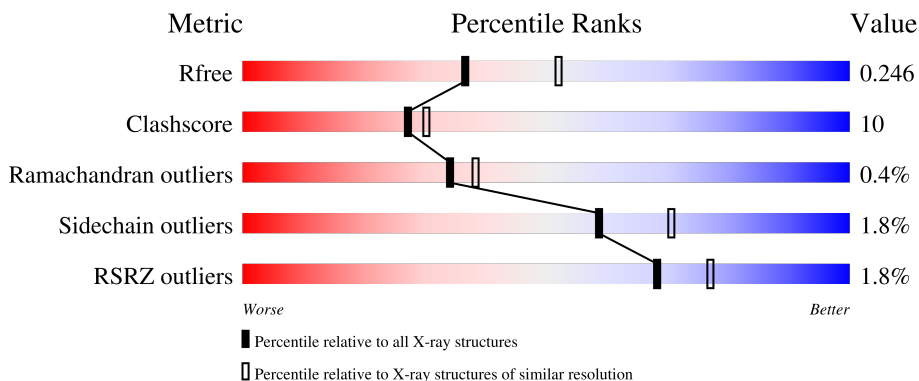|		
PDB ID	:	3DVA
Title	:	Snapshots of catalysis in the E1 subunit of the pyruvate dehydrogenase multi-enzyme complex
Authors	:	Pei, X.Y.; Titman, C.M.; Frank, R.A.W.; Leeper, F.J.; Luisi, B.F.
Deposited on	:	2008-07-18
Resolution	:	2.35 Å(reported)

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.35 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	Percentile Ranks	Value
Rfree		0.246
Clashscore		10
Ramachandran outliers		0.4%
Sidechain outliers		1.8%
RSRZ outliers		1.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	369	5% 79% 19% ••
1	C	369	2% 86% 12% •
1	E	369	2% 82% 14% •
1	G	369	.% 80% 18% ••
2	B	325	77% 22% •

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Mol	Chain	Length	Quality of chain
2	D	325	82% 17%
2	F	325	76% 23%
2	H	325	82% 17%
3	I	428	2% 90%
3	J	428	2% 91%

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 23282 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 Pyruvate dehydrogenase E1 component subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2895	1850	491	546	8			
1	C	365	Total	C	N	O	S	0	0	0
			2895	1850	491	546	8			
1	E	354	Total	C	N	O	S	0	0	0
			2798	1791	473	526	8			
1	G	365	Total	C	N	O	S	0	0	0
			2895	1850	491	546	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ALA	ILE	engineered mutation	UNP P21873
C	206	ALA	ILE	engineered mutation	UNP P21873
E	206	ALA	ILE	engineered mutation	UNP P21873
G	206	ALA	ILE	engineered mutation	UNP P21873

- Molecule 2 is a protein called Pyruvate dehydrogenase E1 component subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	324	Total	C	N	O	S	0	0	0
			2488	1586	424	470	8			
2	D	324	Total	C	N	O	S	0	0	0
			2488	1586	424	470	8			
2	F	324	Total	C	N	O	S	0	0	0
			2488	1586	424	470	8			
2	H	324	Total	C	N	O	S	0	0	0
			2488	1586	424	470	8			

- Molecule 3 is a protein called Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	42	Total 314	C 195	N 62	O 56	S 1	0	0	0
3	J	40	Total 294	C 180	N 59	O 54	S 1	0	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Mg 2	0	0
4	C	1	Total 1	Mg 1	0	0
4	E	2	Total 2	Mg 2	0	0
4	G	1	Total 1	Mg 1	0	0

- Molecule 5 is 2-{4-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-3-METHYL THIOPHEN-2-YL}ETHYL TRIHYDROGEN DIPHOSPHATE (three-letter code: TPW) (formula: $C_{13}H_{19}N_3O_7P_2S$).
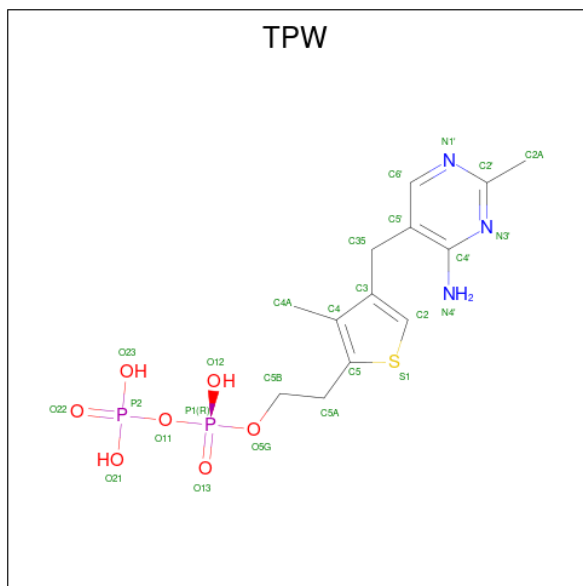
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 26	C 13	N 3	O 7	P 2	S 1	0	0
5	C	1	Total 26	C 13	N 3	O 7	P 2	S 1	0	0
5	E	1	Total 26	C 13	N 3	O 7	P 2	S 1	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	G	1	Total 26	C 13	N 3	O 7	P 2	S 1	0	0

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	K 1	0	0
6	D	1	Total 1	K 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	150	Total 150	O 150	0	0
7	B	139	Total 139	O 139	0	0
7	C	148	Total 148	O 148	0	0
7	D	161	Total 161	O 161	0	0
7	E	100	Total 100	O 100	0	0
7	F	126	Total 126	O 126	0	0
7	G	139	Total 139	O 139	0	0
7	H	155	Total 155	O 155	0	0
7	I	5	Total 5	O 5	0	0
7	J	4	Total 4	O 4	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, ye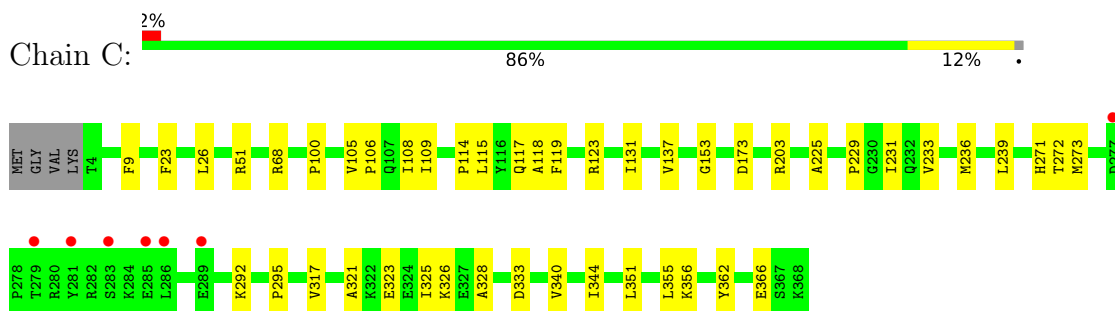llow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha

- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha

- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha

- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha

Chain G:

• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta

Chain B:

• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta

Chain D:

• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta

Chain F:

• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta
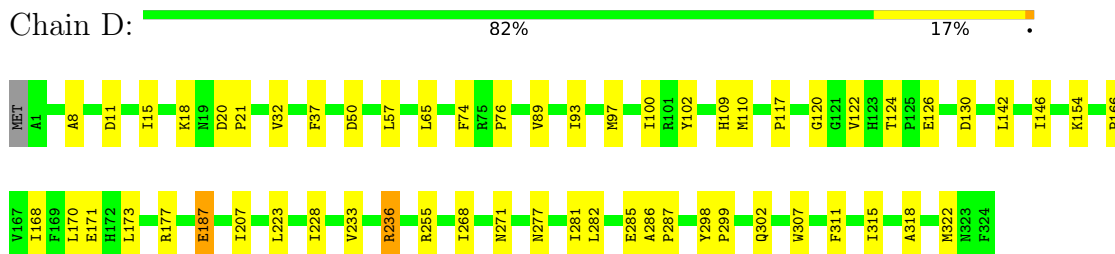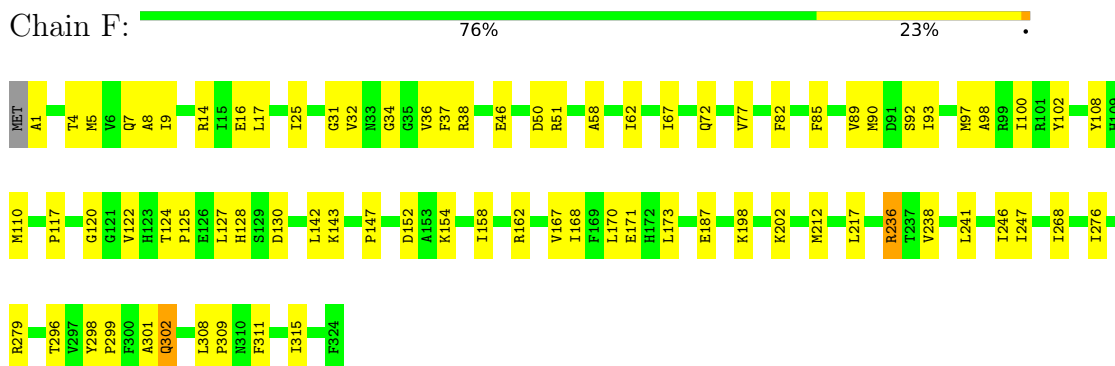
Chain H:

82% 17%

MET A1 D20 P21 I25 V52 L65 A70 F74 R75 P76 V89 M90 D91 S92 I93 Q96 M97 Y102 P111 R115 S116 P117 G120 G121 V122 H123 T124 L127 D130 Q139 L142 I146 I161 P166 V167 I168 F169 L170 E171

I206 I207 A219 E226 V233 V238 Q239 P240 L241 D242 I246 V250 I257 I268 V272 I276 A286 P287 Y298 P299 W307 F311 I315 K319 F324

• Molecule 3: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex

Chain I:

2% 90%

MET ALA PHE GLU PHE LYS LEU PRO ASP ILE GLY GLU GLY ILE HIS GLU GLY ILE GLU ILE VAL LYS TRP PHE VAL LYS PRO GLY ASP VAL VAL ASN GLU ASP ASP VAL LEU CYS GLU VAL GLN ASN ASP LYS ALA VAL VAL GLU ILE PRO SER PRO VAL LYS GLY LYS VAL LEU GLU ILE LEU

VAL PRO GLU THR VAL ALA THR VAL GLY GLN THR LEU ILE THR LEU ASP ALA PRO GLY TYR GLU ASN MET THR PHE LYS GLY GLN GLU GLU GLU ALA LYS LYS GLU GLU LYS THR GLU THR VAL SER LYS GLU GLU LYS VAL ASP ALA VAL ALA PRO ASN ALA PRO ALA ALA GLU

ALA GLU ALA GLY PRO ASN ARG R128 V129 I130 P133 S134 V135 R136 K137 Y138 A139 R140 E141 V144 D145 I146 R147 L148 G151 K154 N155 G156 R157 V158 L159 K160 E161 D162 I163 F166 L167 A168 G169 GLY ALA LYS PRO ALA ALA ALA GLU GLU LYS ALA ALA PRO ALA

ALA ALA LYS PRO ALA THR THR GLU GLY GLU PHE PRO GLU THR GLY THR ARG GLU GLY LYS MET SER GLY ILE ARG ARG ALA ILE ALA LYS ALA MET VAL HIS SER LYS HIS THR ALA PRO HIS VAL THR LEU MET ASP GLU ALA ASP VAL THR LYS LEU VAL ALA HIS ARG LYS LYS PHE LYS ALA ILE

ALA ALA GLU GLY ILE LYS LEU THR PHE LEU PRO TYR VAL VAL LYS ALA LEU VAL SER ALA LEU ARG GLU TYR PRO VAL LEU ASN THR SER ILE ASP GLY ASP ASP VAL ILE TYR HIS ASN TYR ASN ILE GLY ILE ALA ALA ASP THR ASP ARG GLY LEU LEU VAL PRO

VAL ILE LYS HIS ALA ASP ARG LYS PRO ILE PHE ALA LEU ALA GLN GLU ILE ASN LEU ALA GLU LYS ALA ARG ASP GLY LYS LEU THR PRO GLY GLU MET LYS GLY ALA SER CYS THR ILE THR ASN ILE GLY SER ALA GLY GLY GLN TRP PHE THR PRO VAL ILE ASN HIS PRO GLU

VAL ALA ILE LEU GLY ILE GLY ARG ILE ALA GLU LYS PRO ILE VAL ARG ASP GLY GLU ILE VAL ALA ALA PRO MET LEU ALA LEU SER LEU SER PHE ASP HIS ARG MET ILE ASP GLY ALA THR ALA GLN LYS ALA LEU ASN HIS ILE LYS ARG LEU LEU SER ASP PRO GLU LEU LEU LEU

MET GLU ALA

• Molecule 3: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex

Chain J:

2% 91%

MET ALA PHE GLU PHE LYS LEU PRO ASP ILE GLY GLU GLY ILE HIS GLU GLY ILE GLU ILE VAL LYS TRP PHE VAL LYS PRO GLY ASP VAL VAL ASN GLU ASP ASP VAL LEU CYS GLU VAL GLN ASN ASP LYS ALA VAL VAL GLU ILE PRO SER PRO VAL LYS GLY LYS VAL LEU GLU ILE LEU

VAL PRO GLU THR VAL ALA THR VAL GLY GLN THR LEU ILE THR LEU ASP ALA PRO GLY TYR GLU ASN MET THR PHE LYS GLY GLN GLU GLU GLU ALA LYS LYS GLU GLU LYS THR GLU THR VAL SER LYS GLU GLU LYS VAL ASP ALA VAL ALA PRO ASN ALA PRO ALA ALA GLU

ALA GLU ALA GLY PRO ASN ARG R128 V129 I130 A131 K137 E141 V144 D145 I146 R147 L148 V149 Q150 G151 T152 G153 K154 N155 G156 R157 V158 L159 K160 E161 D162 I163 D164 A165 F166 L167 ALA GLY GLY ALA LYS PRO ALA ALA ALA GLU GLU ALA ALA PRO ALA ALA ALA

LYS PRO ALA THR THR GLU GLY GLU PHE PRO GLU THR GLY THR ARG GLU GLY LYS MET SER GLY ILE ARG ARG ALA ILE ALA LYS ALA MET VAL HIS SER LYS HIS THR ALA PRO HIS VAL THR LEU MET ASP GLU ALA ASP VAL THR LYS LEU VAL ALA HIS ARG LYS LYS PHE LYS ALA ILE ALA ALA

GLU LYS GLY ILE LYS LEU THR PHE LEU PRO TYR VAL VAL LYS ALA LEU VAL SER ALA LEU ARG GLU TYR PRO VAL LEU ASN THR SER ILE ASP ASP GLU THR GLU GLU ILE ILE GLN LYS HIS TYR TYR ASN ILE GLY ALA ALA ASP THR ASP ARG GLY LEU LEU VAL PRO VAL ILE

LYS HIS ALA ASP ARG LYS PRO ILE PHE ALA LEU ALA GLN GLU ILE ASN GLU LEU ALA GLU LYS ALA ARG ASP GLY LYS LEU THR PRO GLY GLU MET LYS GLY ALA SER CYS THR ILE THR ASN ILE GLY SER ALA GLY GLY GLN TRP PHE THR PRO VAL ILE ASN HIS PRO GLU VAL ALA

ILE LEU GLY ILE GLY ARG ILE ALA GLU GLU LYS PRO ILE VAL ARG ASP GLY GLU ILE VAL ALA ALA PRO MET LEU ALA LEU SER LEU SER PHE ASP HIS ARG MET ILE ASP GLY ALA THR ALA GLN LYS ALA LEU ASN HIS ILE LYS ARG LEU LEU SER ASP PRO GLU LEU LEU LEU MET GLU

ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.67Å 232.29Å 91.94Å 90.00° 91.20° 90.00°	Depositor
Resolution (Å)	72.17 – 2.35 72.08 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.9 (72.17-2.35) 98.9 (72.08-2.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	5.04 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.247 0.191 , 0.246	Depositor DCC
R_{free} test set	5906 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.1	EDS
L-test for twinning[2]	$< |L| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.049 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	23282	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 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TPW, K, 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	0.38	0/2958	0.53	1/3995 (0.0%)
1	C	0.35	0/2958	0.48	0/3995
1	E	0.33	0/2858	0.45	0/3859
1	G	0.31	0/2958	0.47	0/3995
2	B	0.40	0/2534	0.55	2/3437 (0.1%)
2	D	0.27	0/2534	0.53	1/3437 (0.0%)
2	F	0.26	0/2534	0.52	1/3437 (0.0%)
2	H	0.28	0/2534	0.51	0/3437
3	I	1.44	1/316 (0.3%)	1.17	1/421 (0.2%)
3	J	1.54	0/295	1.16	1/395 (0.3%)
All	All	0.41	1/22479 (0.0%)	0.53	7/30408 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	138	TYR	CD2-CE2	-5.70	1.30	1.39

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	ASP	CB-CG-OD1	-7.67	111.40	118.30
2	B	234	ASP	CB-CG-OD1	6.80	124.42	118.30
2	B	236	ARG	CB-CA-C	-5.90	98.59	110.40
2	D	236	ARG	CB-CA-C	-5.84	98.72	110.40
3	J	162	ASP	CB-CG-OD1	-5.63	113.23	118.30

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	2895	0	2871	73	0
1	C	2895	0	2871	34	0
1	E	2798	0	2776	44	0
1	G	2895	0	2871	64	0
2	B	2488	0	2515	47	0
2	D	2488	0	2515	46	0
2	F	2488	0	2515	58	0
2	H	2488	0	2515	47	0
3	I	314	0	322	40	0
3	J	294	0	291	36	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
4	E	2	0	0	0	0
4	G	1	0	0	0	0
5	A	26	0	16	1	0
5	C	26	0	16	3	0
5	E	26	0	16	1	0
5	G	26	0	16	3	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	A	150	0	0	3	0
7	B	139	0	0	5	0
7	C	148	0	0	3	0
7	D	161	0	0	7	0
7	E	100	0	0	6	0
7	F	126	0	0	5	0
7	G	139	0	0	10	0
7	H	155	0	0	2	0
7	I	5	0	0	0	0
7	J	4	0	0	2	0
All	All	23282	0	22126	449	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 10.

The worst 5 of 449 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:A:281:TYR:CB	1:A:282:ARG:HA	1.57	1.34
2:D:285:GLU:HG3	3:I:140:ARG:NH2	1.56	1.18
3:J:160:LYS:O	3:J:160:LYS:HG2	1.43	1.17
1:A:281:TYR:HB3	1:A:282:ARG:HA	1.30	1.11
1:A:281:TYR:HB2	1:A:282:ARG:HA	1.30	1.07

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	363/369 (98%)	352 (97%)	11 (3%)	0	100	100
1	C	363/369 (98%)	350 (96%)	13 (4%)	0	100	100
1	E	350/369 (95%)	339 (97%)	11 (3%)	0	100	100
1	G	363/369 (98%)	353 (97%)	10 (3%)	0	100	100
2	B	322/325 (99%)	315 (98%)	6 (2%)	1 (0%)	41	47
2	D	322/325 (99%)	312 (97%)	9 (3%)	1 (0%)	41	47
2	F	322/325 (99%)	307 (95%)	12 (4%)	3 (1%)	17	17
2	H	322/325 (99%)	307 (95%)	15 (5%)	0	100	100
3	I	40/428 (9%)	31 (78%)	4 (10%)	5 (12%)	0	0
3	J	38/428 (9%)	30 (79%)	6 (16%)	2 (5%)	2	0
All	All	2805/3632 (77%)	2696 (96%)	97 (4%)	12 (0%)	34	38

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	236	ARG
3	J	165	ALA
2	F	301	ALA

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Mol	Chain	Res	Type
3	I	161	GLU
3	I	167	LEU

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	301/304 (99%)	293 (97%)	8 (3%)	44	55
1	C	301/304 (99%)	299 (99%)	2 (1%)	84	91
1	E	290/304 (95%)	289 (100%)	1 (0%)	92	96
1	G	301/304 (99%)	298 (99%)	3 (1%)	76	85
2	B	263/264 (100%)	260 (99%)	3 (1%)	73	84
2	D	263/264 (100%)	260 (99%)	3 (1%)	73	84
2	F	263/264 (100%)	260 (99%)	3 (1%)	73	84
2	H	263/264 (100%)	262 (100%)	1 (0%)	91	95
3	I	30/341 (9%)	21 (70%)	9 (30%)	0	0
3	J	28/341 (8%)	20 (71%)	8 (29%)	0	0
All	All	2303/2954 (78%)	2262 (98%)	41 (2%)	59	70

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	147	ARG
3	J	146	ILE
3	I	148	LEU
3	I	159	LEU
3	J	150	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	214	HIS

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Mol	Chain	Res	Type
1	G	271	HIS
2	H	271	ASN
1	G	69	GLN
2	D	109	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\#|Z| > 2$
5	TPW	G	1370	4	23,27,27	1.85	3 (13%)	30,40,40	1.81	9 (30%)
5	TPW	C	1370	4	23,27,27	1.83	3 (13%)	30,40,40	1.92	9 (30%)
5	TPW	A	1370	4	23,27,27	1.48	3 (13%)	30,40,40	1.84	9 (30%)
5	TPW	E	1370	4	23,27,27	1.64	3 (13%)	30,40,40	1.88	8 (26%)

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
5	TPW	G	1370	4	-	5/16/17/17	0/2/2/2
5	TPW	C	1370	4	-	2/16/17/17	0/2/2/2
5	TPW	A	1370	4	-	3/16/17/17	0/2/2/2
5	TPW	E	1370	4	-	0/16/17/17	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	1370	TPW	C5A-C5	6.08	1.53	1.50
5	C	1370	TPW	C5A-C5	5.95	1.53	1.50
5	E	1370	TPW	C5A-C5	4.16	1.52	1.50
5	E	1370	TPW	C2-C3	-3.65	1.34	1.37
5	C	1370	TPW	C2-C3	-3.50	1.34	1.37

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1370	TPW	C3-C2-S1	-3.88	108.13	112.26
5	C	1370	TPW	C35-C5'-C6'	-3.72	116.58	121.73
5	A	1370	TPW	C3-C2-S1	-3.61	108.42	112.26
5	E	1370	TPW	C3-C2-S1	-3.59	108.44	112.26
5	G	1370	TPW	P1-O11-P2	-3.57	120.58	132.83

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1370	TPW	P1-O11-P2-O21
5	A	1370	TPW	P1-O11-P2-O23
5	C	1370	TPW	C5-C5A-C5B-O5G
5	G	1370	TPW	C5-C5A-C5B-O5G
5	G	1370	TPW	C5B-O5G-P1-O12

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	1370	TPW	3	0
5	C	1370	TPW	3	0
5	A	1370	TPW	1	0
5	E	1370	TPW	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 TPW G 1370

Bond lengths

Bond angles

Torsions

Rings

Ligand TPW C 1370

Bond lengths

Bond angles

Torsions

Rings

Ligand TPW A 1370

Bond lengths

Bond angles

Torsions

Rings

Ligand TPW E 1370

Bond lengths

Bond angles

Torsions

Rings
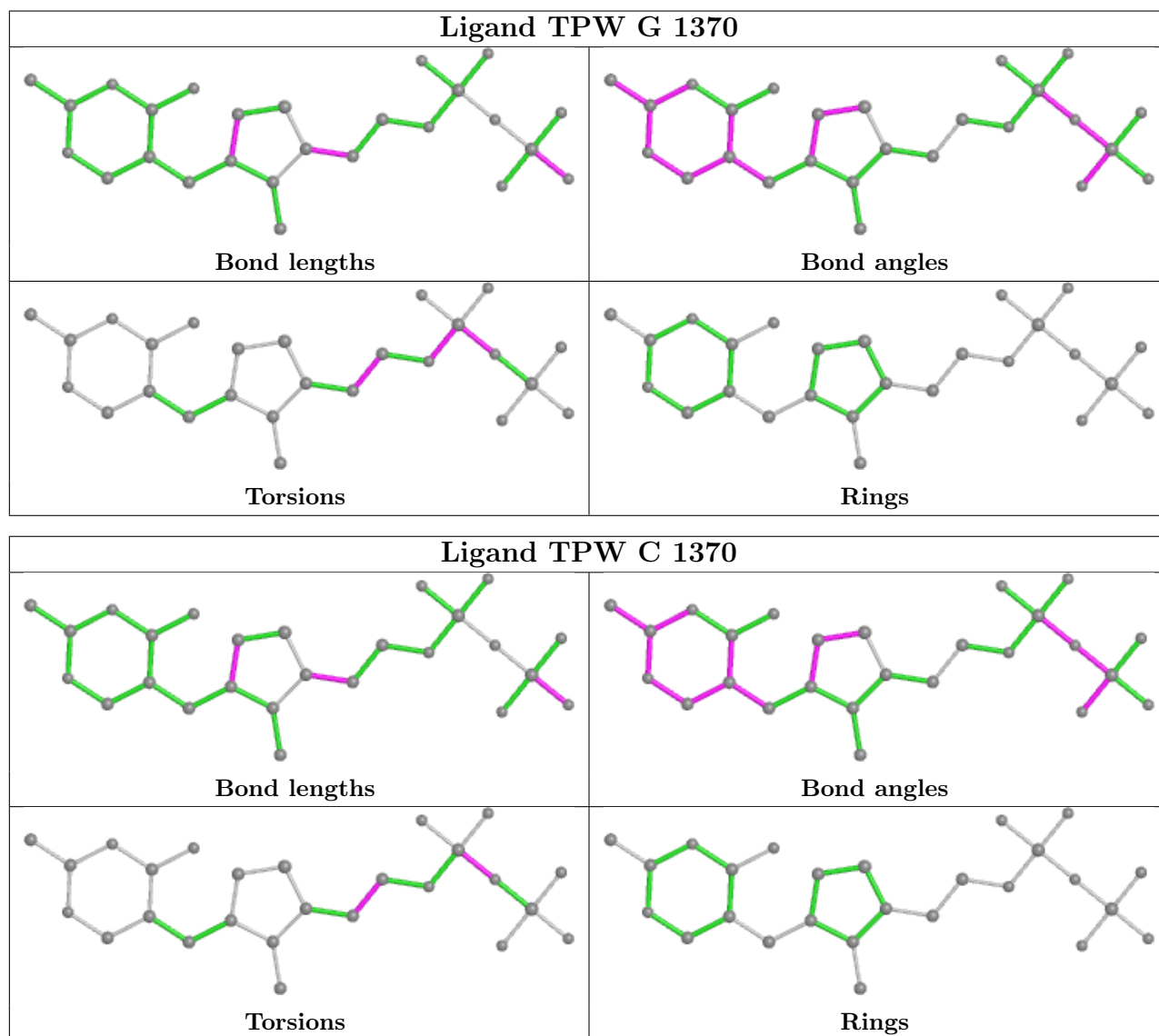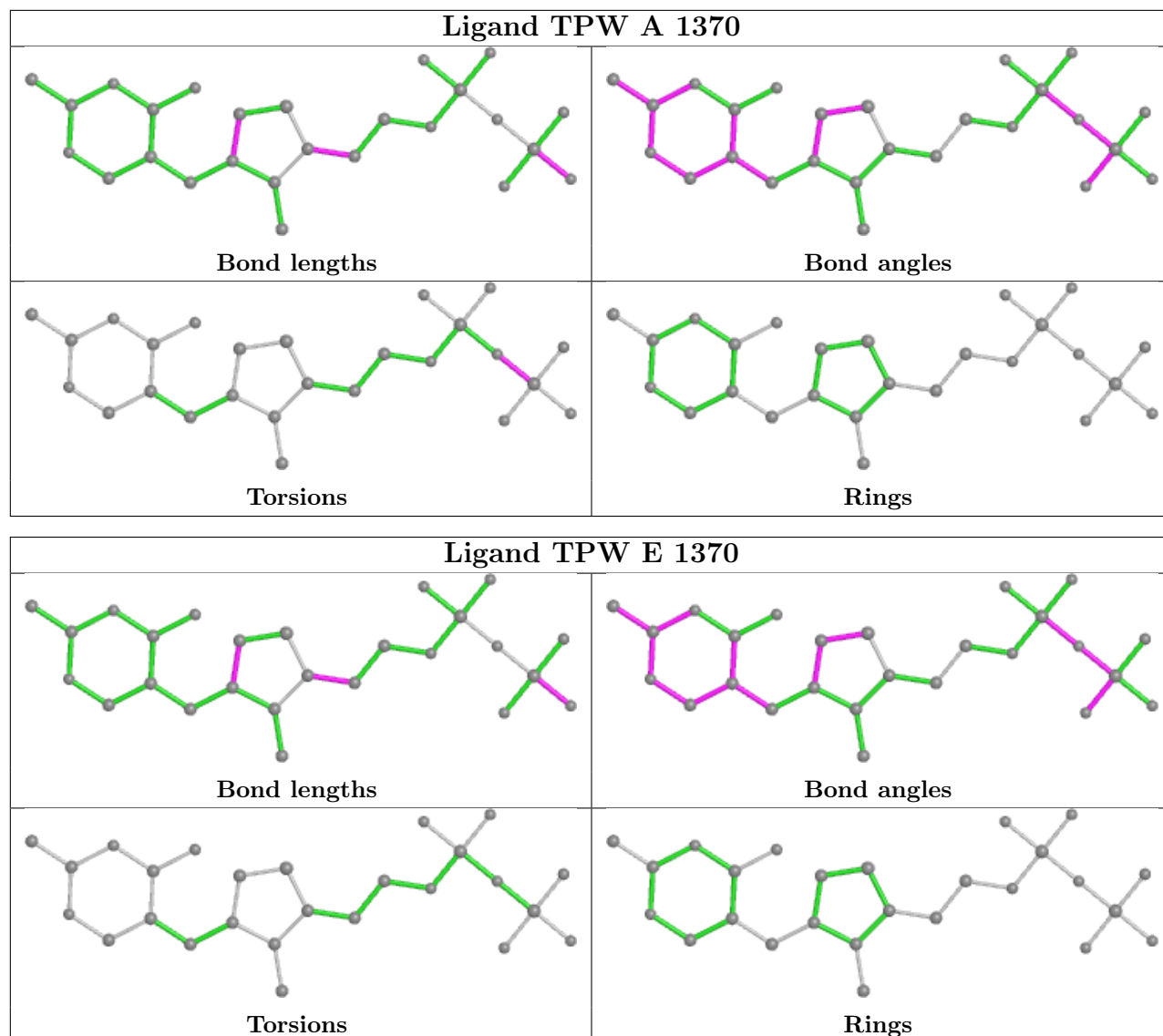
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	365/369 (98%)	0.05	17 (4%)	31	44	15, 25, 44, 58	2 (0%)
1	C	365/369 (98%)	-0.07	7 (1%)	66	76	14, 24, 45, 58	2 (0%)
1	E	354/369 (95%)	0.01	6 (1%)	70	78	21, 32, 48, 60	2 (0%)
1	G	365/369 (98%)	-0.08	4 (1%)	80	87	20, 29, 48, 55	2 (0%)
2	B	324/325 (99%)	-0.28	0	100	100	16, 24, 34, 38	0
2	D	324/325 (99%)	-0.23	0	100	100	15, 20, 27, 30	0
2	F	324/325 (99%)	-0.17	0	100	100	21, 27, 34, 36	0
2	H	324/325 (99%)	-0.17	0	100	100	21, 25, 31, 32	0
3	I	42/428 (9%)	1.12	8 (19%)	1	2	22, 62, 70, 74	0
3	J	40/428 (9%)	0.98	9 (22%)	0	1	20, 53, 75, 78	0
All	All	2827/3632 (77%)	-0.08	51 (1%)	68	77	14, 26, 47, 78	8 (0%)

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	SER	8.1
1	A	281	TYR	6.0
1	A	286	LEU	5.9
1	A	280	ARG	5.3
3	I	128	ARG	5.3

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å²)	Q<0.9
4	MG	E	369	1/1	0.65	0.32	45,45,45,45	0
4	MG	A	1326	1/1	0.85	0.20	30,30,30,30	0
4	MG	G	369	1/1	0.93	0.11	16,16,16,16	0
4	MG	E	370	1/1	0.94	0.08	33,33,33,33	0
4	MG	A	1368	1/1	0.97	0.13	3,3,3,3	0
5	TPW	E	1370	26/26	0.97	0.10	19,20,20,20	0
5	TPW	G	1370	26/26	0.97	0.12	23,23,24,24	0
5	TPW	A	1370	26/26	0.98	0.12	13,13,15,15	0
5	TPW	C	1370	26/26	0.98	0.10	12,12,13,13	0
4	MG	C	1368	1/1	0.99	0.11	7,7,7,7	0
6	K	B	1325	1/1	0.99	0.04	16,16,16,16	0
6	K	D	1325	1/1	0.99	0.06	10,10,10,10	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 TPW E 1370:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
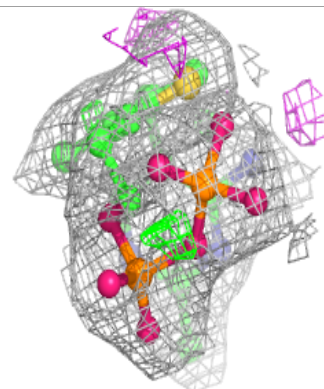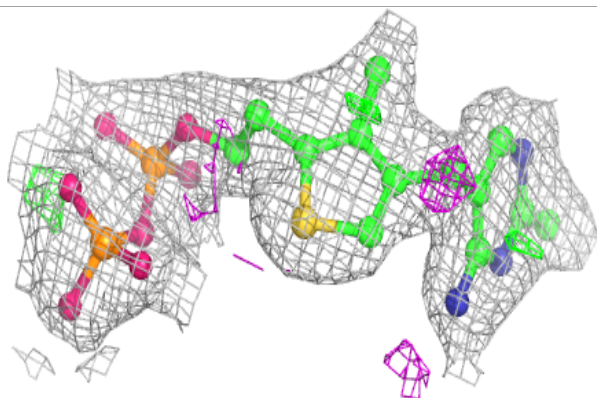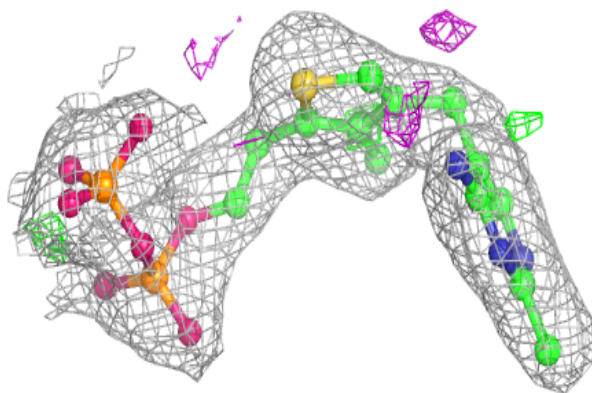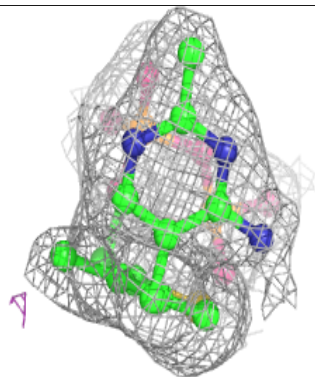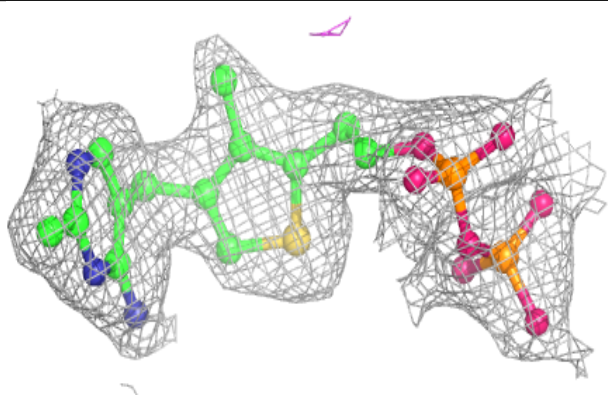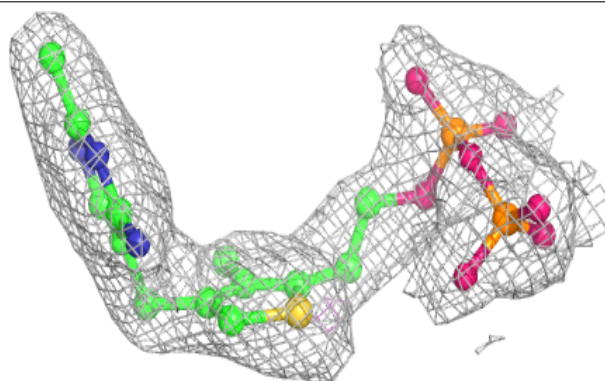mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
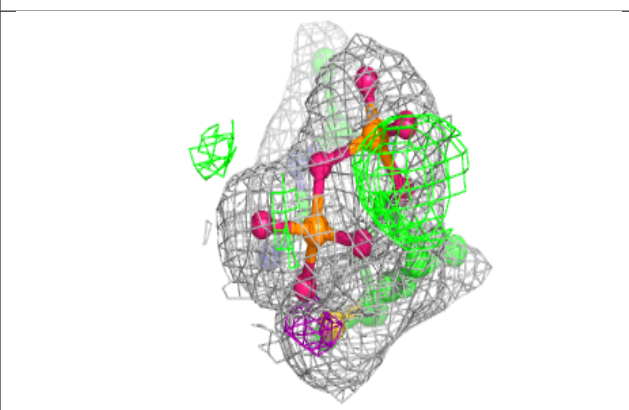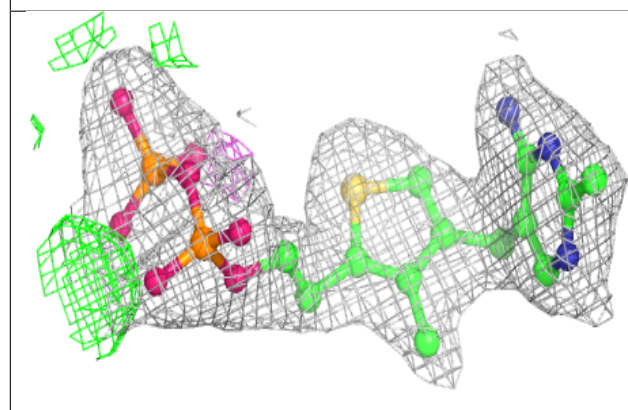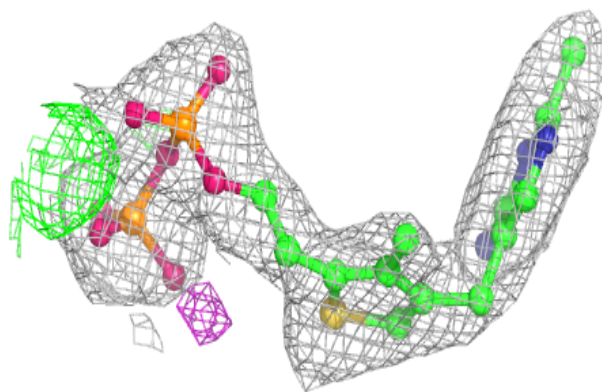
Electron density around TPW G 1370:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
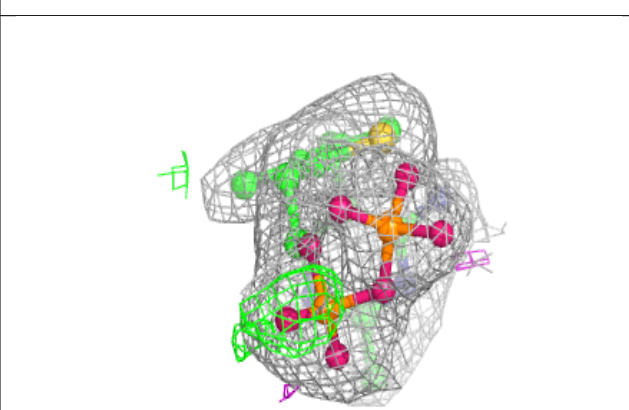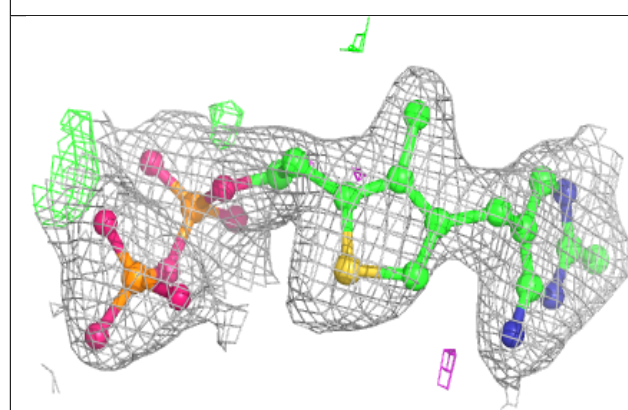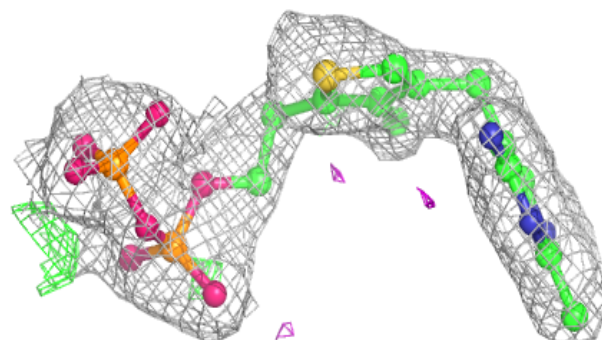
Electron density around TPW A 1370:

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

Electron density around TPW C 1370:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.