



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 02:04 PM UTC

PDB ID : 3DV0 / pdb_00003dv0
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 : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

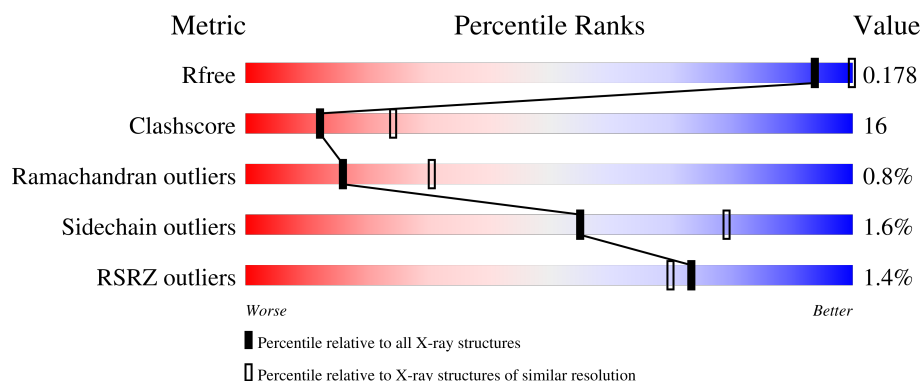
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	369	2% 68% 24% 5%
1	C	369	% 70% 25% 5%
1	E	369	2% 55% 36% 7%
1	G	369	3% 59% 34% 5%
2	B	325	72% 27%

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Mol	Chain	Length	Quality of chain
2	D	325	 79%18%.
2	F	325	 64%34%.
2	H	325	 71%26%.
3	I	428	 5%90%.
3	J	428	 6%90%.

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
7	PYR	D	502	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22633 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	349	Total	C	N	O	S	0	0	0
			2764	1772	466	519	7			
1	C	351	Total	C	N	O	S	0	0	0
			2776	1779	468	522	7			
1	E	344	Total	C	N	O	S	0	0	0
			2698	1728	456	507	7			
1	G	352	Total	C	N	O	S	0	0	0
			2758	1765	466	520	7			

- 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
			2489	1586	424	471	8			

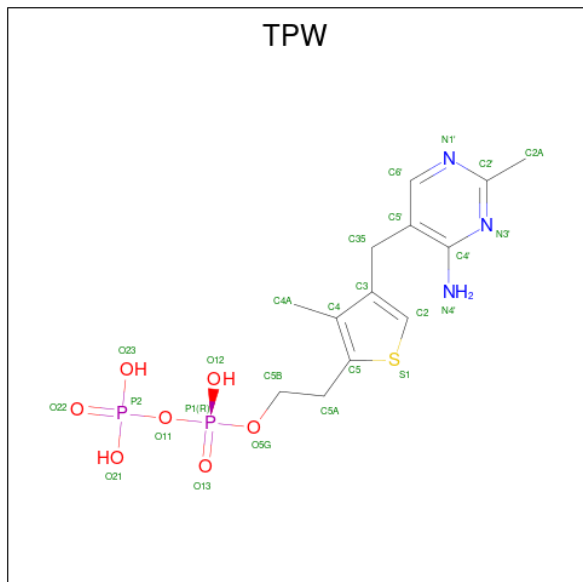
- Molecule 3 is a protein called Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	43	Total	C	N	O	S	0	0	1
			299	188	54	56	1			
3	J	41	Total	C	N	O	S	0	0	0
			269	165	52	51	1			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is 2-{4-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-3-METHYLT HIOPHEN-2-YL}ETHYL TRIHYDROGEN DIPHOSPHATE (CCD ID: TPW) (formula: C₁₃H₁₉N₃O₇P₂S).

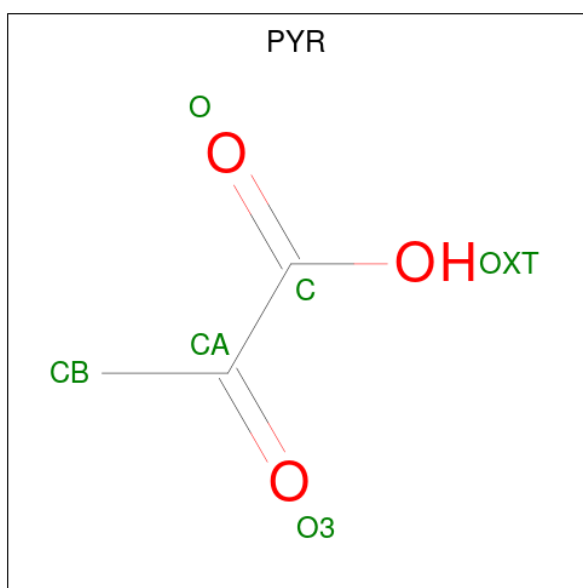


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 26	C 13	N 3	O 7	P 2	S 1	0	0
5	C	1	Total 26	C 13	N 3	O 7	P 2	S 1	0	0
5	E	1	Total 26	C 13	N 3	O 7	P 2	S 1	0	0
5	G	1	Total 26	C 13	N 3	O 7	P 2	S 1	0	0

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 7 is PYRUVIC ACID (CCD ID: PYR) (formula: $C_3H_4O_3$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	125	Total O 125 125	0	0
8	B	143	Total O 143 143	0	0
8	C	146	Total O 146 146	0	0
8	D	151	Total O 151 151	0	0

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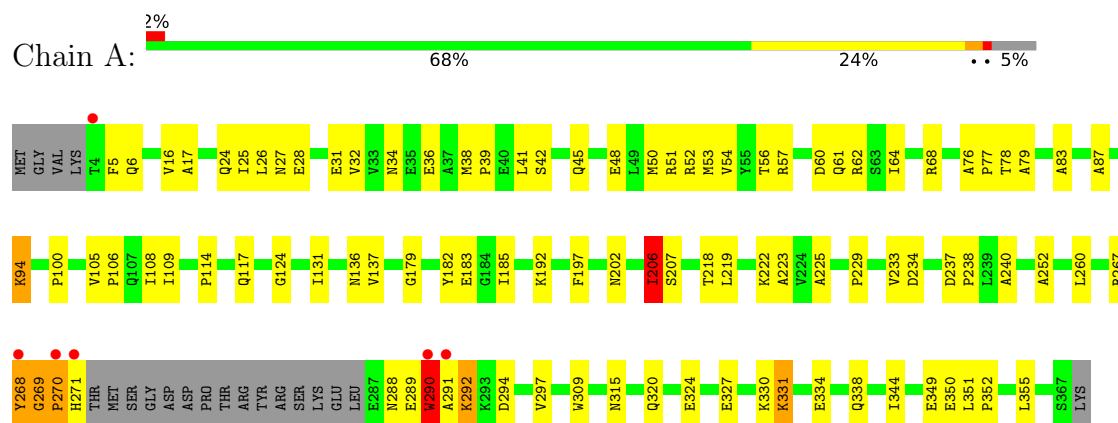
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	76	Total 76	O 76	0	0
8	F	87	Total 87	O 87	0	0
8	G	101	Total 101	O 101	0	0
8	H	127	Total 127	O 127	0	0
8	I	19	Total 19	O 19	0	0
8	J	15	Total 15	O 15	0	0

3 Residue-property plots

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

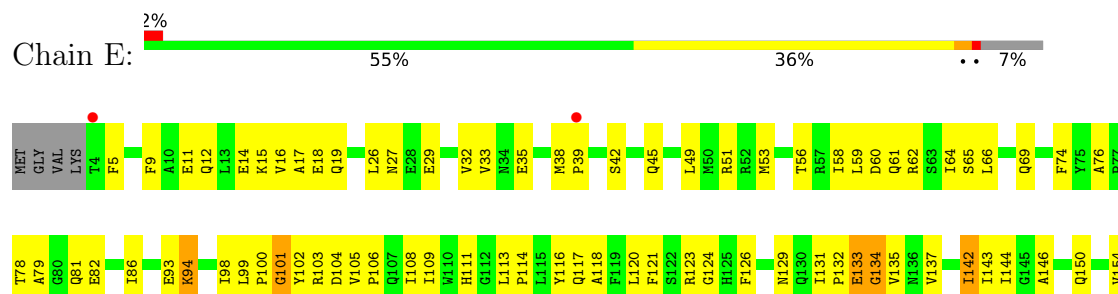
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha

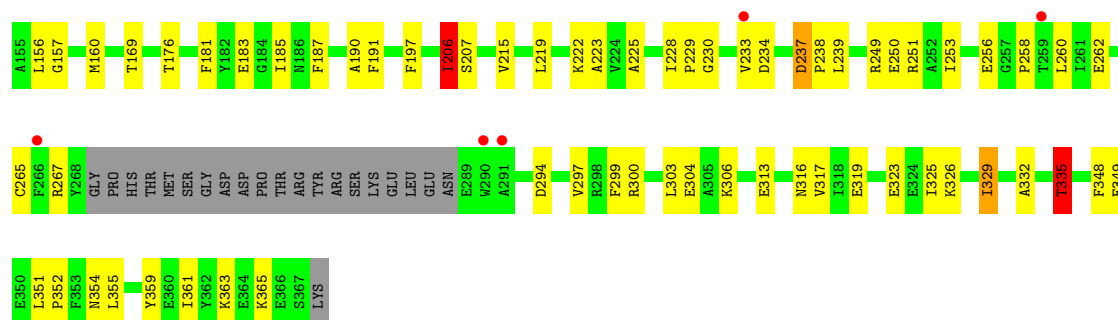


• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha

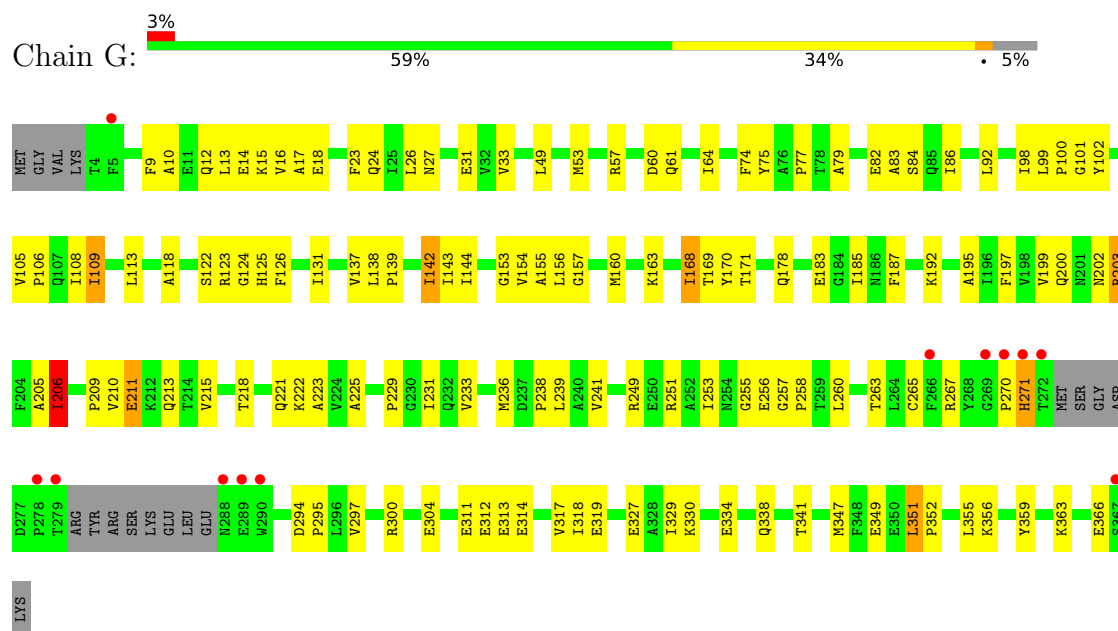


• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha

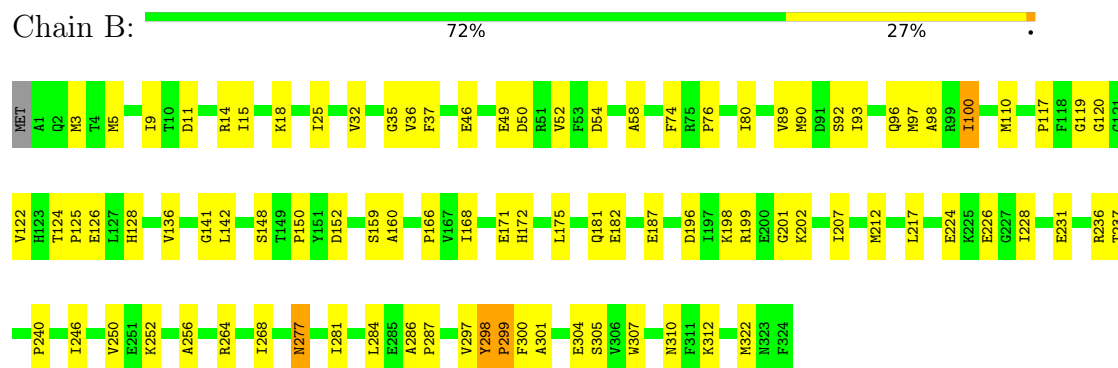




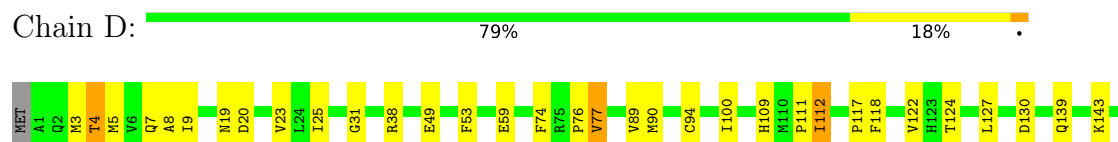
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha



• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta



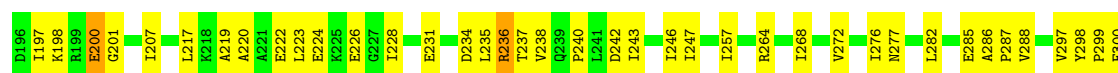
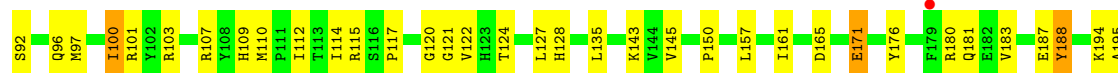
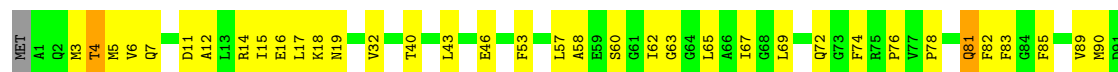
• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta





• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta

Chain F: 64% 34% .



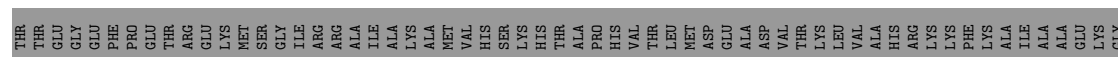
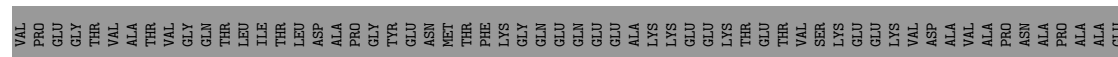
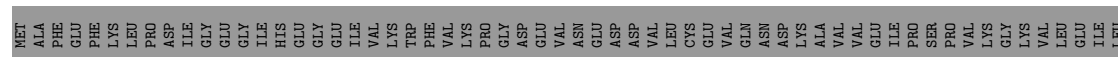
• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta

Chain H: 71% 26% .



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

Chain I: 5% 90% .



[illegible]

ILE	GLY	ARG	ALA	GLU	LYS	PRO	VAL	LEU	ASP	GLY	GLU	ILE	VAL	ALA	ALA	ALA	MET	LEU	ALA	SER	PHE	ASP	HIS	ARG	MET	ILE	ASP	GLY	ALA	THR	GLN	LYS	ALA	LEU	ASN	HIS	ILE	LYS	ARG	LEU	LEU	LEU	MET	GLU
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- Molecule 3: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex



NET	ALA	ALA	PHE	GLU	PHE	LYS	LEU	PRO	ASP	ILE	GLY	GLY	GLY	ILE	HIS	GLU	GLY	GLU	ILE	VAL	LYS	TRP	PHE	VAL	LYS	PRO	GLY	ASP	GLU	VAL	ASN	GLU	VAL	VAL	ASN	GLN	ASP	LYS	ALA	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	ILE	PRO	PRO	SER	SER	VAL	LYS	GLY	LYS	VAL	LEU	GLU	ILE	LEU
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[illegible]

ALA	GLU	ALA	GLY	PRO	ASN	ARG	ARG	V129	L130	P133	S134	R136	I138	R140	V144	D145	I146	V149	Q150	K154	R157	V158	E161	D162	I163	G169	GLY	ALA	LYS	PRO	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	LYS	PRO	THR	THR	GLU
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GLY	GLU	PHE	PRO	GLU	THR	ARG	GLU	LYS	MET	SER	GLY	ILE	ARG	ARG	ALA	ILE	ALA	ALA	LYS	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	PHE	LYS	ALA	ILE	ALA	ALA	GLU	LYS	ILE	GLY	LYS	LEU
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THR	PHE	LEU	PRO	TYR	VAL	VAL	LYS	ALA	LEU	VAL	SER	ALA	LEU	LEU	ARG	GLU	TYR	PRO	VAL	LEU	THR	SER	ILE	ASP	ASP	GLU	ASP	THR	GLU	GLU	ILE	ILE	GLN	LYS	HIS	TYR	TYR	ASN	ASN	GLY	GLY	ARG	THR	ALA	ALA	ASP	ASP	THR	THR	ASP	ASP	GLY	LEU	LEU	VAL	VAL	VAL	ILE	LYS	HIS	ALA	ALA	ASP	ARG	LYS
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PRO	ILE	PHE	LEU	ALA	GLN	GLU	ILE	ASN	GLU	LEU	ALA	GLU	LYS	ALA	ARG	ASP	GLY	LYS	LEU	THR	PRO	GLY	GLU	GLU	MET	LYS	GLY	ALA	GLY	SER	CYS	THR	ILE	THR	THR	ASN	ILE	GLY	GLY	SER	THR	PRO	THR	VAL	ILE	ASN	GLU	VAL	ALA	ALA	ILE	LEU	GLY	ILE	GLY	GLY	PC
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ILE	ALA	GLU	LYS	PRO	ILE	VAL	ARG	ASP	GLY	GLU	ILE	VAL	ALA	ALA	ALA	ALA	PRO	MET	LEU	ALA	LEU	LEU	SER	PHE	ASP	HIS	ARG	MET	ILE	ASP	GLY	ALA	ALA	ALA	ALA	GLN	LYS	ALA	LYS	LEU	ASN	HIS	ILE	LYS	ARG	LEU	LEU	SER	ASP	PRO	GLU	LEU	LEU	MET	GLU	ALA
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.31Å 232.82Å 92.00Å 90.00° 91.83° 90.00°	Depositor
Resolution (Å)	72.17 – 2.50 72.17 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.2 (72.17-2.50) 96.2 (72.17-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.26 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.173 , 0.241 0.176 , 0.178	Depositor DCC
R_{free} test set	5642 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.056 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22633	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PYR, K, TPW, 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	0.42	0/2824	0.91	9/3816 (0.2%)
1	C	0.42	0/2836	0.87	8/3833 (0.2%)
1	E	0.36	0/2754	0.87	8/3719 (0.2%)
1	G	0.37	0/2815	0.90	9/3803 (0.2%)
2	B	0.44	0/2534	0.96	9/3437 (0.3%)
2	D	0.49	0/2534	0.99	13/3437 (0.4%)
2	F	0.39	0/2534	0.92	4/3437 (0.1%)
2	H	0.43	0/2535	0.95	10/3437 (0.3%)
3	I	0.40	0/300	0.93	1/401 (0.2%)
3	J	0.41	0/271	0.93	1/363 (0.3%)
All	All	0.41	0/21937	0.92	72/29683 (0.2%)

There are no bond length outliers.

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	206	ILE	N-CA-C	-10.99	86.47	109.34
2	H	235	LEU	N-CA-C	-8.67	96.95	109.96
1	C	206	ILE	N-CA-C	-8.18	92.33	109.34
2	H	100	ILE	N-CA-C	7.40	118.13	110.36
2	D	237	THR	N-CA-CB	7.24	122.53	110.59

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2764	0	2736	75	0
1	C	2776	0	2745	65	0
1	E	2698	0	2664	127	0
1	G	2758	0	2714	120	0
2	B	2488	0	2515	58	0
2	D	2488	0	2515	48	0
2	F	2488	0	2515	107	0
2	H	2489	0	2515	87	0
3	I	299	0	294	18	0
3	J	269	0	232	13	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	2	0	0	0	0
5	A	26	0	16	2	0
5	C	26	0	16	7	0
5	E	26	0	16	7	0
5	G	26	0	16	3	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
7	B	6	0	0	2	0
7	D	6	0	0	1	0
8	A	125	0	0	11	0
8	B	143	0	0	9	0
8	C	146	0	0	11	0
8	D	151	0	0	6	0
8	E	76	0	0	5	0
8	F	87	0	0	6	0
8	G	101	0	0	11	0
8	H	127	0	0	10	0
8	I	19	0	0	1	0
8	J	15	0	0	0	0
All	All	22633	0	21509	669	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 16.

The worst 5 of 669 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)
2:H:76:PRO:HG2	2:H:112:ILE:HG12	1.48	0.95
2:F:122:VAL:HG23	2:F:124:THR:HG23	1.51	0.91
1:A:292:LYS:H	1:A:292:LYS:HD2	1.35	0.91
1:G:27:ASN:HD21	1:G:31:GLU:HB2	1.38	0.86
1:A:77:PRO:HD2	1:A:271:HIS:HA	1.57	0.85

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	345/369 (94%)	329 (95%)	13 (4%)	3 (1%)	14	27
1	C	347/369 (94%)	330 (95%)	15 (4%)	2 (1%)	21	38
1	E	340/369 (92%)	320 (94%)	17 (5%)	3 (1%)	14	27
1	G	346/369 (94%)	320 (92%)	23 (7%)	3 (1%)	14	27
2	B	322/325 (99%)	308 (96%)	14 (4%)	0	100	100
2	D	322/325 (99%)	307 (95%)	13 (4%)	2 (1%)	21	38
2	F	322/325 (99%)	303 (94%)	15 (5%)	4 (1%)	10	20
2	H	322/325 (99%)	307 (95%)	15 (5%)	0	100	100
3	I	39/428 (9%)	34 (87%)	4 (10%)	1 (3%)	4	7
3	J	39/428 (9%)	26 (67%)	9 (23%)	4 (10%)	0	0
All	All	2744/3632 (76%)	2584 (94%)	138 (5%)	22 (1%)	16	31

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	TRP
3	J	150	GLN
2	F	81	GLN

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Mol	Chain	Res	Type
1	G	270	PRO
3	J	154	LYS

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	286/305 (94%)	279 (98%)	7 (2%)	43	70
1	C	287/305 (94%)	284 (99%)	3 (1%)	68	86
1	E	277/305 (91%)	271 (98%)	6 (2%)	45	73
1	G	283/305 (93%)	278 (98%)	5 (2%)	51	77
2	B	263/264 (100%)	259 (98%)	4 (2%)	57	80
2	D	263/264 (100%)	263 (100%)	0	100	100
2	F	263/264 (100%)	261 (99%)	2 (1%)	73	88
2	H	263/264 (100%)	259 (98%)	4 (2%)	57	80
3	I	27/341 (8%)	23 (85%)	4 (15%)	3	6
3	J	19/341 (6%)	18 (95%)	1 (5%)	20	42
All	All	2231/2958 (75%)	2195 (98%)	36 (2%)	55	79

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	171	GLU
3	J	130	ILE
2	H	235	LEU
3	I	137	LYS
1	C	160	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	239	GLN

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Mol	Chain	Res	Type
2	H	81	GLN
1	G	24	GLN
1	G	316	ASN
2	H	139	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	TPW	C	1370	-	25,27,27	1.23	2 (8%)	37,40,40	1.82	10 (27%)
5	TPW	G	1370	-	25,27,27	1.25	2 (8%)	37,40,40	1.85	10 (27%)
7	PYR	D	502	-	5,5,5	2.89	1 (20%)	3,6,6	0.82	0
5	TPW	E	1370	-	25,27,27	1.25	2 (8%)	37,40,40	1.86	10 (27%)
5	TPW	A	1370	-	25,27,27	1.27	3 (12%)	37,40,40	1.78	10 (27%)
7	PYR	B	502	-	5,5,5	2.89	1 (20%)	3,6,6	0.89	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
5	TPW	C	1370	-	-	0/17/17/17	0/2/2/2
5	TPW	G	1370	-	-	2/17/17/17	0/2/2/2
7	PYR	D	502	-	-	0/4/4/4	-
5	TPW	E	1370	-	-	1/17/17/17	0/2/2/2
5	TPW	A	1370	-	-	3/17/17/17	0/2/2/2
7	PYR	B	502	-	-	0/4/4/4	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	502	PYR	O3-CA	5.83	1.36	1.23
7	D	502	PYR	O3-CA	5.82	1.36	1.23
5	A	1370	TPW	C2-C3	-2.56	1.33	1.36
5	E	1370	TPW	C2-C3	-2.54	1.33	1.36
5	G	1370	TPW	C2-C3	-2.50	1.33	1.36

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1370	TPW	C5-C4-C3	4.07	115.45	112.50
5	E	1370	TPW	C3-C2-S1	-4.06	108.89	113.46
5	G	1370	TPW	C3-C2-S1	-4.02	108.93	113.46
5	C	1370	TPW	C5-C4-C3	3.86	115.30	112.50
5	C	1370	TPW	C3-C2-S1	-3.84	109.14	113.46

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

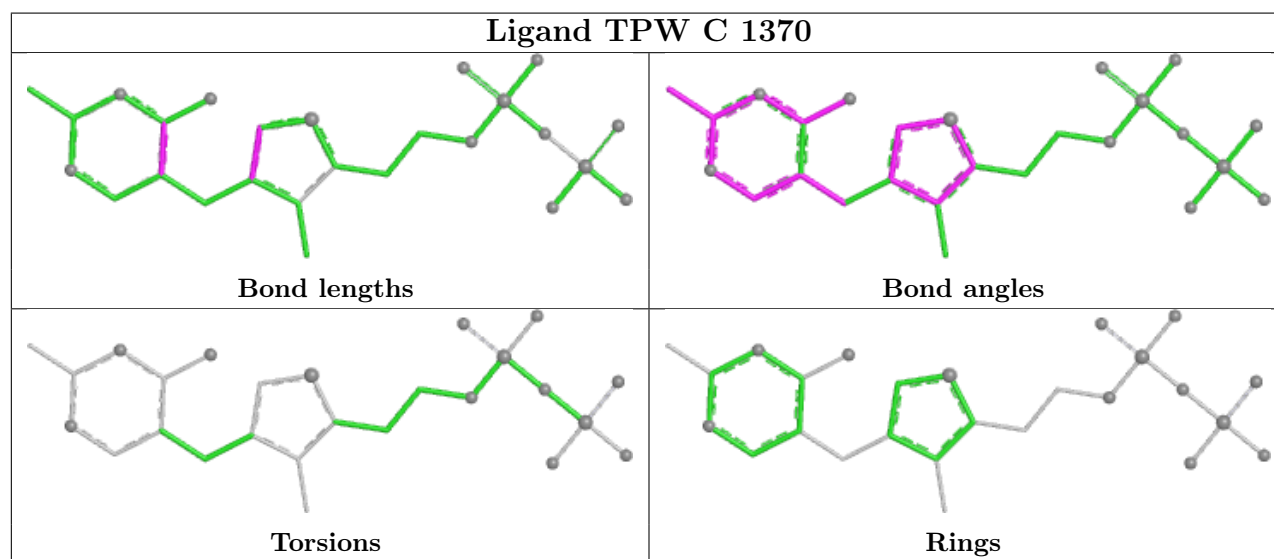
Mol	Chain	Res	Type	Atoms
5	A	1370	TPW	P1-O11-P2-O21
5	E	1370	TPW	P1-O11-P2-O23
5	G	1370	TPW	P1-O11-P2-O21
5	A	1370	TPW	P1-O11-P2-O22
5	A	1370	TPW	P1-O11-P2-O23

There are no ring outliers.

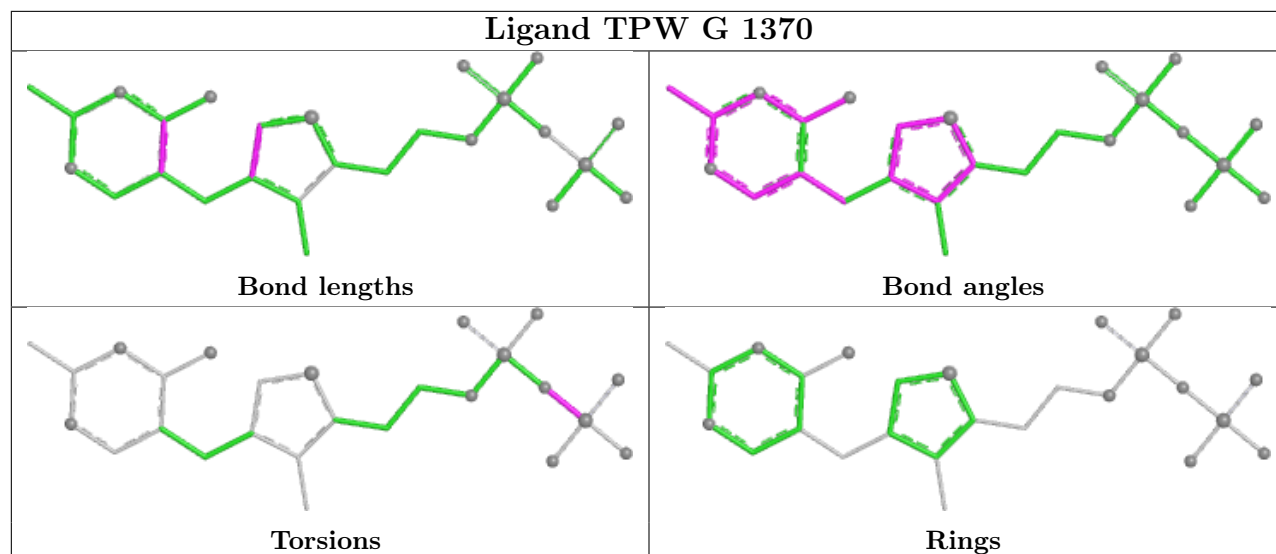
6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1370	TPW	7	0
5	G	1370	TPW	3	0
7	D	502	PYR	1	0
5	E	1370	TPW	7	0
5	A	1370	TPW	2	0
7	B	502	PYR	2	0

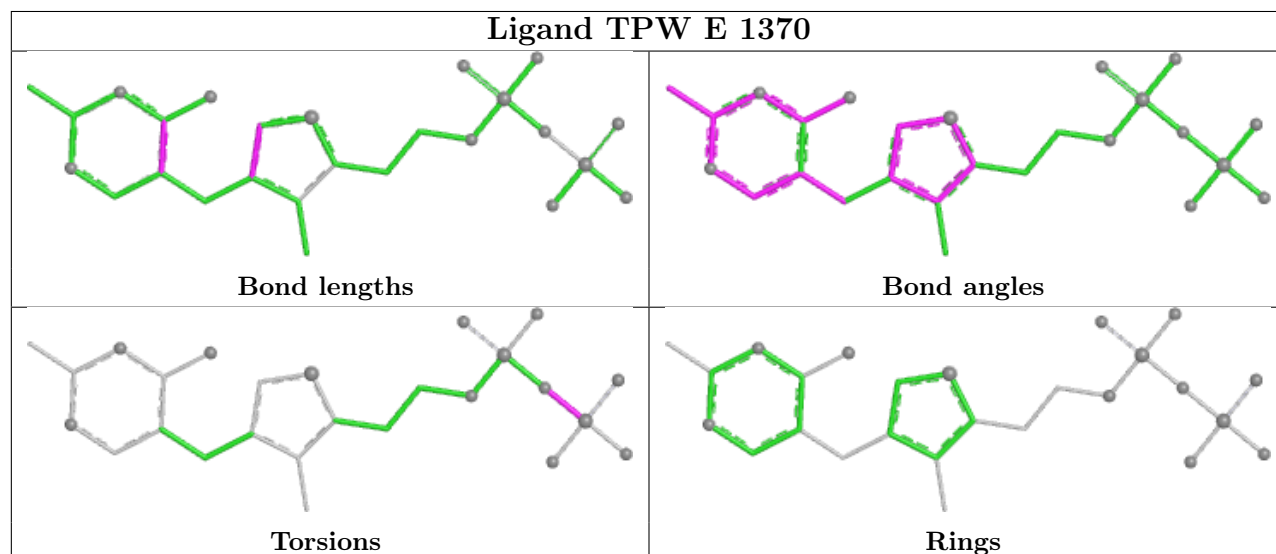
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



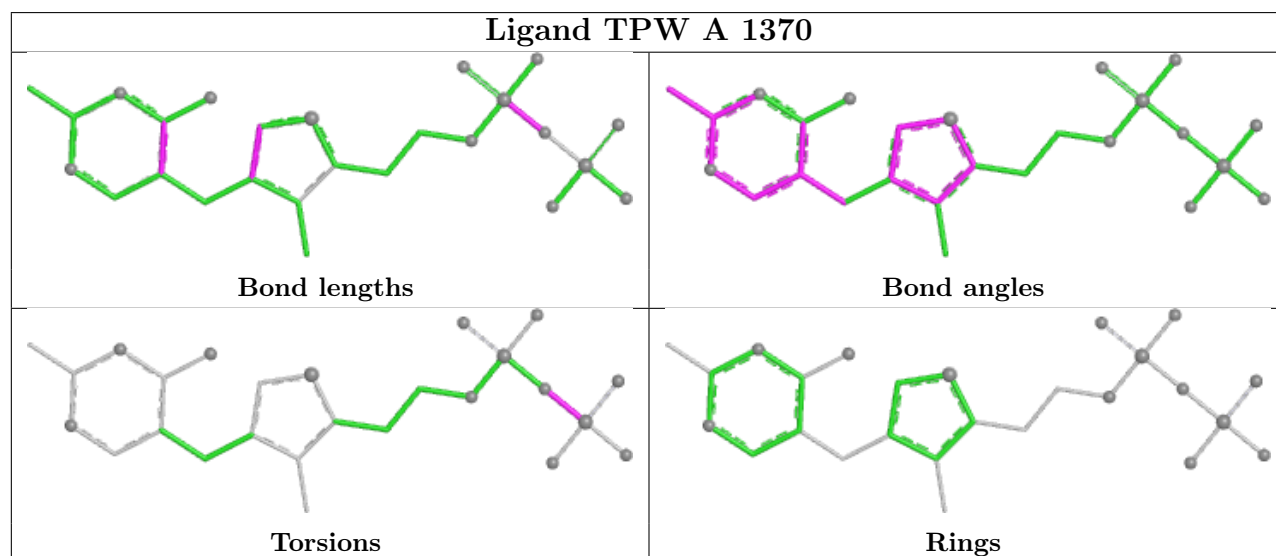
Ligand TPW G 1370



Ligand TPW E 1370



Ligand TPW A 1370



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	349/369 (94%)	-0.42	6 (1%) 69 65	11, 26, 60, 99	2 (0%)
1	C	351/369 (95%)	-0.47	5 (1%) 73 70	8, 24, 60, 100	2 (0%)
1	E	344/369 (93%)	0.33	7 (2%) 65 61	27, 52, 80, 94	2 (0%)
1	G	352/369 (95%)	0.02	12 (3%) 48 43	21, 40, 73, 100	2 (0%)
2	B	324/325 (99%)	-0.56	0 100 100	8, 24, 43, 58	0
2	D	324/325 (99%)	-0.72	0 100 100	8, 19, 35, 47	0
2	F	324/325 (99%)	-0.07	1 (0%) 90 87	21, 40, 61, 81	0
2	H	324/325 (99%)	-0.54	0 100 100	14, 27, 42, 56	0
3	I	43/428 (10%)	0.80	2 (4%) 36 32	39, 61, 73, 82	0
3	J	41/428 (9%)	1.29	6 (14%) 6 4	43, 65, 81, 86	0
All	All	2776/3632 (76%)	-0.26	39 (1%) 73 70	8, 31, 68, 100	8 (0%)

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	TRP	4.2
1	A	270	PRO	4.1
1	G	269	GLY	3.8
2	F	179	PHE	3.7
1	G	272	THR	3.6

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

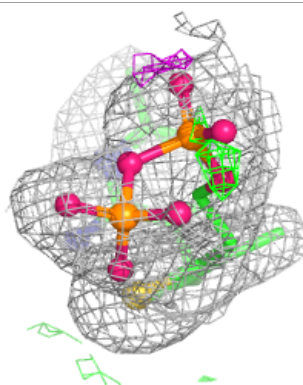
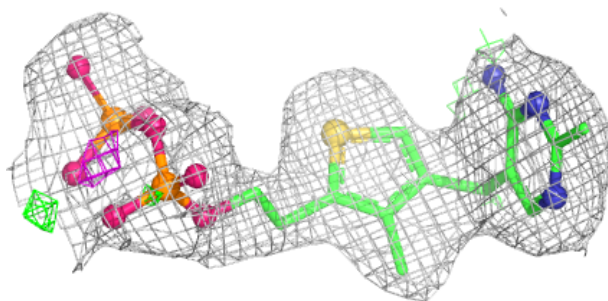
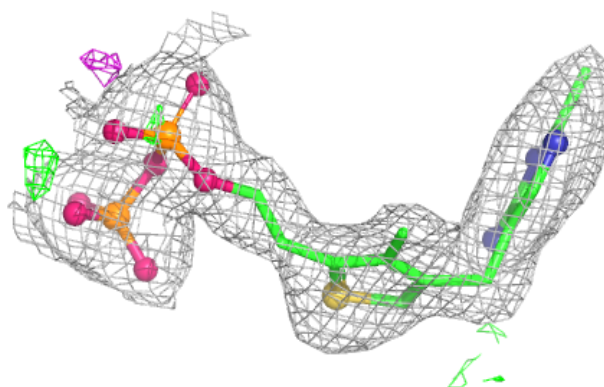
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
7	PYR	D	502	6/6	0.56	0.68	44,49,53,61	6
4	MG	C	1368	1/1	0.74	0.26	59,59,59,59	0
7	PYR	B	502	6/6	0.85	0.31	37,41,44,57	6
4	MG	E	1368	1/1	0.88	0.12	54,54,54,54	0
4	MG	B	1326	1/1	0.93	0.12	48,48,48,48	0
5	TPW	E	1370	26/26	0.95	0.08	19,37,59,72	0
4	MG	G	1326	1/1	0.95	0.13	45,45,45,45	0
4	MG	G	1367	1/1	0.95	0.06	36,36,36,36	0
5	TPW	G	1370	26/26	0.96	0.07	21,39,46,52	0
6	K	B	1325	1/1	0.96	0.05	32,32,32,32	0
4	MG	A	1368	1/1	0.97	0.07	12,12,12,12	0
6	K	F	1325	1/1	0.97	0.04	46,46,46,46	0
5	TPW	C	1370	26/26	0.98	0.05	13,20,27,42	0
6	K	H	1325	1/1	0.98	0.03	26,26,26,26	0
5	TPW	A	1370	26/26	0.99	0.05	2,16,28,31	0
6	K	D	1325	1/1	0.99	0.03	15,15,15,15	0

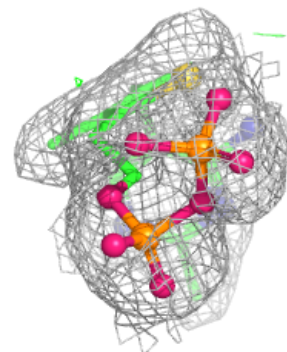
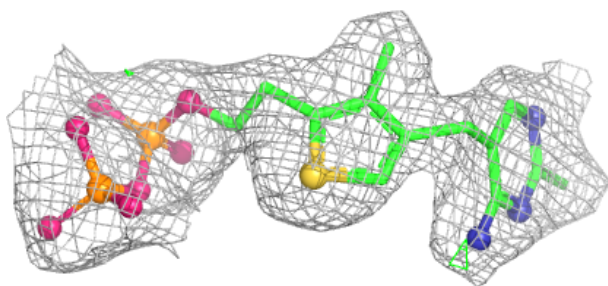
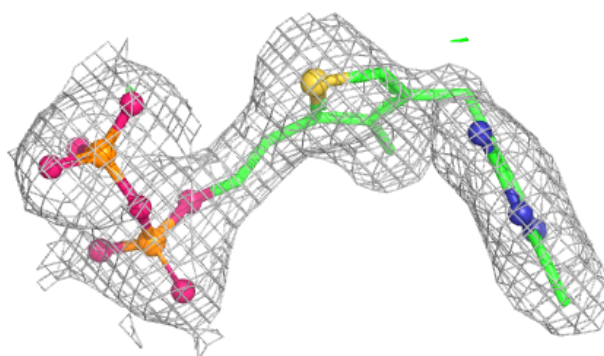
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

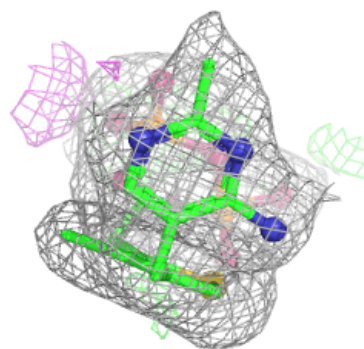
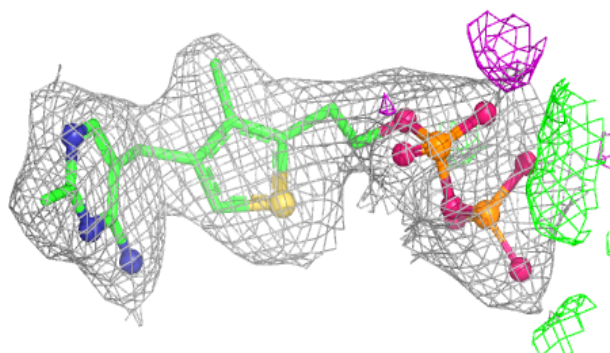
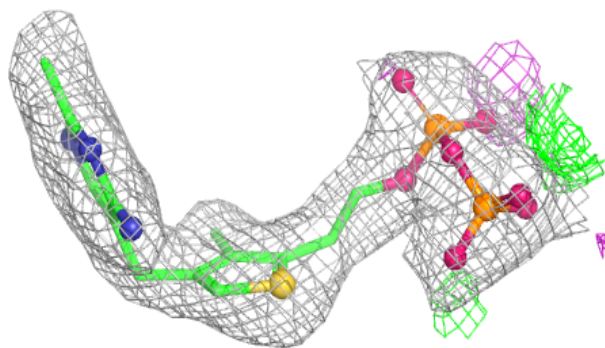
**Electron density around TPW G 1370:**

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

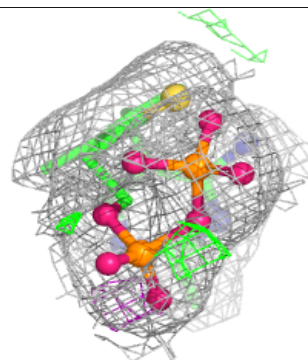
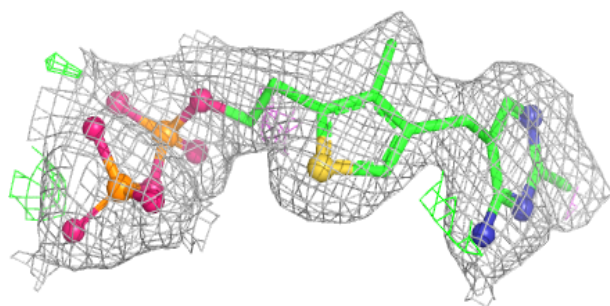
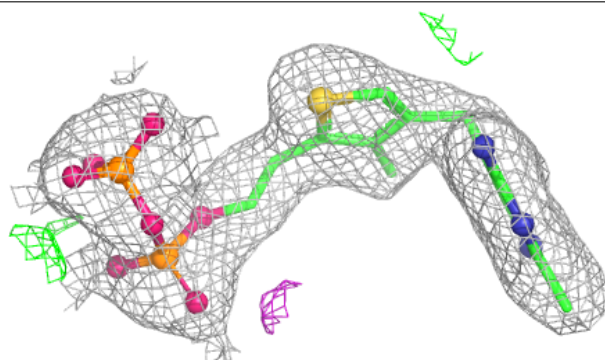


Electron density around TPW C 1370:

$2mF_o-DF_c$ (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:**

$2mF_o-DF_c$ (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.